TENDL applications libraries

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CCFE is the fusion research arm of the **United Kingdom Atomic Energy Authority.**
This work was funded by the RCUK Energy Programme [grant number EP/I501045] .

Overview

1. The need for TENDL in fusion

2. TENDL Processing Methodology

3. Summary

The need for TENDL in fusion

Currently:

- 14 MeV fusion neutrons open up significantly more reaction channels than typically found in fission
- Experimentally derived nuclear data used for fusion modelling is:
  - fragmented and incomplete
  - expensive and slow to produce
  - lacking in terms of uncertainty quantification

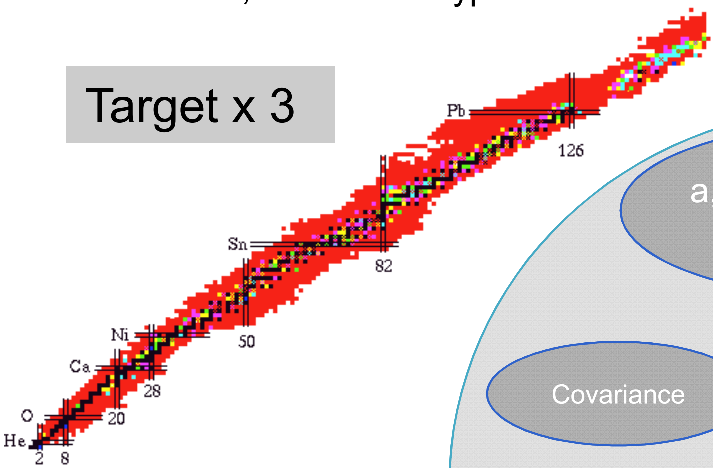
With TENDL:

- Comprehensive nuclear data upto 200 MeV
- Production of nuclear data libraries is ***relatively*** fast and cheap to produce
- Full covariance data available (for codes that handle it)

EASY-II &TENDL-2014, -2013

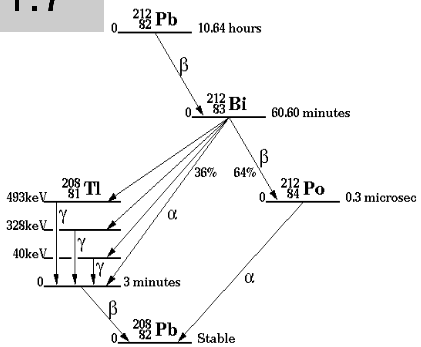
- 2630 (2434) targets (H^1 to Ds^{281})
- Cross section, 90 reaction types

Target x 3



- Decay data: 3873 nuclides; 24 types
- Stables and isomeric states; g, m, n, o,..

Decay x 1.7



a, g, n, p, d-TENDL-2014 (-2013)

