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Continuous-Energy Data Checks

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Contents

1 Introduction

1.1 Objectives

The purpose of this report is to provide an overview of all Quality Assurance tests that have to be performed on a nuclear data set to be transformed into an ACE formatted nuclear data file. The ACE file is capable of containing different types of data such as continuous energy neutron data, thermal scattering data, etc. Within this report, we will limit ourselves to continuous energy neutron data.

The main goal of these tests is to check whether or not the nuclear data set subjected to the tests is ACE capable. The tests therefore focus on both the format parameters of the data (representation types, etc.) as well as the physics represented by the data to check the consistency of the data.

The present document is the result of a collaboration between Los Alamos National Laboratory (LANL) in the US and the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) in France. The Nuclear Criticality Safety Program (NCSP) in the United States is responsible for the nuclear criticality safety research and development. This collaboration is under the auspices of NCSP and works to contribute to criticality safety research.

1.2 ACE QA tests at LANL

Currently at LANL, the verification and validation of ACE-formatted data files is performed by a script called CHECKACE [1]. This is a Perl script that runs a series of small Fortran routines that check various pieces of the ACE-formatted data. The errors found by CHECKACE are reported to the screen and are *not* written to a file for later retrieval.

In addition to the CHECKACE test suite used at LANL for ACE QA testing, NJOY [5] also provides a number of consistency tests in the ACER module (these consistency tests are implemented in the consis routine). The NJOY ACE consistency tests specifically tests the following data:

- Comparison of reaction thresholds against the reaction's Q value
- Checking whether or not the cross section energy grid is monotonic
- Checking angular distributions (reference frame, cosine values, cdf values)
- Checking energy distributions
- Checking delayed neutron data (fractions and energy distributions)
- Checking photon data (production cross section and distributions)
- Checking particle production cross sections and distributions

1.3 ACE QA tests at IRSN

GAIA is a computer software developed at IRSN to minimise the effort on the generation of nuclear data libraries using NJOY and provide additional quality assurance. The library files produced consist of ACE files (which will be used by MCNP, MCNPX and MORET 5) and PENDF files (which will only be used by VESTA). GAIA not only automates the entire NJOY processing path, but it will also perform a number of additional operations to verify the produced files and add any missing data required for the applications in question.

The software generates a tailor made NJOY input file for each nuclide without intervention of the user using data found in the nuclide's ENDF file (such as the initial temperature of the ENDF file, whether or not the nuclide is fissile, whether or not it has unresolved resonances, etc.). When the library files have been generated, GAIA will also process the output from NJOY and extract all messages and warnings from NJOY that are deemed important. A print out including a short explanation of the messages in question is then printed to the listing (the user can, if needed, override this setting to extract all messages and errors regardless of their importance). The most important test provided by the software is the verification of the unresolved resonance probability tables. GAIA will check for the presence of any negative cross section values in the tables. If such negative values are detected, GAIA will rerun NJOY but omit the generation of the unresolved resonance probability tables.

Once the library files pass the NJOY processsing and verification stage, GAIA will add data from the original ENDF file to the final PENDF file for use by VESTA:

- the average number of neutrons per fission (the MF1 MT452 section of the original ENDF file if the nuclide is fissile)
- the components of energy release per fission (the MF1 MT458 section of the original ENDF file if the nuclide is fissile)
- the isomeric branching ratio data (the MF9 file of the original ENDF file if such data is defined for more than one isomeric state different from the ground state). It should be noted that the data from MF10 is already added to the PENDF by NJOY itself.

As a final operation, GAIA will also organise the data into a comprehensive structure of directories in which it will save both the final library files (`ACE` and PENDF files) as well as the input, output and postscript files produced during the NJOY runs. Entries for an xsdir file for use by MCNP(X) and an XML formatted cross section directory file for use by VESTA and MORET 5 are also produced by GAIA.

After the `ACE` files have been produced, they are tested using simple MCNP and MORET 5 input files. These tests allow us to identify additional issues, such as negative cross section values outside the resonance range.

1.4 Test related data

For each test, we will briefly describe what is tested, how it is tested, what the conditions for success are, what levels of failure are associated to the test and what the information is that the test should provide in its report.

