Getting started with FISPACT-II

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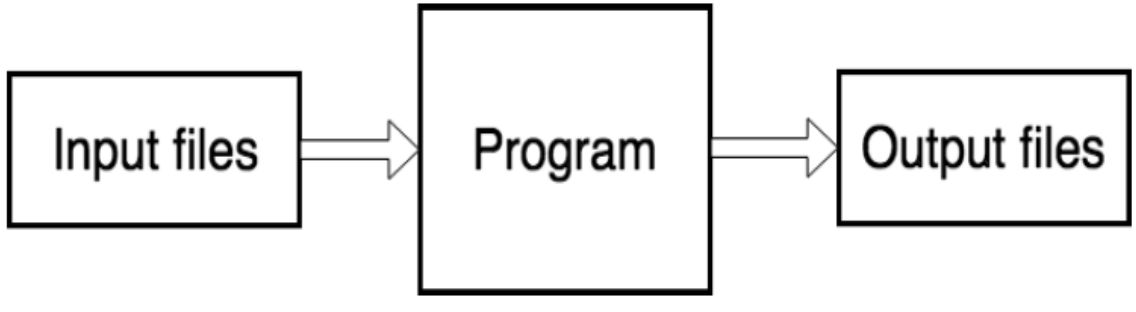
Useful links

- Wiki - FISPACT-II usage
- Forum - Post a question
- Manual - Latest manual
- Nuclear Data - Download the required libraries
- GitHub - Open source related codes
- Docker - Running FISPACT-II in docker

https://fispact.ukaea.uk

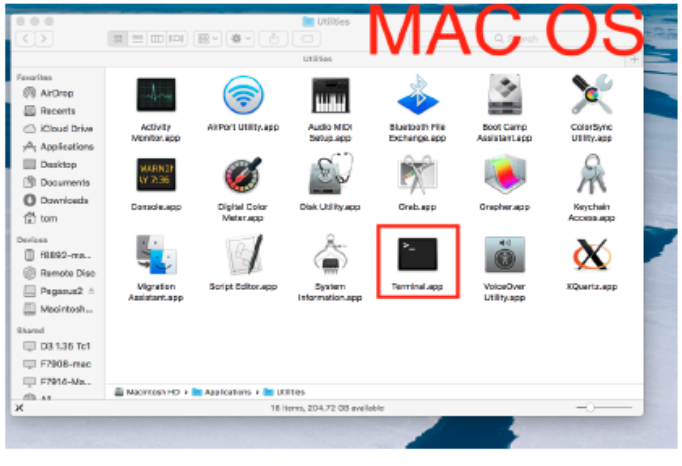
What is FISPACT-II?

- Command line tool only
- Works on Windows, Linux and Mac
- Single binary executable program
- File driven program (via **input files**)
- Produces **output files** (text, TAB and JSON formats)
- Human readable outputs with more structured outputs for parsing



How to run FISPACT-II

- No **GUI** (yet)
- Use via **terminal** (Linux) or **cmd** (Windows)
- Powershell or Cygwin can be used too!



Be aware

- Windows uses **.exe** extension (not the case for Mac and Linux)
- Windows uses **** not **/** (Linux/Mac)
- Important for files file (more on that later). Linux style paths can be used on Windows
- Input and output files are independent of operating system

Running FISPACT-II

- Requires input files as arguments
- Will not run without an input

Mac/Linux

```
[tom@mac:~/Dev/fispact]$ /path/to/fispact # gives an error
```

Windows

```
C:\Dev\fispact> C:\path\to\fispact.exe # gives an error
```

Running FISPACT-II correctly

We need an input file ***myinput.i*** and files file ***myfiles*** (always!)

```
[tom@mac:~/Dev/fispact]$ /path/to/fispact myinput myfiles
Running....
```

Note that ***.i*** is needed for the input file name extension **but** is omitted from cmd line

```
[tom@mac:~/Dev/fispact]$ ls
myinput.i       myfiles
[tom@mac:~/Dev/fispact]$ /path/to/fispact myinput myfiles
```

Running FISPACT-II correctly

- First argument is the input file ***myinput.i***
- Second argument is the files file ***filesfile*** (optional)
- Input file must have *.i* extension
- Files file can have extension (if you want) but normally doesn't
- Files file argument can be omitted **iff** it is named *'files'*, *'Files'*, or *'FILES'*

Note that ***.i*** is needed for the input file name extension **but** is omitted from cmd line

```
[tom@mac:~/Dev/fispact]$ ls
myinput.i       myfiles         FILES
```

```
# uses myfiles file
[tom@mac:~/Dev/fispact]$ /path/to/fispact myinput myfiles
```

```
# uses FILES file
[tom@mac:~/Dev/fispact]$ /path/to/fispact myinput
```

Creating an alias for FISPACT-II

Instead of typing

```
/path/to/fispact
```

Easier to make an alias

Mac/Linux

```
[tom@mac:~/Dev/fispact]$ export FISPACT=/path/to/fispact
```

```
[tom@mac:~/Dev/fispact]$ $FISPACT myinput myfiles
```

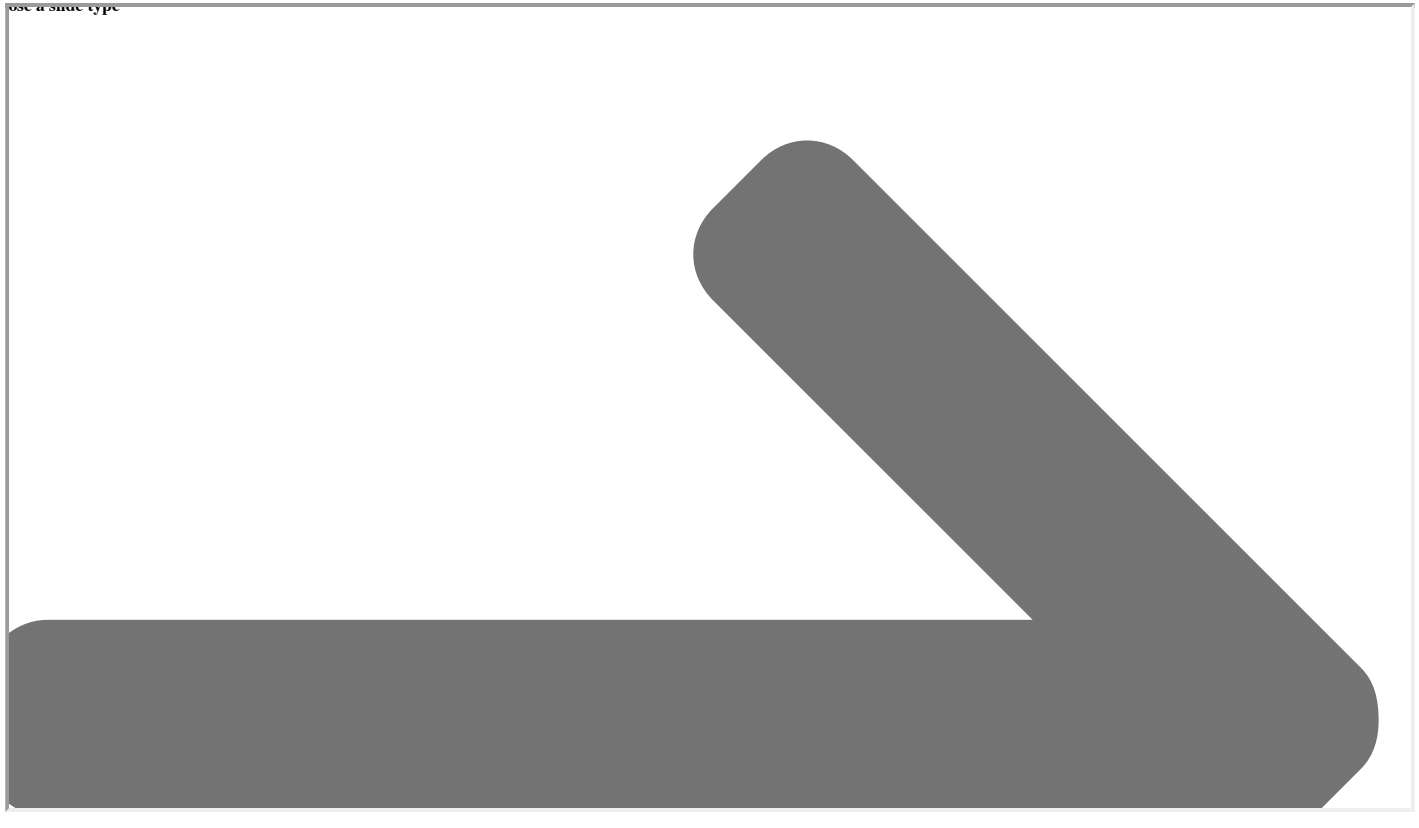
Windows

```
C:\Dev\fispact> set FISPACT=C:\path\to\fispact.exe
```

```
C:\Dev\fispact> %FISPACT% myinput myfiles
```

Poll: FISPACT-II experience

Click here to take the poll



Files file

- We will see later how to make these files from scratch
- But first let's learn more about the **files file**
- Why do we need it?
- What does it do?
- What do we need to put in it?