Covariance

Decay-2012

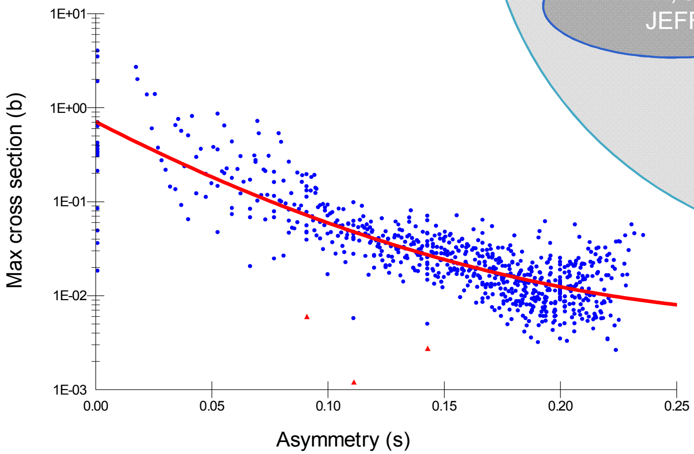
FISPACT-II

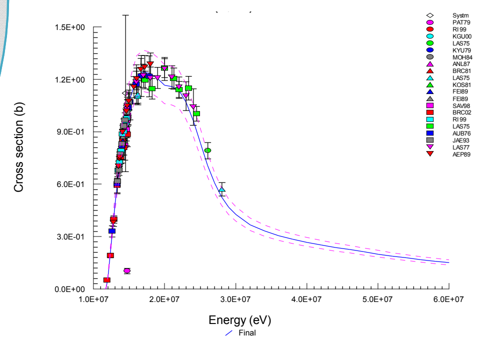
ENDF/B, JENDL, JEFF

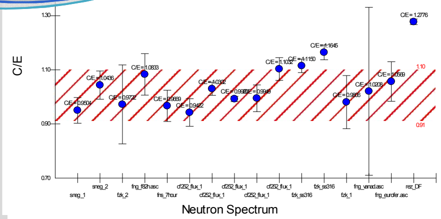
UKFY-4.2 fission yield

Hazard indices

Validation: SACS







V&V, C/E integral and differential with uncertainty

TENDL PROCESSING METHODOLOGY

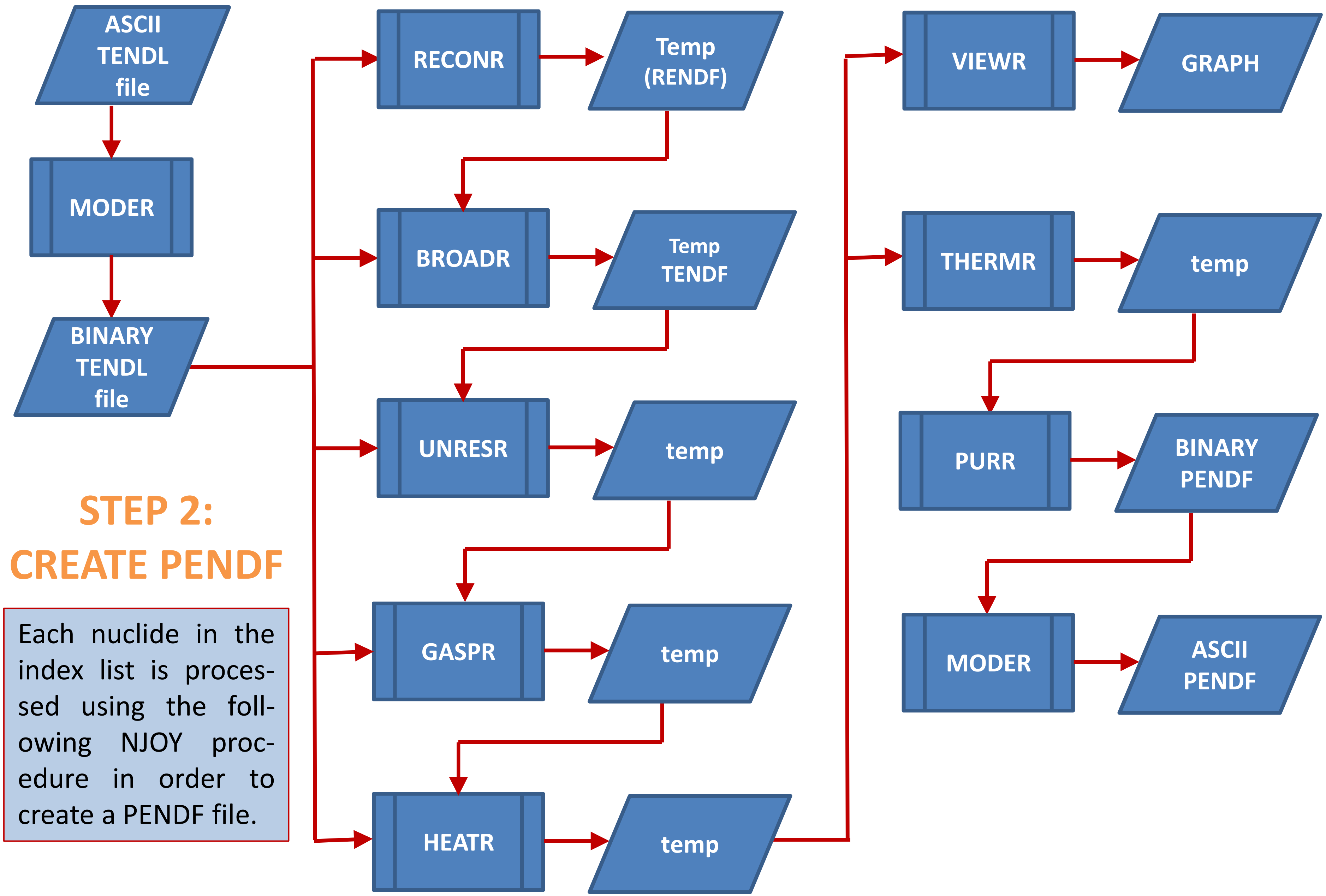
TENDL PROCESSING METHODOLOGY
STEP 1: REDUCED NUCLIDE INDEX SET

- **TENDL14 contains nuclear data for 2633 nuclides**
  - **Perfect to serve the needs of all aspects the nuclear community, however it is bulky and not all nuclides are required for reactor applications**
  - **Hence, a reduced TENDL14_Lite nuclide index is required which contains only the nuclides required for fusion/fission modelling**