The tests are organized by the type of data upon which they will be applied:

reaction data the most general type of data

cross section data this includes transport cross sections, particle production cross sections for secondary particles such as photons and heating data

nubar data

multiplicity data

secondary particle angular and energy distributions
unresolved resonance probability tables

Each test has a unique name used to define the test. The following are defined for each test:

Code whenever the test is currently part of any of the LANL testing codes within `CHECKACE` or if it is a test currently performed inside NJOY, the name of the LANL code in question is indicated here

Description a description of what the test actually does

Type either format or physics

Target the data for which the test needs to be applied (e.g. reaction names, incident particle types, etc.)

Input data values required for the test that can be changed by the user, such as tolerances, etc.

Severity any issues detected when these tests are performed can be categorized into several levels depending on the impact when the test fails:

- **information** an issue with the data that poses no problems but of which the user should be aware (e.g. incomplete heating values, etc.)
- **error** an issue with the data that potentially poses a problem which can be fixed either through user intervention or automatic (this can be a physics error such as negative cross section values)
- **fatal** a fatal issue such as the absence of linearised data or required reactions, etc. When a fatal issue is encountered, it is most likely impossible to transform the nuclear data set into a legal `ACE` file.

Report data data to be included in the test report

It is possible that multiple names are given. This can be due to the fact that the test is performed in multiple codes or the fact that the tests were performed on different data types that use similar representations (e.g. checking for negative cross sections and heating values are performed by CHECKXS and CHECK_HEAT while the data representations of both are the same).

2 Reaction data

The tests described here are for required data without which we cannot produce an `ACE` file.

2.1 `RequiredReactions`

Description a number of reactions have to be present for an `ACE` file to be created: total, elastic, absorption and heating.

Type format

Target reactions

Input data none

Severity fatal

Report data names of the reactions that are missing

2.2 `RequiredNuBar`

Description If fission is defined, total and delayed nubar needs to be given. Prompt nubar is not required but the absence of the data should be flagged.
Type format
Target fission nu
Input data none
Severity fatal
Report data nu type that is missing (missing prompt nu is an information message only)

2.3 `RequiredReactionsForProbabilityTables`

Description a probability table contains data for the following reactions: total, elastic, fission (if defined), capture and heating. Only these should be given in the probability table.
Type format
Target probability tables
Input data none
Severity error
Report data energy value of the probability table and missing reaction names.

3 Cross section data

The cross section data stored in a continuous energy neutron `ACE` file consists of an energy grid and corresponding cross section values for each reaction. The cross section data is linearized.

3.1 `LinearisedCrossSectionData`

Description Each cross section to be included in the `ACE` file needs to be represented as a linear-linear interpolatable table.
Type format
Target all cross section
Input data none
Severity fatal
Report data The names of the reactions that have no linearized cross section associated to them.

3.2 `UnionisedEnergyGrid`

Description All cross sections to be included in the `ACE` file need to be defined on a common energy grid. A special case concerns threshold reactions for which all energy values starting from the threshold energy must be included in the common energy grid.
Type format

Target all cross sections.
Input parameters none
Severity fatal
Report data The names of the reactions that have energy points that are not on the common energy grid. The additional energy points should not be written to the report because it can potentially be a very large list.

3.3 `MonotonicIncreasingEnergyGrid`

Code `NJOY`
Description The common energy grid to be included in the `ACE` file must be monotonically increasing but does not require a strict monotonic grid to allow for cross section jumps. Cross section jumps are tolerated but are signaled (this is something MCNP actually checks for).
Type format
Target all cross sections.
Input parameters none
Severity fatal
Report data Any sequence of energy values that are not monotonic along with the indices of these energy values in the common energy grid. Duplicate energy values are reported as information.

3.4 `StrictlyPositiveEnergyValues`

Description All energy values in the common energy grid must be strictly positive. Negative or zero values are not allowed.
Type physics
Target all cross sections.
Input parameters none
Severity fatal
Report data Any energy values that are not strictly positive along with the indices of these energy values in the common energy grid.

3.5 `NoNegativeCrossSectionValues`

Code `CHECKXS`, `CHECK_HEAT`
Description The cross section values not be negative.
Type physics
Target each cross section.
Input parameters none
Severity error
Report data The names of the reactions, the energy values and cross section values for which the test fails.

3.6 `NoZeroHeatingValues`

Code `CHECK_HEAT`
Description Heating values that are zero are due to incomplete data.
Type physics
Target each heating cross section.
Input parameters none
Severity information
Report data reaction names for which the test fails.