Files file

*The files file declares the nuclear data libraries to be used in the fispact run**

(*mainly -it also tells FISPACT-II the names and locations of files to read and write)

FISPACT-II is useless without nuclear data!

Files file

- A text file
- With a list of keys and values
- Typically named 'files', 'Files' or 'FILES'
- But can be named anything e.g. files.tendl2015.run1
- Order of paths does not matter
- Use linux style '/' for paths
- Don’t use tab to indent – causes parsing problems!

Files file

Nuclear data paths...

```
# index of nuclides to be included
ind_nuc /home/F-II/nuclear_data/TENDL2015data/tendl15_decay12_i

# Library cross section data
xs_endf /home/F-II/nuclear_data/TENDL2015data/tal2015-n/gxs-709

# Library decay data
dk_endf /home/F-II/nuclear_data/decay/decay_2012
```

Files file

Other data paths...

```
# fluxes file to be read in
fluxes fluxes

# collapsed cross section data (in and out)
collapxi COLLAPX
collapxo COLLAPX

# condensed decay and fission
arrayx ARRAYX
```

Files file

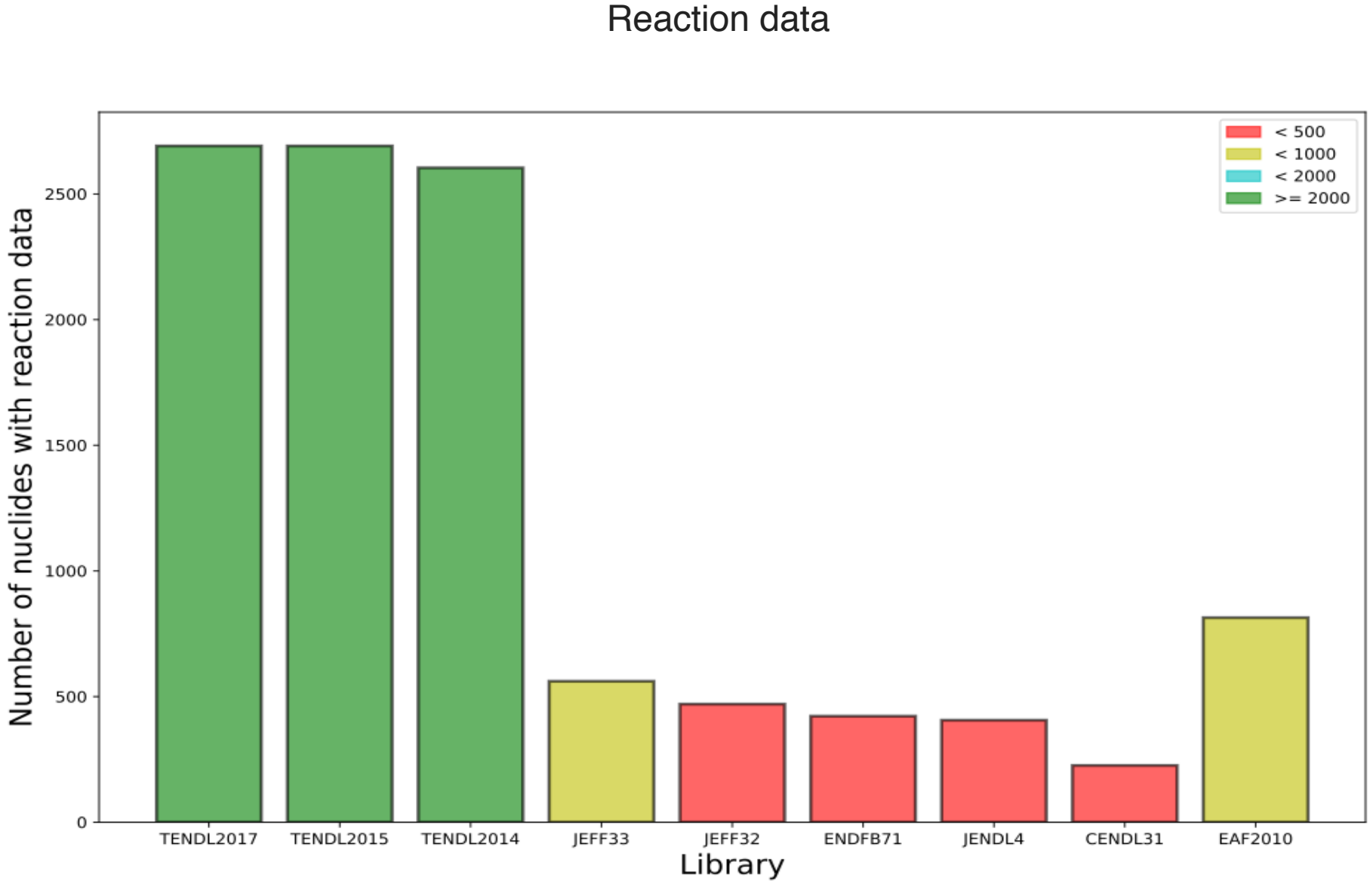
- Normally use about **12 - 16** key-value pairs needed
- Over 40 possible options
- See advanced usage for details on the others
- In most examples here, we will use no more than 16.

Nuclear data

- FISPACT-II can process a lot of different nuclear data libraries
- Can process both **ENDF-6** format and **EAF** format libraries
- A large number are shipped with version 4.0 already
- FISPACT-II uses group wise data, not point wise

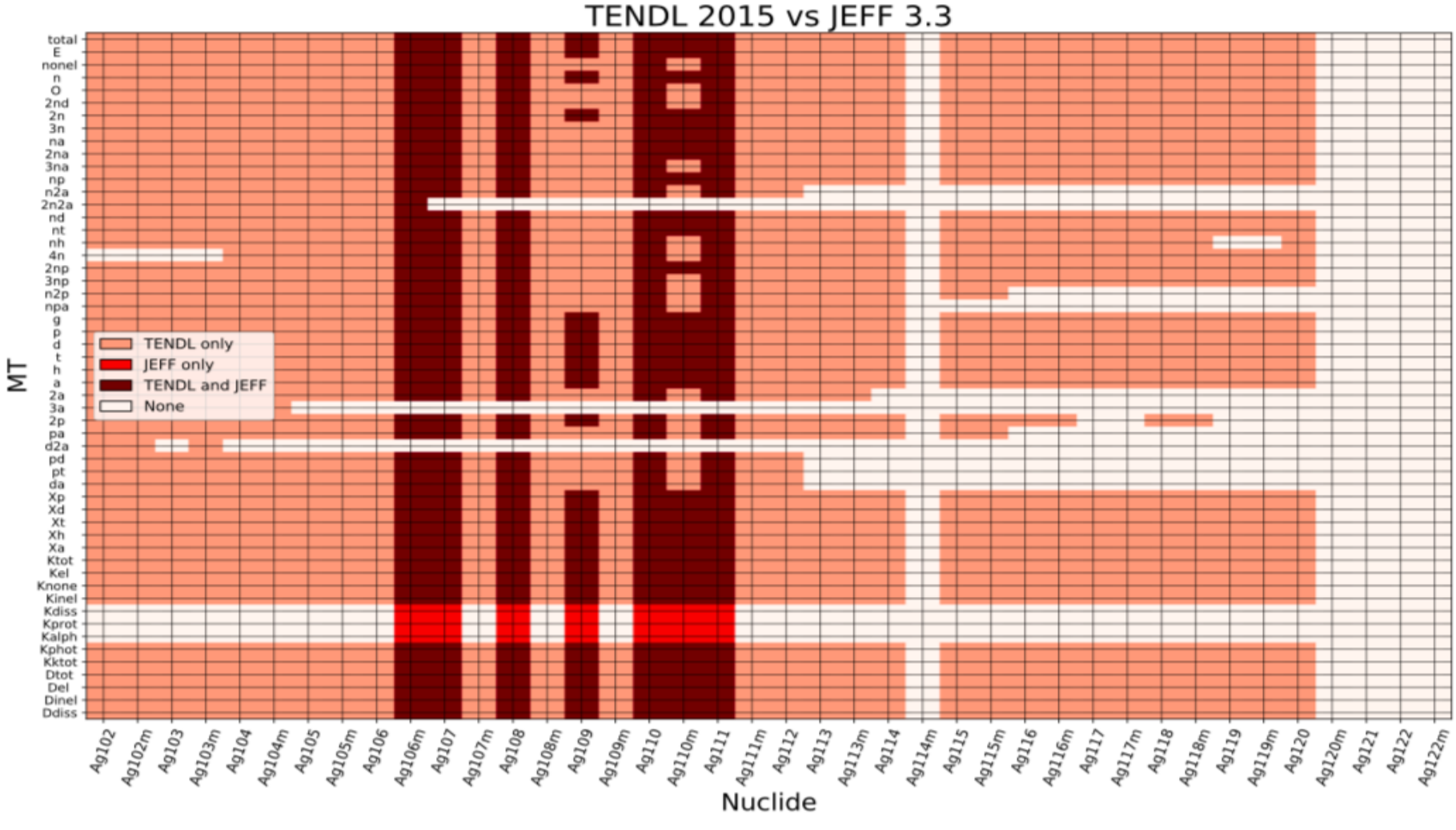
Disclamer: FISPACT-II does not hold responsibility for nuclear data errors/issues, it is simply a consumer of nuclear data