- **Nuclide index list**
  - **JENDL (406)**
  - **ENDFB7.1 (423)**
  - **JEFF32 (472)**

- **TENDL14_Lite nuclide index set is created from the union of the JENDL, ENDF and JEFF nuclide sets**
  - **TENDL_Lite (496)**

- **The TENDL14_Lite nuclide index set is then split into N separate files, in order to run each set through NJOY in parallel.**

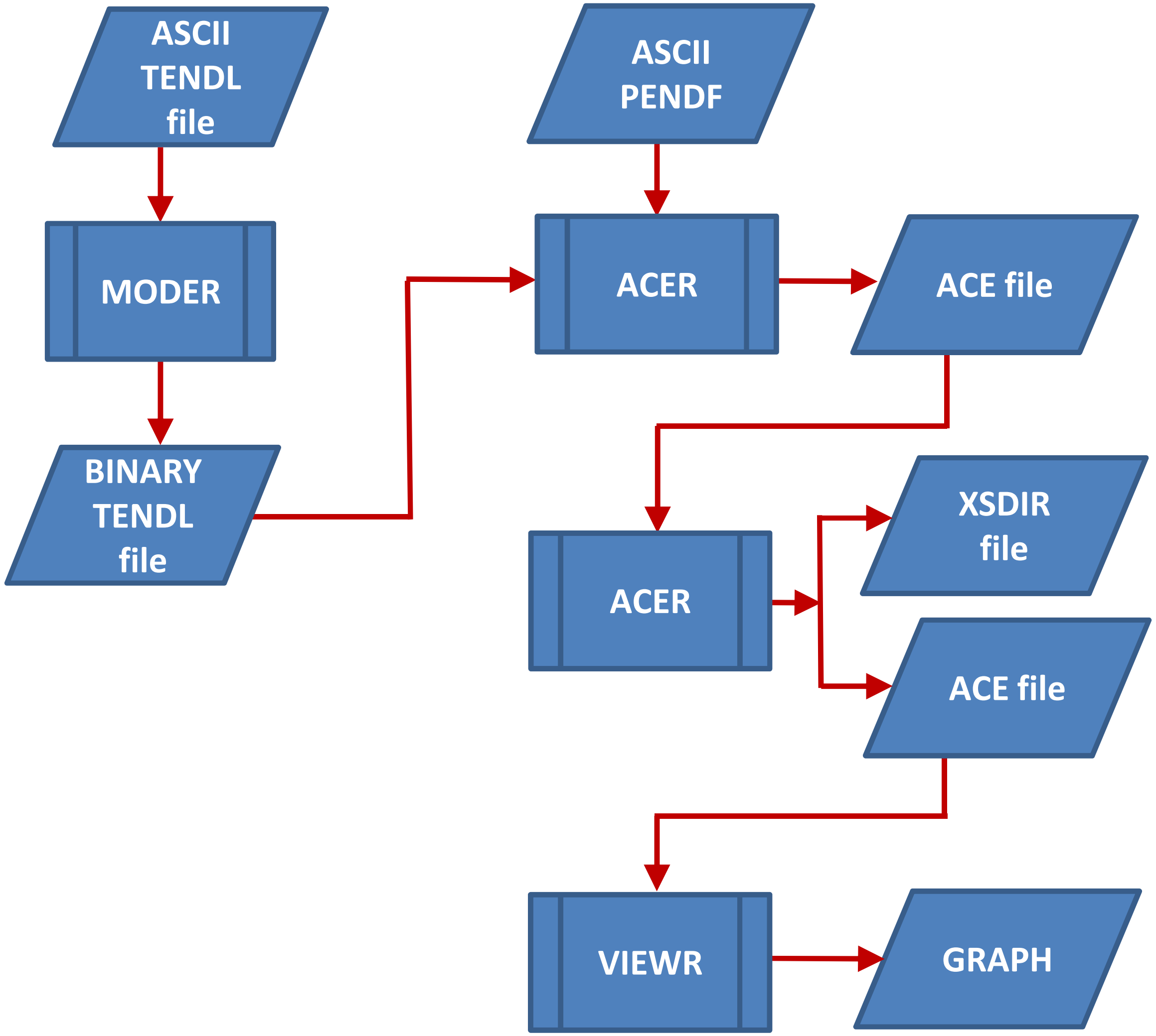


STEP 2: CREATE PENDF

Each nuclide in the index list is processed using the following NJOY procedure in order to create a PENDF file.