3.7 `NoAbnormallyLargeCrossSectionValues`

Code `CHECKXS`
Description The cross section values cannot take abnormally large values, see [1] for more information.
Type physics
Target each cross section.
Input parameters test tolerance and high value
Severity information
Report data reaction names, energy values and cross section values for which the test fails.

3.8 `InitialZeroCrossSectionForThresholdReaction`

Code `CHECK0`
Description The first cross section value for a threshold reaction should be zero.
Type physics
Target each threshold reaction
Input parameters none
Severity error
Report data The reaction names, energy values and cross section values for which the test fails.

3.9 `KinematicThresholdForThresholdReaction`

Code `NJOY`, `CHECKTHRESH`
Description The kinematic threshold defined as $-Q\frac{A+A_n}{A}$ should be equal to the threshold energy of the threshold reaction. In this equation, A and A_n are given in atomic mass units or neutron mass units. In this last case, the A value is equal to the AWR value in the ENDF file and the A_n is equal to one. It is important to use a tolerance in this test, otherwise we will run into a lot of cases related to simple roundoff problems.
Type physics
Target each threshold reaction
Input parameters comparison tolerance

Severity error

Report data The reaction names, threshold energy, kinematic threshold and difference between both values when the test fails.

3.10 `PartialCrossSectionsSumToTotal`

Code `CHECKXS`, `CHECK_HEAT`

Description At each energy value in the common energy grid and at each midpoint for each interval in the grid, the partial cross sections and heating values that make up a summation cross section sum up to the summation cross section within a given tolerance.

Type physics

Target each cross section defined as the sum of other cross sections. This includes the total cross section, the absorption cross section, the total inelastic reaction, the inelastic scattering cross section and the fission cross section. The total cross section is defined as the sum of all its partials (which turn can be defined as the sum of its own partials).

Input parameters comparison tolerance

Severity error

Report data reaction names, energy values and cross section values for which the test fails.

4 Fission nu data

Fission nu data is "basically" multiplicity data but it is treated as a special case.

4.1 `LinearisedOrPolynomialTotalAndPromptNuData`

Description the total and prompt nu needs to be represented as either a linear-linear interpolatable table or as a polynomial series.

Type format

Target total and prompt nu

Input parameters none

Severity fatal

Report data nu types that have no linearized table or polynomial series associated to them

4.2 `LinearisedDelayedNuData`

Description the delayed nu needs to be represented as a linear-linear interpolatable table (only if it is present).

Type format

Target delayed nu

Input parameters none

Severity fatal
Report data delayed nu has no linearized table associated to it

4.3 `MonotonicIncreasingEnergyGridInNuData`

Description The energy values of the fission nu data must be monotonically increasing and all energy values in nu data must be strictly positive. Negative or zero values are not allowed.
Type physics
Target all nu data represented as linearised data.
Input parameters none
Severity error
Report data nu type as well as any energy sequence that is not monotonic or any energy value that is not strictly positive along with the indices of these energy values in the common energy grid. Duplicate energy values are reported as information.

4.4 `NoNegativeNuValues`

Code `CHECKXS`
Description The nu values may not be negative.
Type physics
Target total, prompt and delayed nu.
Input parameters none
Severity error
Report data nu type, energy values and nu values for which the test fails.

4.5 `NoAbnormallyLargeNuValues`

Code `CHECKXS`
Description A nu value is considered abnormally high if above 11.0. This last value is the default value but can be set as an input parameter. Note: this is an implementation specific issue in MCNP but not necessarily in other Monte Carlo codes that use `ACE` formatted data.
Type physics
Target total, prompt and delayed nu.
Input parameters test tolerance and high value
Severity information
Report data nu type, energy values and nu values for which the test fails.

4.6 `DelayedNeutronFractionsSumToOne`

Code `NJOY`
Description The delayed neutron fractions sum to 1.
Type physics
Target delayed nu.

Input parameters test tolerance
Severity error
Report data delayed neutron fractions, their sum and the difference with 1.

5 Secondary particle multiplicity

5.1 `AllowedRepresentationInMultiplicity`

Description A seconday particle's multiplicity should be of one of the allowed representation types.
Type format
Target all secondary particle multiplicities
Input parameters none
Severity fatal
Report data reaction name, secondary particle type for which the multiplicity is given in an incorrect representation type.