Nuclear data: quick compare

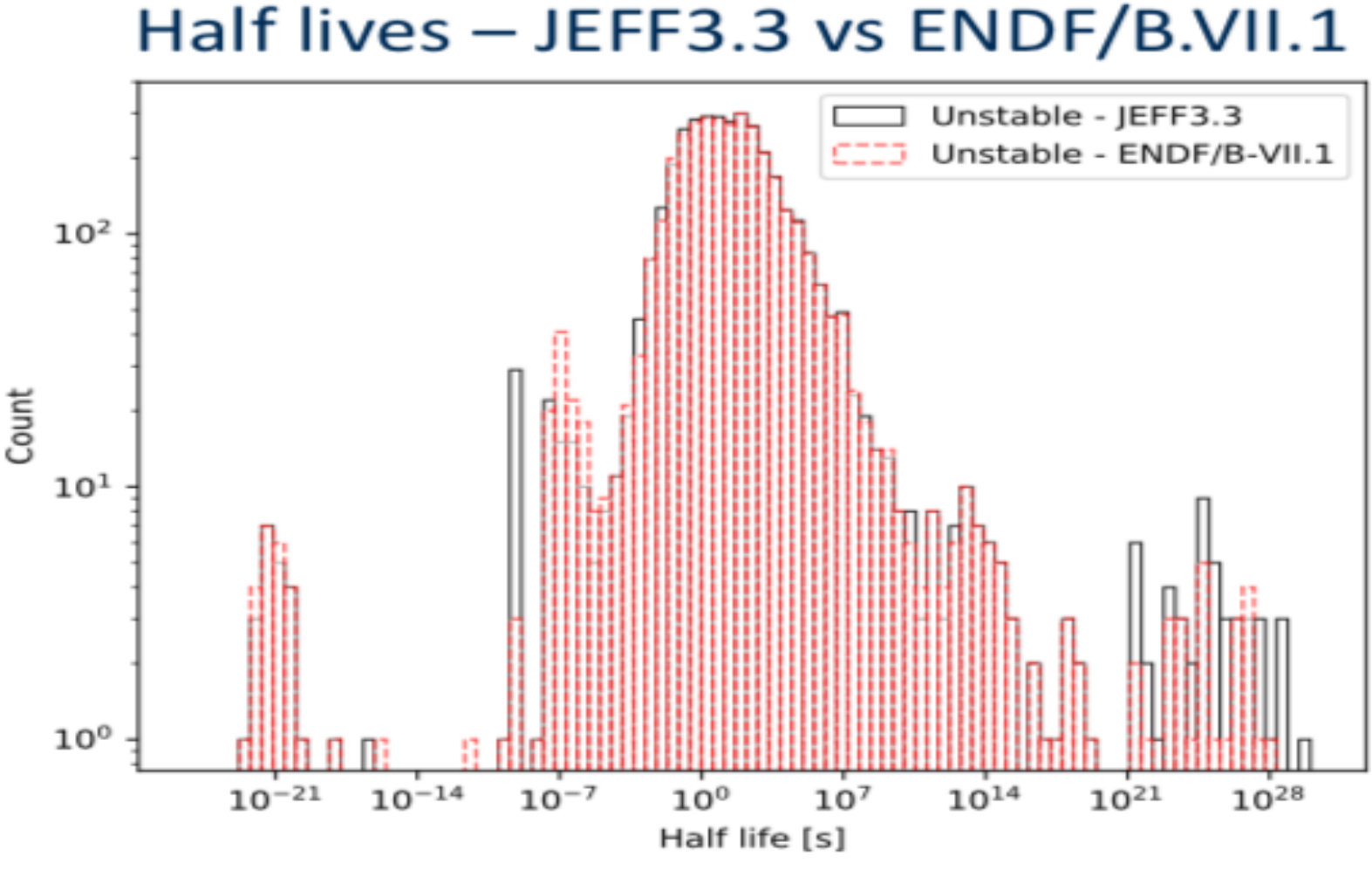


Nuclear data: in depth compare

Reaction data for Silver

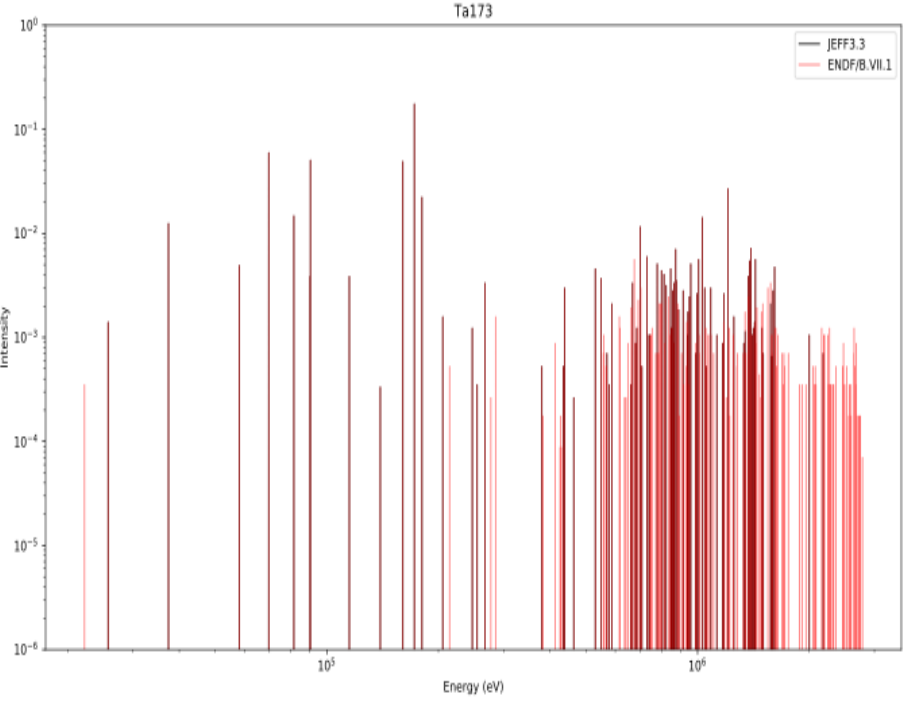


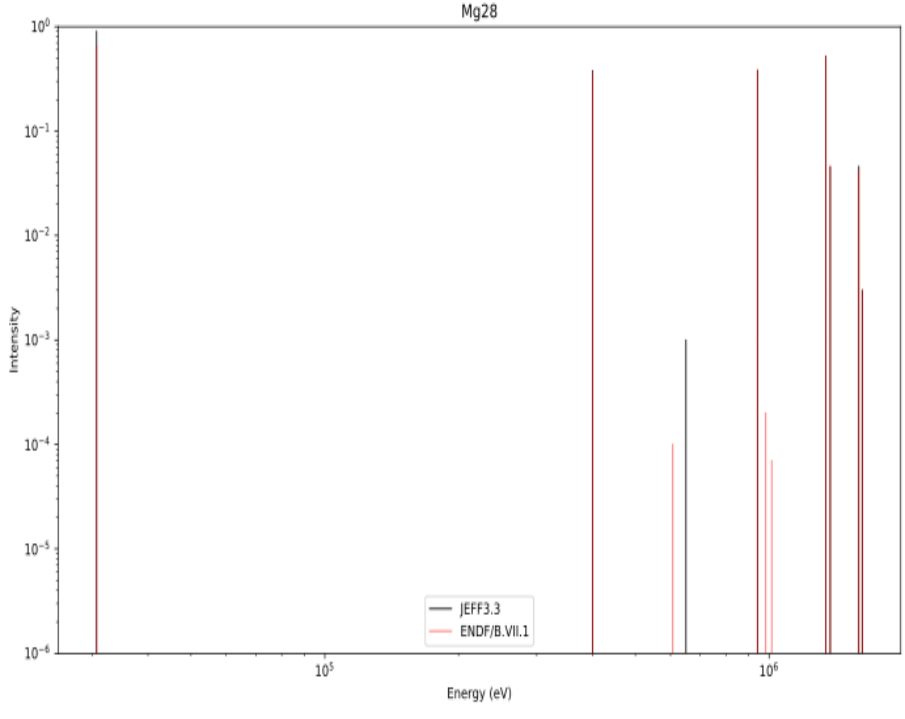
Decay data is different too



Gamma lines

JEFF3.3 vs ENDFB VII





A final note on nuclear data

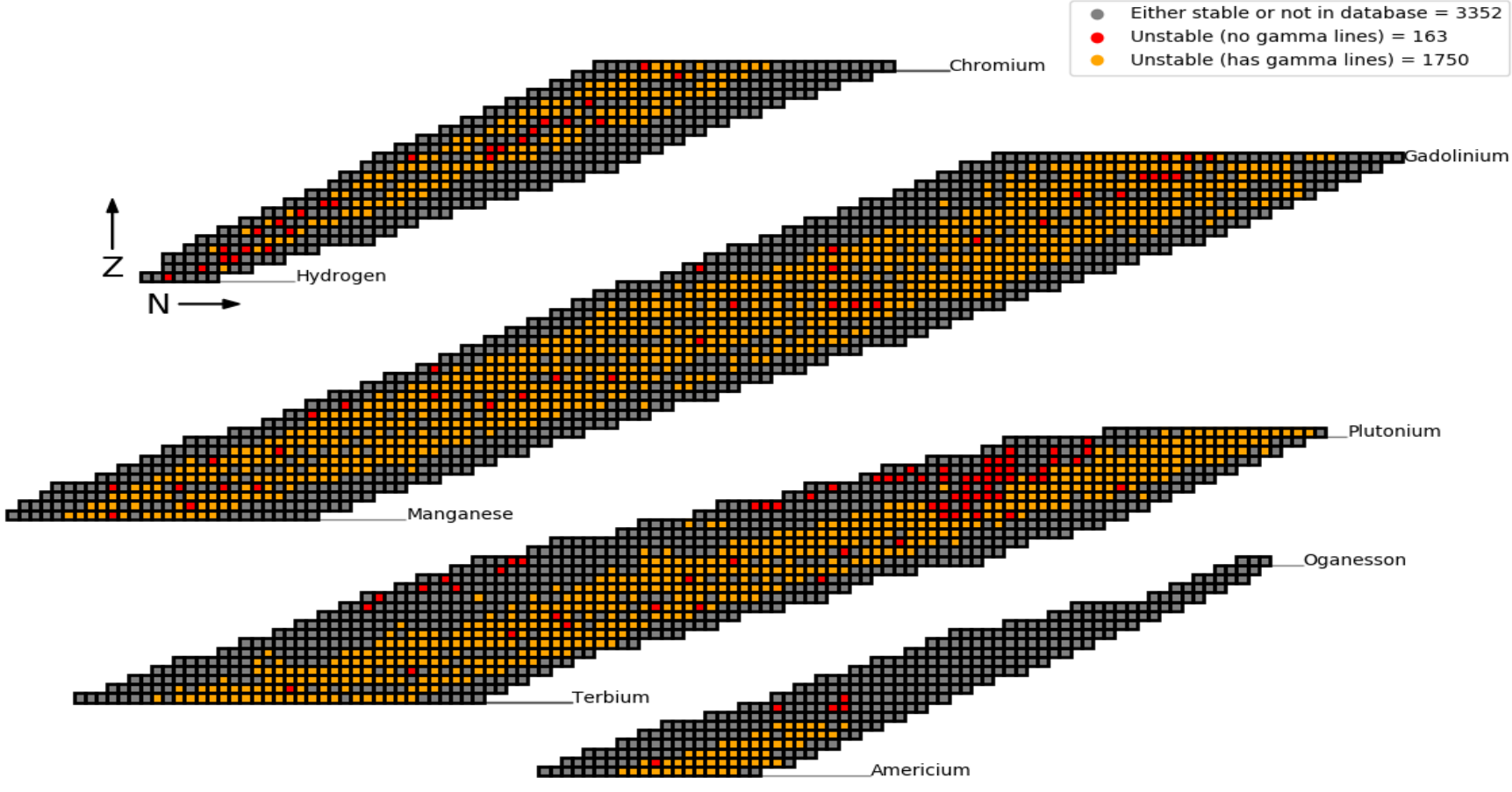
TENDL recommended

- FISPACT-II development has run in parallel with that of the **TALYS-based Evaluated Nuclear Data Library** – TENDL*
- It is the largest and most complete nuclear data library!
- 2014, 2015 and 2017 included with FISPACT-II
- 2019 also now available

* A. J. Koning, D. Rochman, et al. - https://tendl.web.psi.ch/tendl_2017/tendl2017.html

3850+ nuclides

Full decay_2012 library



Compressing nuclear data

- Large nuclear data libraries (such as TENDL) can take a while to read
- Sometimes up to 2 minutes for TENDL 2017
- This can be improved by up to **60%** using the compress_xs_endf tool
- Separate tool shipped with FISPACT-II
- Turns nuclear data text files into binary equivalent
- Note: they are OS dependant
- Use GETXS -1 for binary files

Core nuclear data

- **ind_nuc** = Index file – tells what nuclides to include in the simulation