TENDL PROCESSING METHODOLOGY
STEP 3: CREATE ACE +XSDIR

Each nuclide in the index list is processed using the following NJOY procedure in order to create an ACE file from a PENDF.



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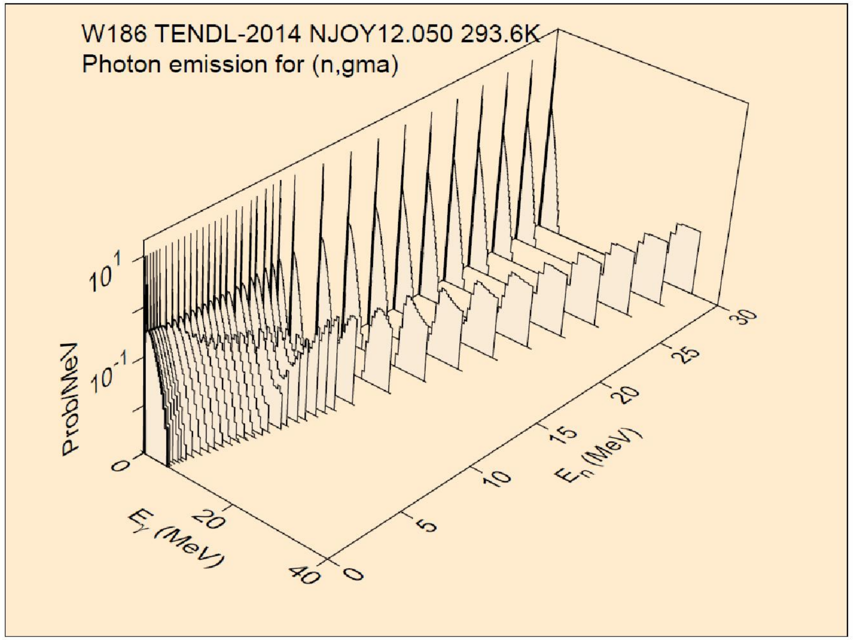
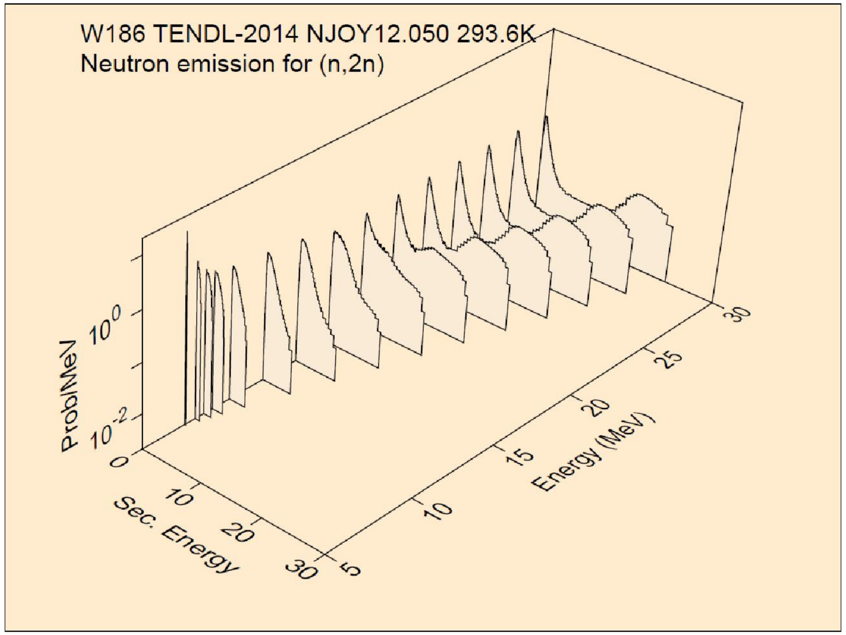
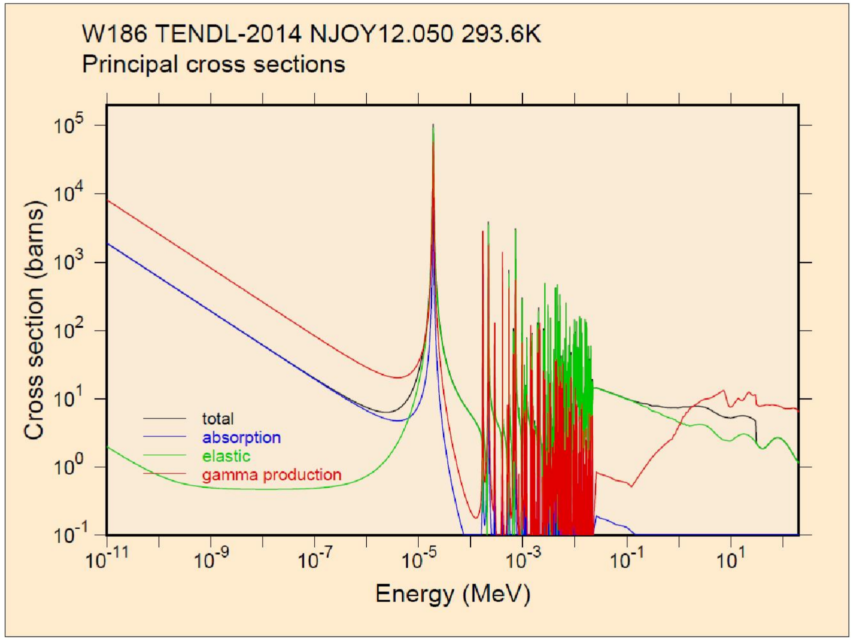
TENDL PROCESSING METHODOLOGY
STEP 3b: Checking Data