5.2 `MonotonicIncreasingEnergyGridInMultiplicity`

Description The energy values of the secondary particle multiplicity must be monotonically increasing and all energy values of the secondary particle multiplicity must be strictly positive. Negative or zero values are not allowed.
Type physics
Target all secondary particle multiplicity represented as linearised data.
Input parameters none
Severity error
Report data Reaction name and secondary particle type as well as any energy sequence that is not monotonic or any energy value that is not strictly positive along with the indices of these energy values in the energy grid. Duplicate energy values are reported as information.

5.3 `NoNegativeMultiplicityValues`

Description The multiplicity values may not be negative.
Type physics Target:all multiplicities.
Input parameters none
Severity error
Report data reaction name, particle type, energy values and multiplicity values for which the test fails.

5.4 `InitialZeroMultiplicityAtThreshold`

Code `CHECK5`
Description the secondary neutron multiplicity of a reaction should be zero at the threshold energy.

Type physics
Target each threshold reaction
Input parameters test tolerance
Severity error
Report data reaction names, particle type, energy values and multiplicity values for which the test fails.

5.5 `NoAbnormallyLargeMultiplicityValues`

Code `CHECK5`
Description A multiplicity value is considered abnormally high if above 11.0. This last value is the default value but can be set as an input parameter. Note: this is an implementation specific issue in MCNP but not necessarily in other Monte Carlo codes that use `ACE` formatted data.
Type physics
Target all threshold reactions. Note: CHECK5 only tests the MT5 reaction.
Input parameters test tolerance and high value
Severity error
Report data nu type, energy values and nu values for which the test fails.

6 Secondary particle angular and energy data

6.1 `AllowedRepresentationInAngularDistribution`

Description Angular distribution data should be of one of the allowed representation types: isotropic, equal probability bins, linearised or histogram data with pdf and cdf
Type format
Target all secondary angular distributions (excluding coupled energy-angle distributions)
Input parameters none
Severity fatal
Report data reaction name, secondary particle type for which the angular distribution is given in an incorrect representation type.

6.2 `CorrectReferenceFrameInAngularDistribution`

Code `NJOY`
Description The angular distribution of any inelastic scattering level (excluding the continuum) must be given in the centre of mass system. In all other cases, they should be given in the laboratory system.
Type physics
Target all secondary angular distributions (excluding coupled energy-angle distributions)

Input parameters none
Severity information
Report data reaction name and secondary particle type for which the angular distribution is given in an incorrect frame.

6.3 `MonotonicIncreasingCosineGridInAngularDistribution`

Code `NJOY`
Description The cosine values of an angular distribution must be monotonically increasing and the values must be between -1 and 1.
Type physics
Target all secondary angular distributions (excluding coupled energy-angle distributions).
Input parameters none
Severity error
Report data reaction name, secondary particle type and reaction name for which the angular distribution has abnormal cosine values.

6.4 `AllowedRepresentationInEnergyDistribution`

Description A seconday particle's energy distribution data should be of one of the allowed representation types.
Type format
Target all secondary energy distributions (excluding coupled energy-angle distributions)
Input parameters none
Severity fatal
Report data reaction name, secondary particle type for which the energy distribution is given in an incorrect representation type.

6.5 `MonotonicIncreasingEnergyGridInEnergyDistribution`

Code `NJOY`
Description The energy values of a secondary particle's energy distribution must be monotonically increasing and all energy values in a secondary particle's energy distribution must be strictly positive. Negative or zero values are not allowed.
Type physics
Target all secondary energy distributions (excluding coupled energy-angle distributions).
Input parameters none
Severity error
Report data reaction name and secondary particle type as well as any energy sequence that is not monotonic or energy value that is not strictly positive along with the indices of these energy values in the common energy grid. Duplicate energy values are reported as information.

6.6 `MonotonicIncreasingCumulativeProbabilityValues`

Code `NJOY`, `CHECK61`, `CHECKND`, `CHECKND_NEUT`, `CHECKISO`

Description The cumulative probability values of the cumulative density function (cdf) are monotonically increasing. The first value must be equal to zero and the last value must be equal to one.

Type physics

Target all secondary angular and energy distributions using tabulated pdf and cdf.