- **xs_endf** = Cross section data directory (ENDF-6 format)
- **xs_endfb** = Cross section data directory (compressed binary format)
- **dk_endf** = Decay data directory (ENDF-6 format)
- **a2data** = file path of transportation values of radioactive material
- **clear** = file path of clearance values of radioactive material
- **hazards** = file path of ingestion and inhalation values for radionuclides
- **absorp** = file path of air attenuation data for nuclides
- **fy_endf** = neutron fission yield data directory
- **sf_endf** = spontaneous fission yield data directory
- **prob_tab** = directory path to probability table data for self shielding

Note: For EAF keywords can differ. For example, xs_endf -> crossec

Other important data

As mentioned before, files file has other data

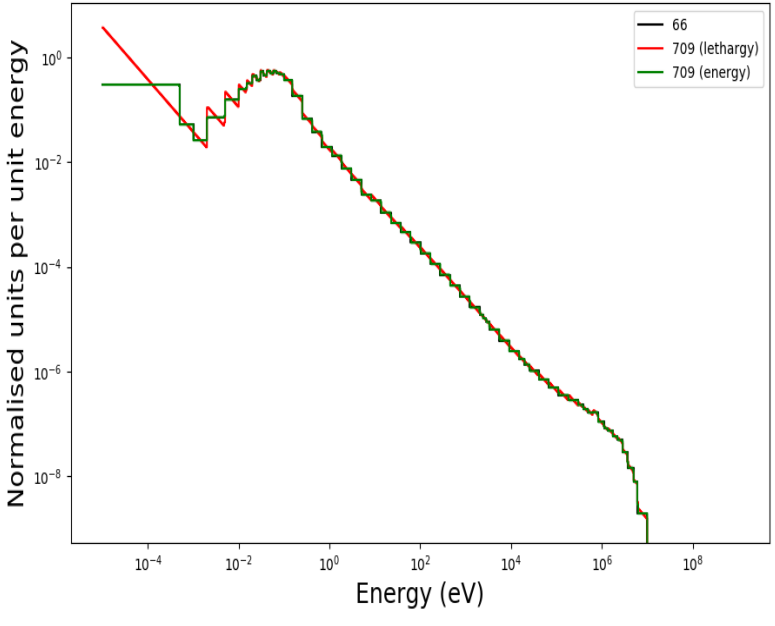
- **fluxes** = Defines your flux (incident particle energy spectrum) - always needed for irradiation simulations
- **collapxi** = if using a pre collapsed binary file, use this instead (more details later)
- **collapxo** = pre collapsed binary file output path
- **arrayx** = binary file for decay data output path