TENDL PROCESSING METHODOLOGY
STEP 4: CREATE SINGLE, CONCATENATED ACE + XSDIR to be used by MCNP6

- In order to reduce disk I/O and create a compact nuclear data library, a single large ACE file is created which is a concatenation of all single xsdir entries produced by NJOY.
  - The TENDL14_Lite nuclide index set results a single ACE file with size of approximately 8 Gb.
  - A script is used to detect all files with '.xsdir' extensions in a particular directory
  - The script reads each xsdir entry into a XSDIR object and rewrites a single concatenated xsdir file with Filename, access_route and address modified.
  - ENDFB7 mass tables are used

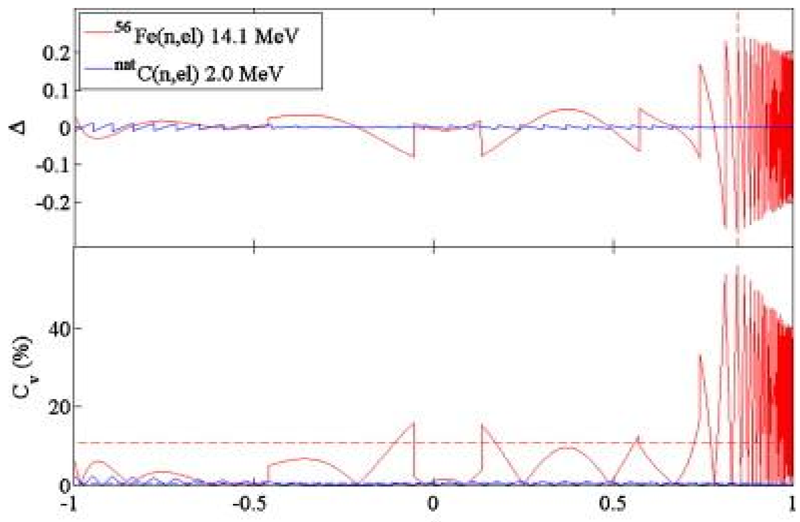
TENDL PROCESSING METHODOLOGY
STEP 4: CREATE XSDIR file to be used by SERPENT

- Although MCNP6 and SERPENT both read ACE files, the xsdir files have a different format
  - Mass tables are not present in the SERPENT XSDIR, unlike MCNP
  - MCNP allows a single concatenated XSDIR, whereas SERPENT requires individual xs files for each nuclide.