Input parameters none

Severity error

Report data reaction name and secondary particle type for which the cdf of the angular distribution monotonically increasing and between zero and 1.

6.7 `ConsistentProbabilityAndCumulativeProbabilityValues`

Description The probability values and cumulative probability values are consistent.

Type physics

Target all secondary angular and energy distributions using tabulated pdf and cdf.

Input parameters toterance

Severity error

Report data reaction name and secondary particle type for which the pdf and cdf of the angular distribution are not consistent.

6.8 `OutgoingEnergyEqualOrSmallerThanIncidentEnergy`

Code `NJOY`, `CHECK61`, `CHECKND`, `CHECKND_NEUT`

Description TODO

Type format

Target outgoing neutrons only, exclude some reactions such as MT5 or fission. Note: upscattering for light nuclei is still possible.

Input parameters test tolerance

Severity error

Report data reaction name, secondary particle type and energy values for which this test fails.

6.9 `NoNegativeAngularProbabilityValues`

Code `NJOY`, `CHECK61`, `CHECKND`, `CHECKND_NEUT`, `CHECKISO`

Description The probability value for a given cosine value cannot be negative (this can occur when the Legendre expansion has not enough terms in it).

Type physics

Target all linearised or histogram data with pdf and cdf

Input parameters none

Severity error

Report data reaction name and secondary particle type for which this test fails.

6.10 `NoAbnormallySmallAngularProbabilityValues`

Code `CHECKISO`
Description TODO
Type physics
Target all linearised or histogram data with pdf and cdf
Input parameters small value and test tolerance
Severity error
Report data reaction name and secondary particle type for which this test fails.

7 Unresolved resonance probability tables

Sometimes the energy values of the probability table are flagged by a minus sign (indicating overlap of resolved/unresolved). What should be done?

7.1 `AllowedRepresentationInProbabilityTables`

Description A probability table should be of one of the allowed representation types.
Type format
Target all probability tables
Input parameters none
Severity fatal
Report data The energy value of the probability table

7.2 `CompetitionReactionExists`

Code `CHECK_URES`
Description the competition reaction defined for the probability table exists.
Type physics
Target each probability table
Input parameters none
Severity error
Report data Message to indicate that the competition reaction does not exist

7.3 `StrictMonotonicIncreasingProbabilitiesInProbabilityTable`

Code `CHECK_URES`
Description the probabilities given in the table are monotonically increasing and sum to one.
Type format
Target each probability table
Input parameters test tolerance
Severity error
Report data The energy value of the probability table as well as any sequences of probabilities that are not strict monotonic.

7.4 `PartialsSumToTotalInProbabilityTable`

Code `CHECK_URES`
Description the total cross section for each row in the probability table is equal to the sum of the elastic, capture, fission and competition (if defined) cross section within a given tolerance.
Type physics
Target each probability table
Input parameters test tolerance
Severity error
Report data the energy value, probability and cross section values from the probability table that do not sum correctly as well as the difference.

7.5 `NoNegativeOrZeroProbabilityTableValues`

Code `CHECK_URES`
Description check for negative and zero values in the total, elastic, capture, fission cross section and heating values.
Type physics
Target each probability table
Input parameters test tolerance
Severity error
Report data the energy value of the probability table, probability and cross section values from the probability table that do not satisfy this test.

7.6 `NoAbnormalProbabilityTableHeatingValues`

Code `CHECK_URES`
Description check if the heating values are larger than a defined value (e.g. 210 MeV/collision).
Type physics
Target each probability table
Input parameters test tolerance and high value
Severity error
Report data the energy value of the probability table, probability and heating values from the probability table that do not satisfy this test.

7.7 `AverageFromTableEqualToInfiniteDilute`

Code `CHECK_URES`
Description the average cross section values for the total, elastic, capture and fission cross sections calculated from the probability table are compared to the infinite dilute cross section values (from the regular cross section tables).
Type physics
Target each probability table
Input parameters test tolerance and infinite dilute value

Severity error

Report data the energy value of the probability table, reaction name, average cross section computed from the probability table, the infinite dilute cross section and the difference.

8 Things to be resolved

"tyr" test from CHECK_ISO

secondary photon distributions: number and values of discrete energy photons at adjacent neutron energies [4]

consis: "check energy distributions"

consis: "particle production sections"

remark: should the tests correct things or simply signal them - to be specified in the introduction

9 Bibliography

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