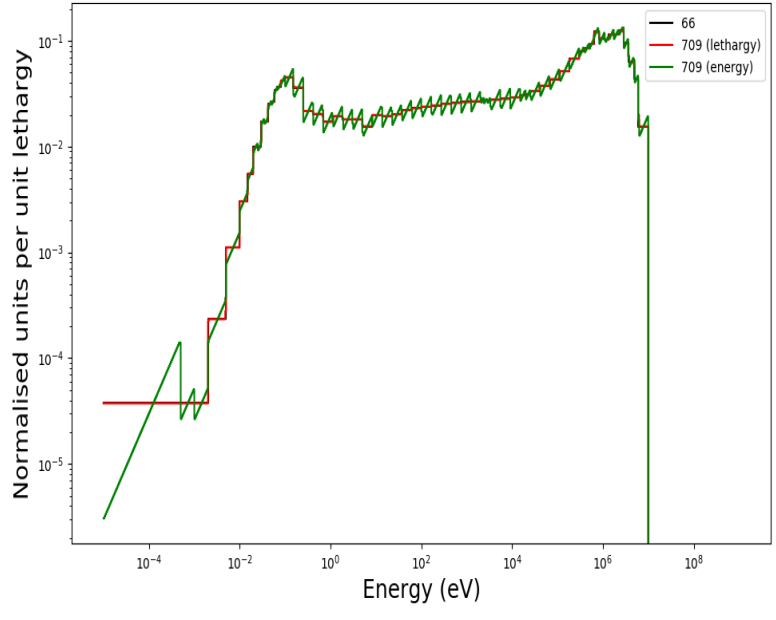
Fluxes file

Defines your incident particle energy spectrum

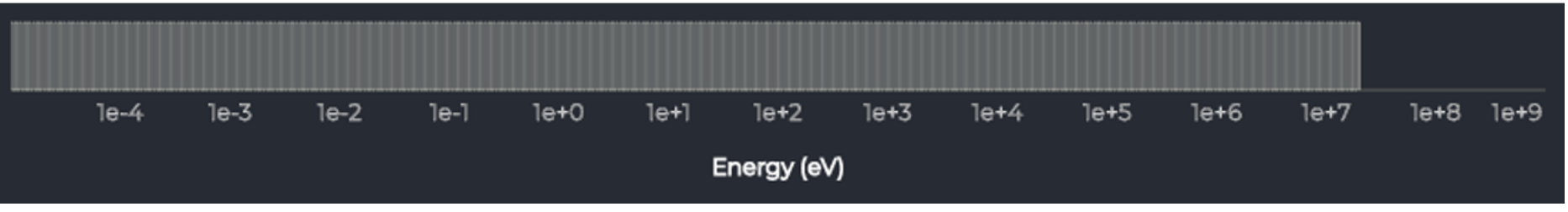
- If you want to do irradiation then a fluxes file is needed
- We have to tell FISPACT-II in the **files file** about the **fluxes file**
- The file contains the group wise data as a list of values
- Note: Data must be specified in descending order (high to low energy)!
- Group structure must match that of nuclear data
    - e.g. If using TENDL2017 then you will need your spectra defined in 709 group.
    - Group convert (GRPCONVERT) can change group structure (more on this later)

Fluxes file

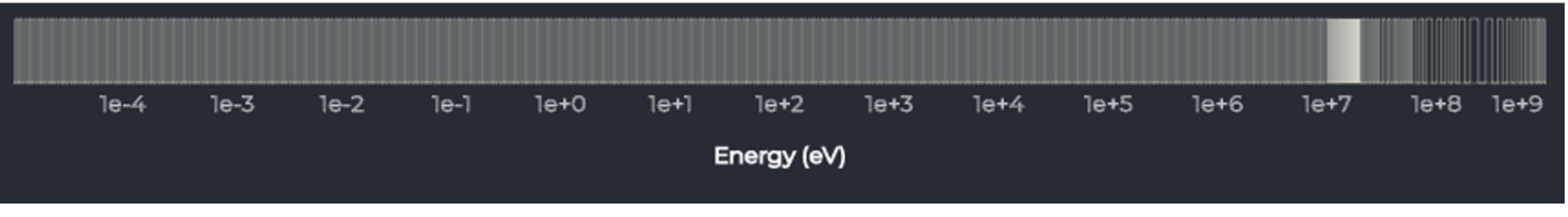

66
709 (lethargy)
709 (energy)
Normalised units per unit energy
Energy (eV)


66
709 (lethargy)
709 (energy)
Normalised units per unit lethargy
Energy (eV)

group 616



group 709

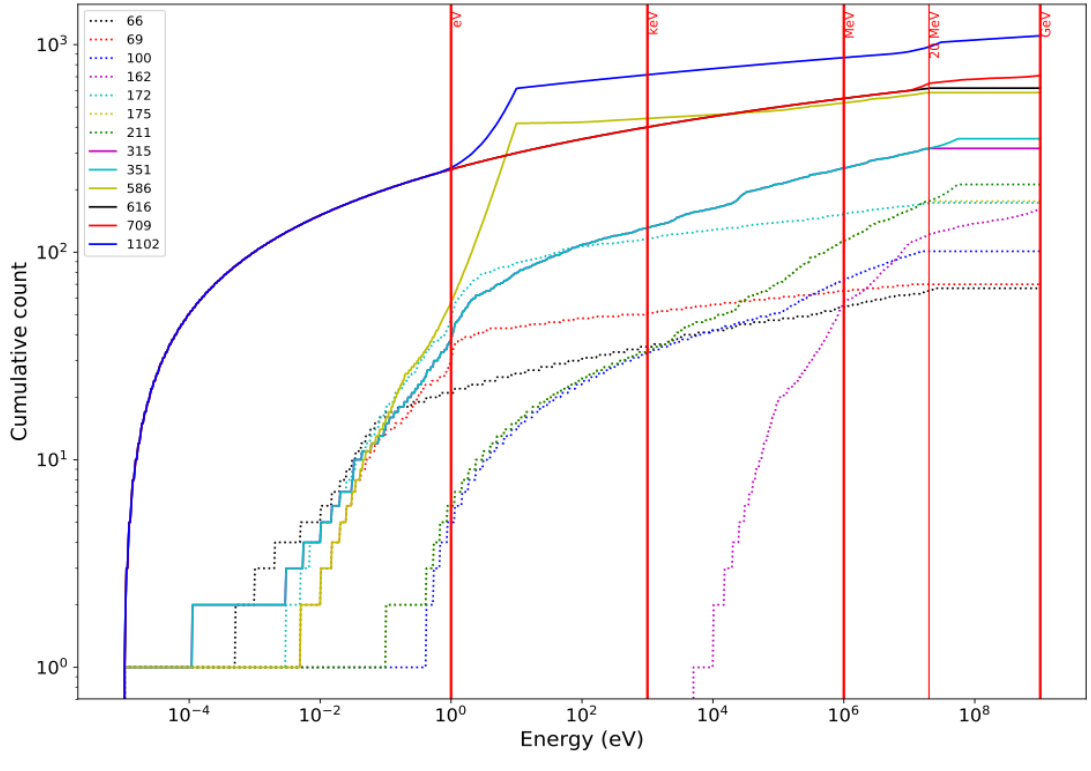


Group structures

Different group structures cover different energy regimes

Some libraries are provided in a given energy range best suited for certain applications

709 group covers up to 1 GeV – most libraries shipped in this structure



Input file

The input file governs everything for the run

- Material definition
- Irradiation schedule
- Log options
- Uncertainties
- Solver settings
- Self shielding
- Pathways
- Output types – TAB, JSON, graph files

Input file

- A text file
- List of keywords and arguments
- No default name, unlike the files file
- Input file must have .i extension
- Order of paths does matter (unlike files file)
- Allows comments with '<< comment here >>'
- Note: **There is a limit of 120 characters per line!**
- 92 keywords in all!

Input file

3 sections to the input file

- Control - 32 possible keywords
- Initialisation - 64 possible keywords
- Inventory - 41 possible keywords

32 + 64 + 41 ≠ 92

Many keywords can be used in each input section, but some can only be used in one section!

Full list: https://fispact.ukaea.uk/wiki/FISPACT-II_keywords

Simple example

```
<< CLOBBER tells fispact to overwrite >>
<< existing files of same name >>
CLOBBER
<< GETXS 1 tells fispact to get the cross section>>
<< data and do collapse >>
GETXS 1 709
<< GETDECAY 1 tells fispact to get the decay>>
<< data and do condense >>
GETDECAY 1
<< FISPACT signals end of control section >>
FISPACT
* example 1
<< END is required to signal end of input >>
END
* end of example
```

Control only - no Initialisation or inventory sections here

Collapse

The nuclear data collapse with GETXS takes the extensive reaction cross section data and probability tables for resonance self-shielding and folds (collapses) them with irradiation spectrum in fluxes. Producing a single scalar value (1-group).

Collapse

Produces a binary COLLAPX file of 1-group data with uncertainties which is given by the ***collapxo*** file in the files file