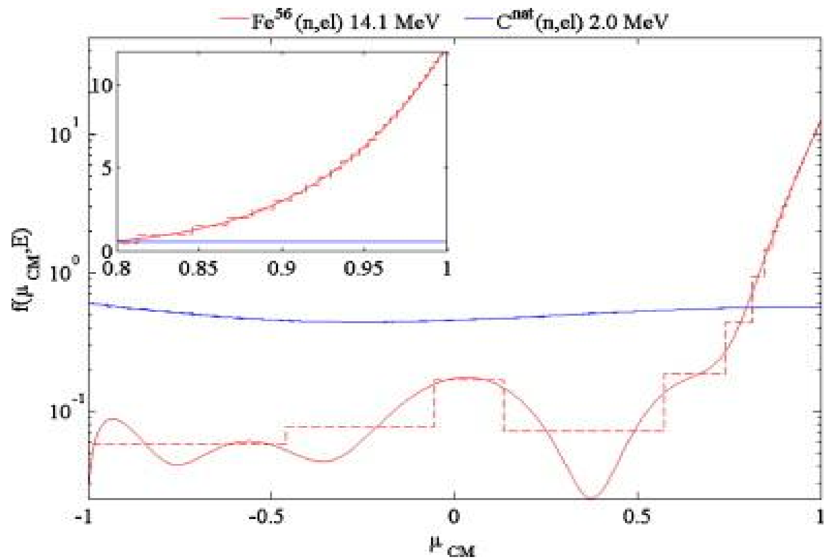
- Use xsdirconvert.pl utility, provided in the SERPENT package to covert MCNP-style xsdir to SERPENT-style xsdir.

TENDL PROCESSING METHODOLOGY
STEP 4: Angular scattering in more detail

- Law 61 specified in NJOY script in order to simulate scattering of neutronics as accurately as possible, which is important for shielding calculations.



Top: Difference between the functional and histogrammed distributions. Bottom: Coefficients of variation for the histogram



Normalised probability distribution functions f(μ, E) for the elastic scatter of neutrons from 56Fe at 14.1 MeV (red) and natC at 2.0 MeV (blue) [1] (Law 4 - equal probability 32 bin).

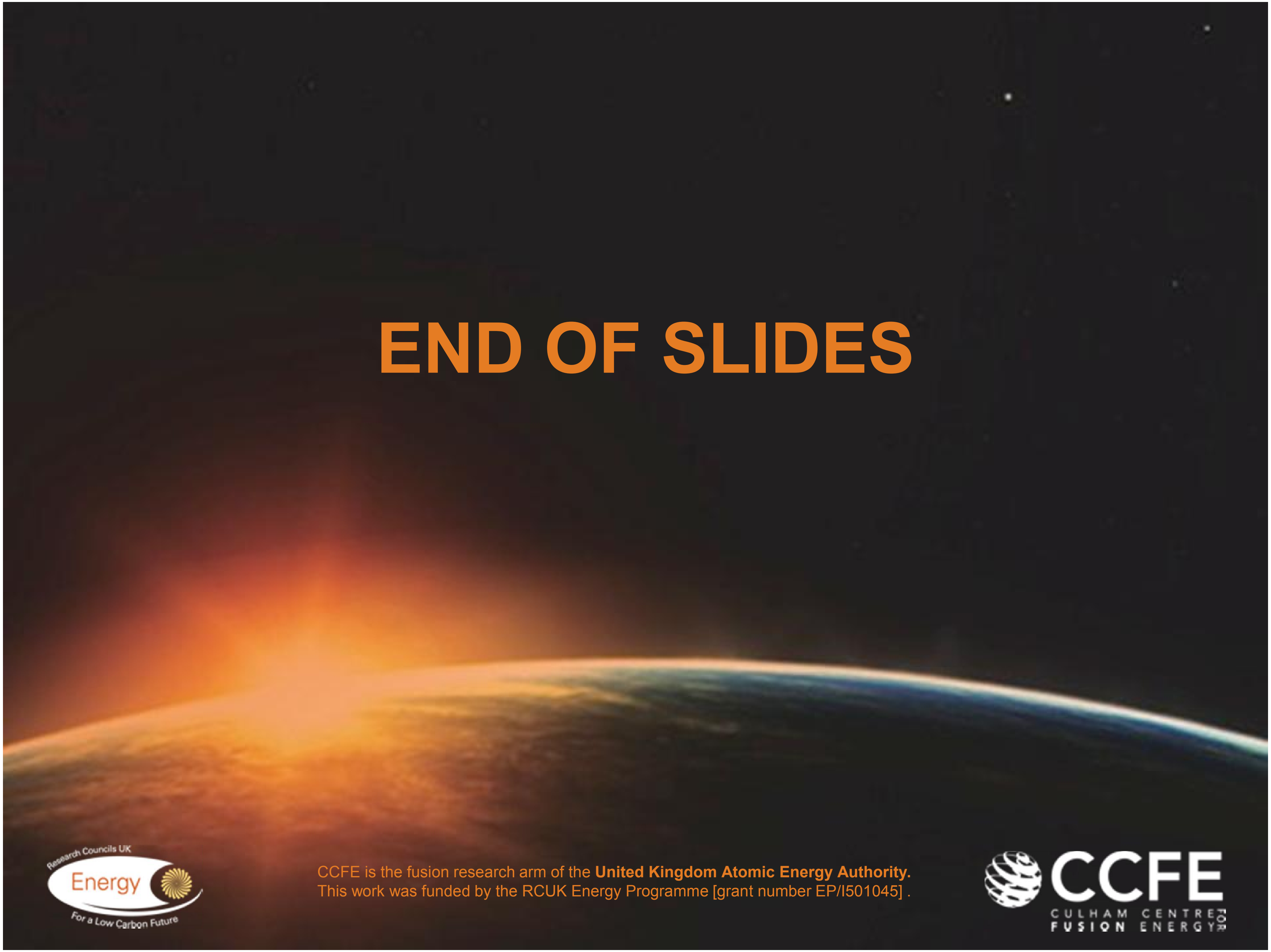
[1] T. Hutton, J.C. Sublet, L. Morgan & T.W. Leadbeater. Nuclear data for fusion: Validation of typical pre-processing methods for radiation transport calculations, Fusion Engineering and Design, In Press.