$$\bar{\sigma} = \frac{\sum_i^N \sigma_i \phi_i}{\sum_i^N \phi_i}$$

Exercise: printlib

Printlib 4 prints all collapsed cross sections to disk

The cross sections are given for each reaction

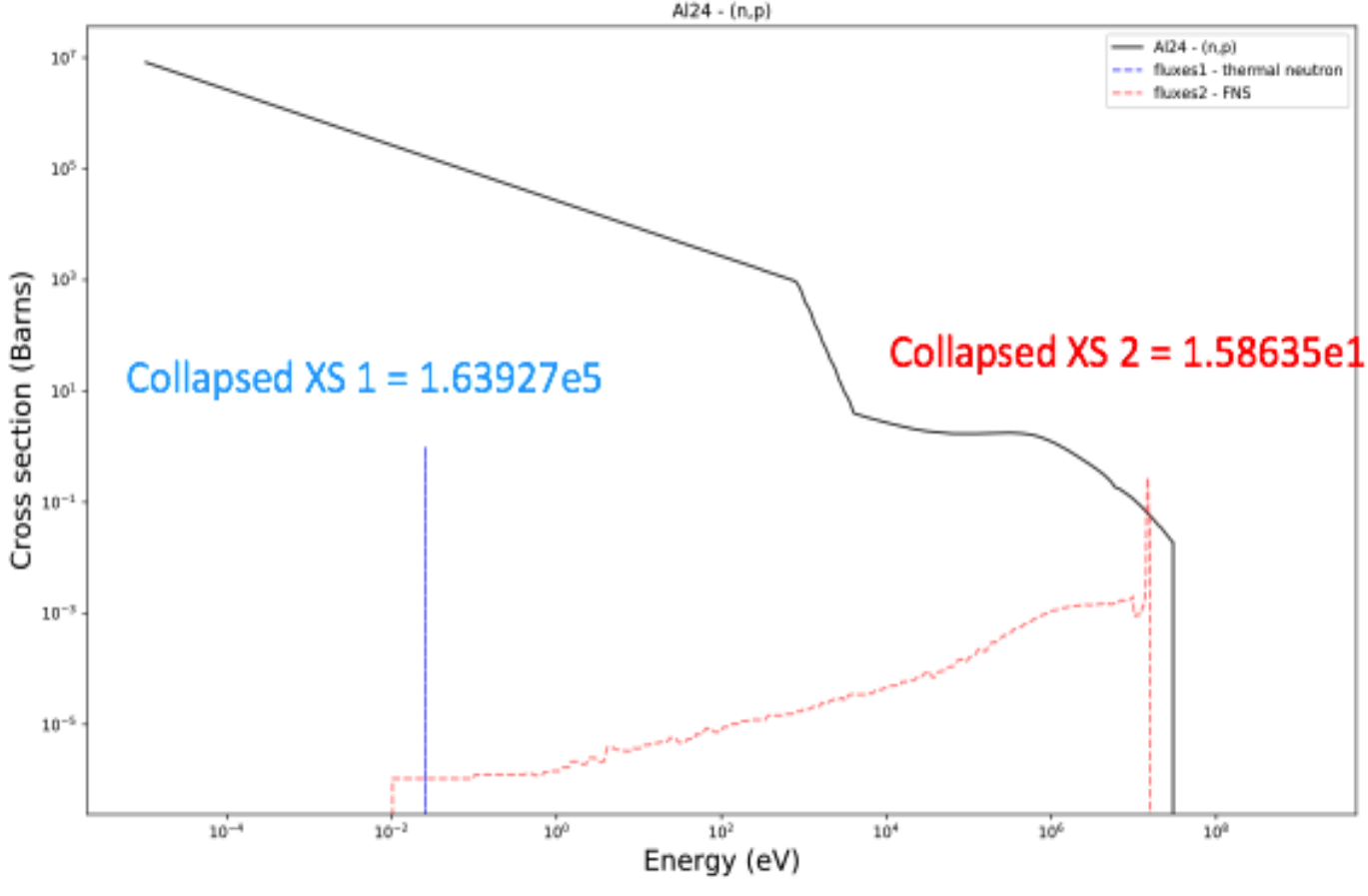
See the exercise on this.

```
 |                                                                                                    |
 | THIS RUN                                                                                           |
 | timestamp:                  09:52:10 5 June 2018                                                   |
 | fileroot :                  ex2                                                                    |
 | name of FILES file:         files                                                                  |
 | FISPACT title:              * example 1                                                            |
 |                                                                                                    |
 | See the ex2.log file                                                                               |
 | and summary details at the end of this file for further information on files used by this run      |
 |                                                                                                    |
 ====================================================================================================

1                C O L L A P S E D    C R O S S    S E C T I O N S    I N    B A R N S

       NOTE: The diagnostic cross-sections for dpa (n,D--) and for kerma (n,K--) reactions are given in barns-eV.

       The cross section for the specified reaction is given in barns, followed by the error in percent.

 parent reaction  daughter cross section   +-error          parent reaction  daughter cross section   +-error
 H   1  (n,Dtot )          1.73063E+02+- 0.00000E+00        H   1  (n,Ddiss)          1.73063E+02+- 0.00000E+00
 H   1  (n,Ktot )          7.32927E+05+- 0.00000E+00        H   1  (n,Kel  )          3.84884E-01+- 0.00000E+00
 H   1  (n,Knone)          7.32926E+05+- 0.00000E+00        H   1  (n,Kphot)          7.32493E+05+- 0.00000E+00
 H   1  (n,Kktot)          7.32927E+05+- 0.00000E+00        H   1  (n,Xd   )          3.29462E-01+- 0.00000E+00
 H   1  (n,total)          3.02774E+01+- 0.00000E+00        H   1  (n,E    )  H   1   2.99480E+01+- 2.96233E-01
 H   1  (n,g    )  H   2   3.29417E-01+- 2.55297E+00        H   2  (n,Dtot )          5.18112E-01+- 0.00000E+00
 H   2  (n,Ddiss)          5.18112E-01+- 0.00000E+00        H   2  (n,Ktot )          3.14013E+03+- 0.00000E+00
 H   2  (n,Kel  )          4.82672E-02+- 0.00000E+00        H   2  (n,Knone)          3.14009E+03+- 0.00000E+00
 H   2  (n,Kktot)          3.53743E+00+- 0.00000E+00        H   2  (n,Xt   )          5.01819E-04+- 0.00000E+00
 H   2  (n,total)          4.22333E+00+- 1.50000E+00        H   2  (n,nonel)          5.01748E-04+- 0.00000E+00
 H   2  (n,E    )  H   2   4.22283E+00+- 2.00000E+00        H   2  (n,g    )  H   3   5.01748E-04+- 3.00000E+00
 H   3  (n,Ktot )          1.87166E-02+- 0.00000E+00        H   3  (n,Kel  )          1.87166E-02+- 0.00000E+00
 H   3  (n,Kktot)          1.87166E-02+- 0.00000E+00        H   3  (n,total)          1.93838E+00+- 0.00000E+00
 H   3  (n,E    )  H   3   1.93838E+00+- 0.00000E+00        He  3  (n,Dtot )          1.05921E+07+- 0.00000E+00
 He  3  (n,Ddiss)          1.05921E+07+- 0.00000E+00        He  3  (n,Ktot )          4.02870E+09+- 0.00000E+00
 He  3  (n,Kel  )          3.72152E-02+- 0.00000E+00        He  3  (n,Knone)          4.02870E+09+- 0.00000E+00
 He  3  (n,Kktot)          4.02870E+09+- 0.00000E+00        He  3  (n,Xp   )          5.27488E+03+- 0.00000E+00
 He  3  (n,Xt   )          5.27488E+03+- 0.00000E+00        He  3  (n,Xa   )          5.45646E-05+- 0.00000E+00
 He  3  (n,total)          5.27801E+03+- 0.00000E+00        He  3  (n,p    )  H   3   5.27415E+03+- 0.00000E+00
 He  3  (n,E    )  He  3   3.85381E+00+- 0.00000E+00        He  3  (n,g    )  He  4   5.45572E-05+- 0.00000E+00
 He  4  (n,Ktot )          7.12495E-03+- 0.00000E+00        He  4  (n,Kel  )          7.12495E-03+- 0.00000E+00
 He  4  (n,Kktot)          7.12495E-03+- 0.00000E+00        He  4  (n,total)          8.62086E-01+- 0.00000E+00
 He  4  (n,E    )  He  4   8.62086E-01+- 1.10339E+00        Li  6  (n,Dtot )          5.61809E+06+- 0.00000E+00
 Li  6  (n,Ddiss)          5.61809E+06+- 0.00000E+00        Li  6  (n,Ktot )          4.45511E+09+- 0.00000E+00
 Li  6  (n,Kel  )          4.91128E-03+- 0.00000E+00        Li  6  (n,Knone)          4.45511E+09+- 0.00000E+00
 Li  6  (n,Kktot)          4.45483E+09+- 0.00000E+00        Li  6  (n,Xt   )          9.31233E+02+- 0.00000E+00
 Li  6  (n,Xa   )          9.31233E+02+- 0.00000E+00        Li  6  (n,total)          9.31920E+02+- 0.00000E+00
 Li  6  (n,nonel)          9.31143E+02+- 0.00000E+00        Li  6  (n,t    )  He  4   9.31105E+02+- 1.35019E-01
 Li  6  (n,E    )  Li  6   7.76787E-01+- 2.00988E+00        Li  6  (n,g    )  Li  7   3.81990E-02+- 8.00000E+00
```

Exercise: printlib

Can actually calculate this by hand

Getting the group wise XS data can be done using another tool with FISPACT-II
extract_xs_endf



Collapse and condense

Common practice is to separate out collapse and condense.

collapse.i input file – GETXS 1

condese.i input file – GETDECAY 1

Computationally expensive to do these processes. If flux is not changing, then no need to redo collapse. We just did the collapse in the previous example.