TENDL PROCESSING METHODOLOGY
STEP 5: Regression Tests

- Each isotope in the TENDL library is regression tested individually
- A script runs a MCNP or SERPENT model of a sphere of a single isotope, for each isotope in the TENDL_lite index
- Each model is run for one minute
  - The output file is checked for error keywords and file size criteria
- A list of passed/failed isotopes is produced
  - Output files of error producing input files are kept, others are deleted
- Work on non-regression testing of nuclear libraries is ongoing.

Summary

- The full TENDL-14 library contains nuclear data for 2633 nuclides.
  - Extensive but bulky!
- TENDL_Lite has been created based on the nuclides found in the most recent JEFF, JENDL and ENDF libraries.
- TENDL_Lite libraries have been produced to serve both MCNP6 and SERPENT2
- In order to faithfully perform MCNP and SERPENT fusion benchmarking, both codes should read exactly the same nuclear data
- TENDL libraries have been regression tested using MCNP6 and SERPENT2.
- Ideally, LAW 61 should be implemented in SERPENT-2 nuclear data libraries .


END OF SLIDES
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Acknowledgements

This work was funded by the RCUK Energy Programme under Grant EP/I501045 and the European Communities under the contract of Association between EURATOM and CCFE. The views and opinions expressed herein do not necessarily reflect those of the European Commission. To obtain further information on the data and models underlying this paper please contact PublicationsManager@ccfe.ac.uk.

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TENDL PROCESSING METHODOLOGY
STEP 4: CREATE XSDIR

- In terms of the NJOY input file the difference between LAW 4 and LAW 61 is small

```
acer
-21 -24 0 31 32
1 0 1 0.14 0/
'Ace $isma[$c1] TENDL-2014‘
$isma[$c2] 293.6/
0 1/
/
```

LAW 4

```
acer
-21 -24 0 31 32
1 0 1 0.14 0/
'Ace $isma[$c1] TENDL-2014‘
$isma[$c2] 293.6/
1 1/
/
```

LAW 61

  - Law 4 represents the distribution of outgoing particle angles with N equiprobable channels (N=32 for ACE).i.e. for each incident neutron outgoing angle, μ_i, a PDF exists which defines E_i'.
  - LAW 61 represents the distribution of outgoing particles (E’,μ) with a tabulated CDF.
- For fission analysis this will make little difference to the result, however the impact for fusion may be of importance