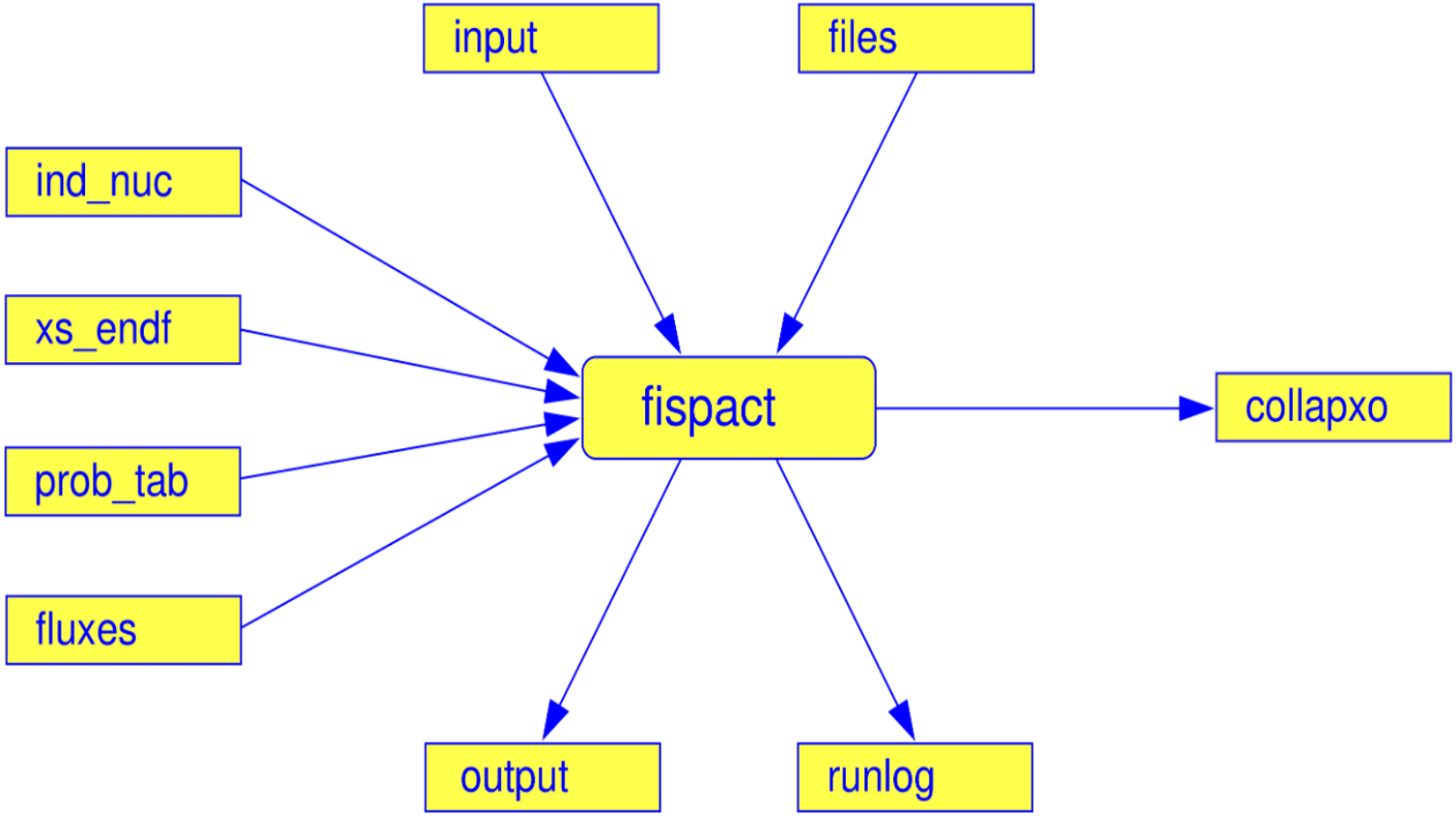
```
[tom@mac:~/exercises/basic/inventory]$ $FISPACT collapse
[tom@mac:~/exercises/basic/inventory]$ $FISPACT condense
[tom@mac:~/exercises/basic/inventory]$ $FISPACT input1
[tom@mac:~/exercises/basic/inventory]$ $FISPACT input2
```

Condense

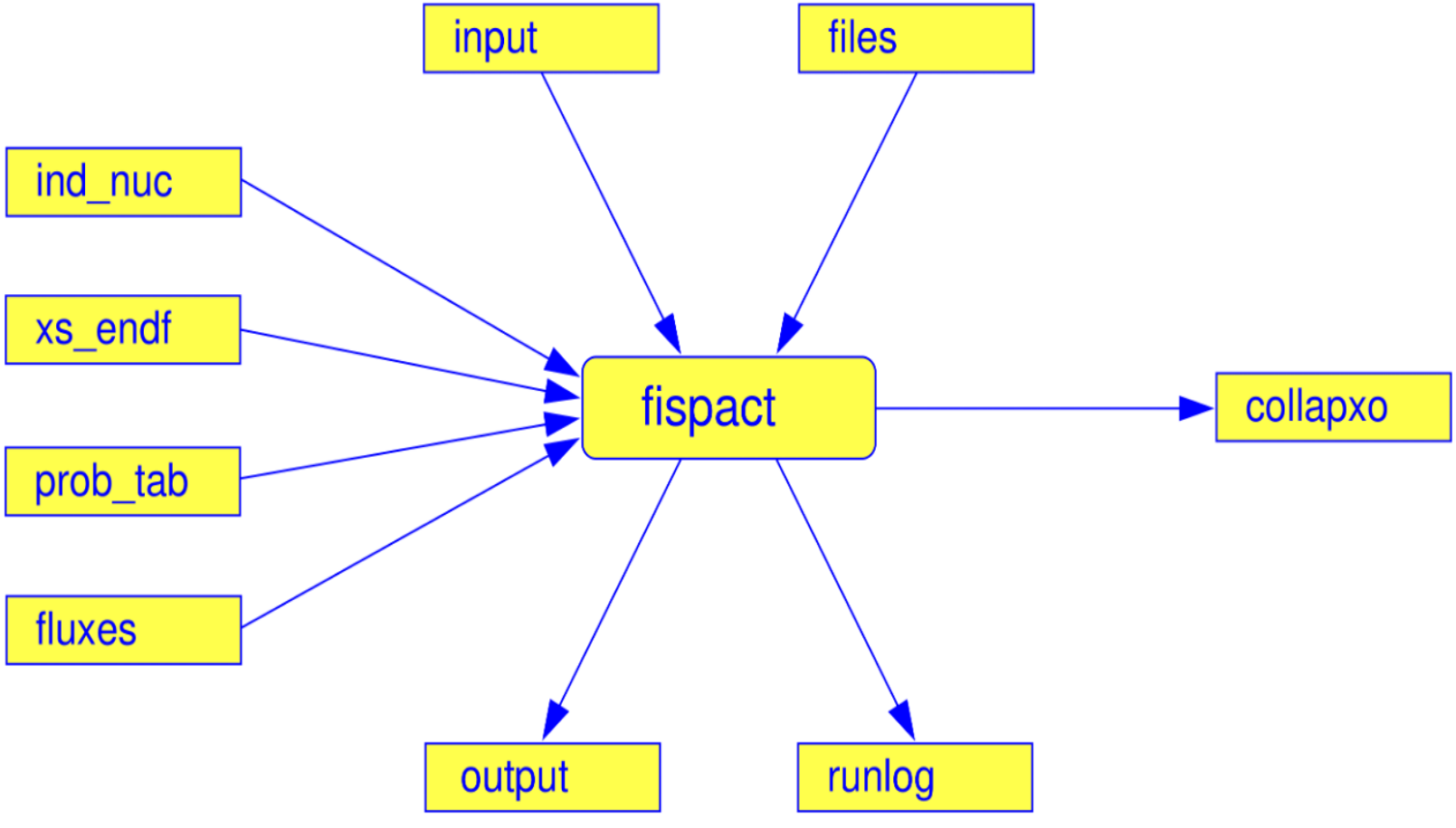
The nuclear data condense via GETDECAY produces a binary ARRAYX file from the extensive decay and fission yield data

May also require an irradiation spectrum (fluxes) to calculate spectrum-dependent fission yields but is not normally the case

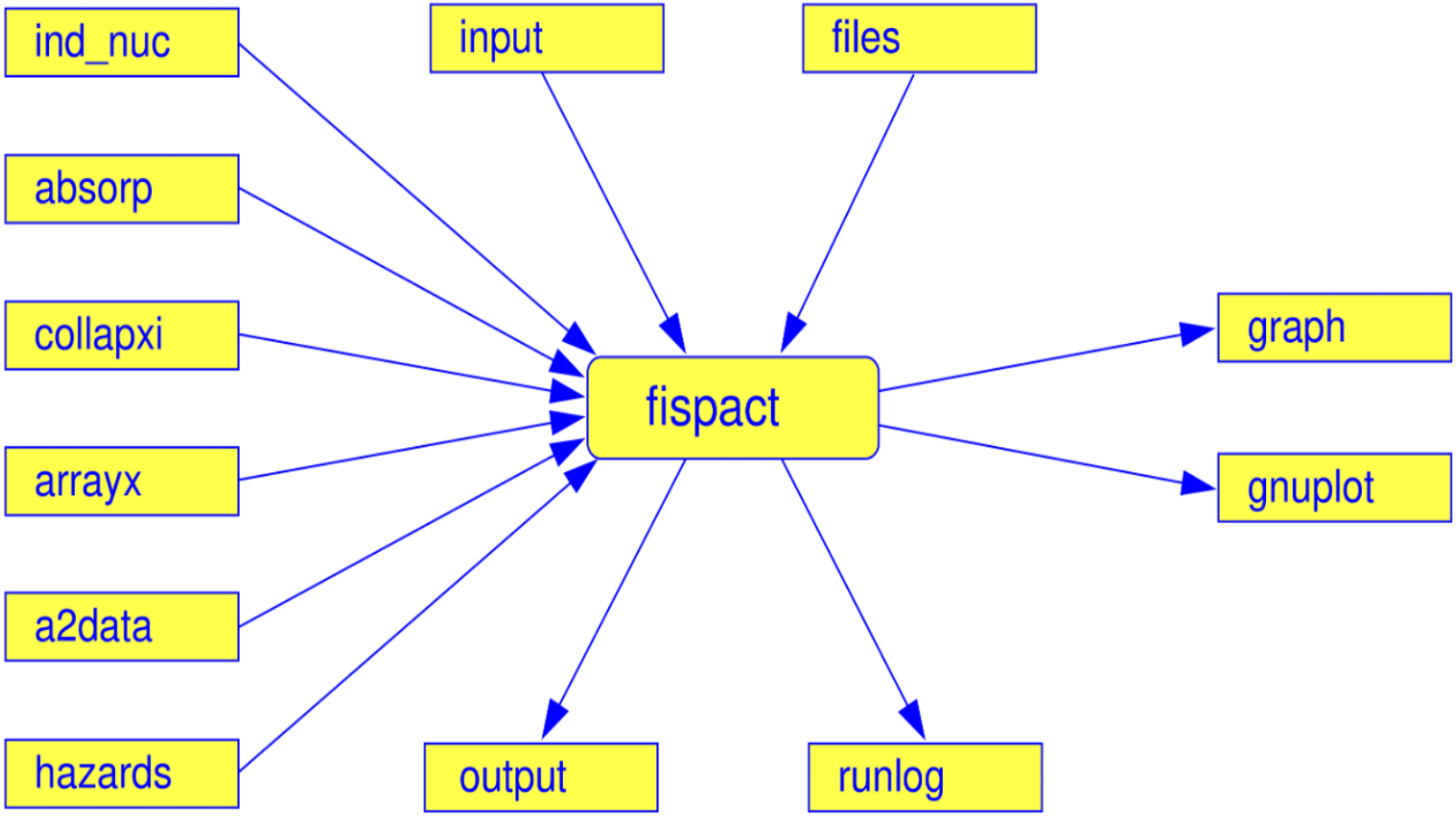
Collapse summary



Condense summary



Inventory summary



Summary so far

- What FISPACT-II is
- Some of what FISPACT-II can do
- What files FISPACT-II needs
    - Files file
    - Fluxes file
    - Input file
- How to run FISPACT-II

In the basic exercises we will use the fluxes and nuclear data to calculate all of the effective cross sections and prepare the decay data for time-dependent simulations.

However, all of this is not very interesting. No actual irradiation yet.

Worked example

FNS Inconel (from getting started)

Contains 4 input files

- collapse.i
- condense.i
- printlib.i
- inventory.i

First 3 have been covered, focus on the inventory run

Worked example - control

```
<< Overwrite any existing output file >>
CLOBBER
<< we also want a JSON output file >>
JSON
<< read in COLLAPX file>>
GETXS 0
<< read in ARRAYX file>>
GETDECAY 0
<< end of control section >>
FISPACT
* FNS 5 Minutes Inconel-600
```

Worked example - initial conditions I

```
<< Inconel 600 with density of 8.42 g/cc >>
DENSITY 8.42
<< 1 gram  with 4 elements >>
MASS 1.0E-3 4
<< 75.82% Ni >>
NI  75.82
<< 15.97% Cr >>
CR  15.97
<< 7.82% Fe >>
FE   7.82
<< 0.39% Mn >>
MN   0.39
```

Worked example - initial conditions II

```
<< ignore nuclides with inventory < 1000 atoms >>
MIND 1E3
<< create gnuplot data and file >>
GRAPH 1 2 1 3
<< pathways analysis >>
UNCERTAINTY 2
<< output half lives >>
HALF
<< output ingestion and inhalation >>
HAZARDS
```

Worked example - irradiation phase

```
<< irradiate material at 1.116e10 n/cm2/s >>
FLUX 1.116E+10
<< initial inventory (t=0) >>
ATOMS
<< want output after 5 minutes irradiation >>
TIME 5.0 MINS
<< solves rate equation matrix and >>
<< outputs initial inventory at time=5 mins>>
ATOMS
```

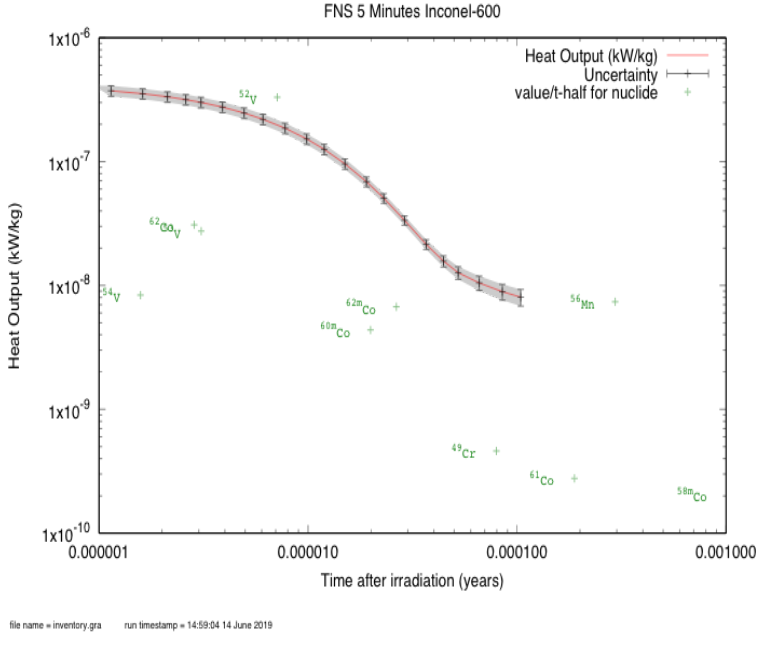
Note: Without either ATOMS, STEP, or SPECTRUM, nothing will be calculated! For less verbose output, use STEP, instead of ATOMS.

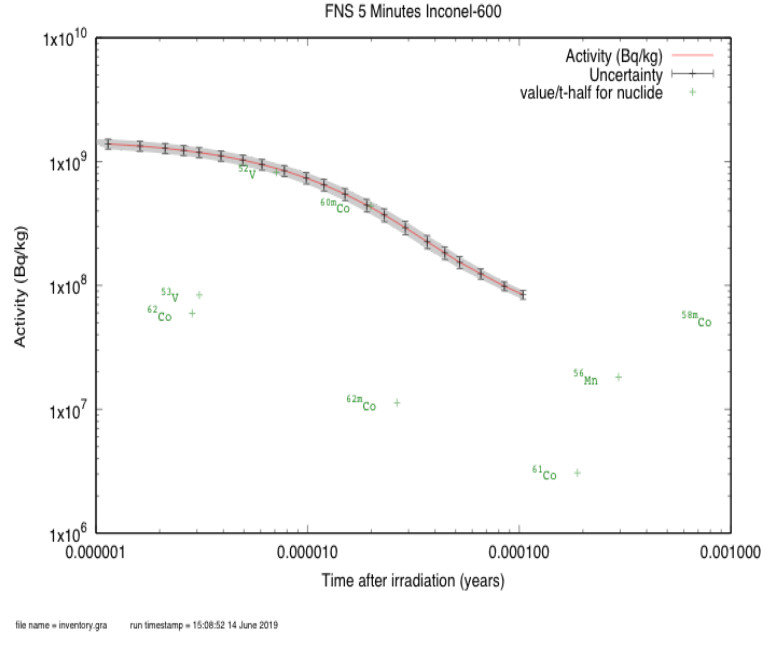
Worked example - cooling phase

```
<< turn flux off - decay only >>
FLUX 0.
<< tells FISPACT-II we are cooling >>
ZERO
<< cooling time intervals >>
<< 38 seconds after irradiation ended >>
TIME    36 ATOMS
<< 15 seconds after previous time >>
TIME    15 ATOMS
<< 16 seconds after previous time >>
TIME    16 ATOMS
...
<< end of input file >>
END
* END
```

Note: Times are **intervals**. It is time difference not cumulative time

Worked example - graph outputs





Worked example summary

Able to irradiate a material and generate graphs

But what if we want custom graphs?

- Generated graphs and plots are good, but limited
- We can look and copy values from the output file, but difficult for big simulations
- Output file can be tricky to parse
- Other output files – TAB and JSON to help file reading issues
- FISPACT-II official parser - pypact

Pypact

Can make parsing legacy FISPACT-II files easy - python3 package