UK Atomic
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FISPACT-II

Extended Usage

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Additional tools

Not just FISPACT-II, additional tools included:

- **compress_xs_endf** – Turn nuclear data into binary format for quicker processing
- **extract_xs_endf** – Get the energy dependent cross section per reaction
- **listreactions** – Prints information about reaction data in ENDF-6 file
- **makenuclideindex** – Create a new index file given nuclide names

Other tools online and open source:

- GitHub - https://github.com/fispact/
  - **Pypact** – python3 package to parse output file and other functions
  - **SPECTRA-PKA** – primary knock-on atom spectra
  - **FFM** – Fispact File Maker
- **Docker** – premade container environments with nuclear data included
  - DockerHub - https://hub.docker.com/u/fispact/

Extract_xs_endf

Previously we compared different incident particle spectra and how this caused different collapsed cross section values. We showed the energy dependent cross section for Al 24 (n,p), but I did not show how to get this data.

FISPACT-II has a tool – extract_xs_endf, which will allow you to extract this data.

- Needs a lightweight files file
- No input file, just command line args
- **Does need a fluxes file** – even if you just want the XS

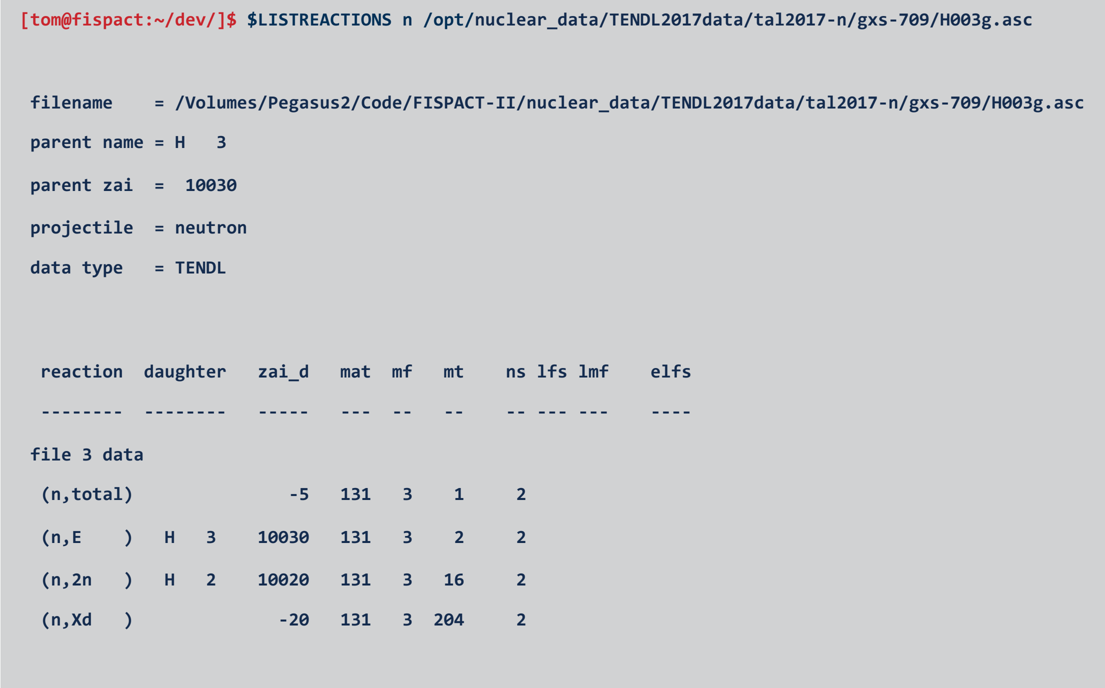
Try the exercise in ‘extended’ folder, to understand how to use it and plot cross sections.

Listreactions

FISPACT-II has a tool – listreactions, which will allow you to print available channels in ENDF-6 files.

- No input files, just two args:
    1. “n”, “p”, “d”, “g”, “t”, “a”
    2. ENDF-6 file path

First argument is really redundant, since you can give it a proton file and input “g”, but for correctness use the correct particle for that file.



```
[tom@fispact:~/dev/]$ $LISTREACTIONS n /opt/nuclear_data/TENDL2017data/tal2017-n/gxs-709/H003g.asc


filename    = /Volumes/Pegasus2/Code/FISPACT-II/nuclear_data/TENDL2017data/tal2017-n/gxs-709/H003g.asc
parent name = H   3
parent zai  =  10030
projectile  = neutron
data type   = TENDL


 reaction  daughter   zai_d   mat  mf   mt    ns lfs lmf    elfs
 --------  --------   -----   ---  --   --    -- --- ---    ----
file 3 data
 (n,total)                -5   131   3    1     2
 (n,E    )   H   3     10030   131   3    2     2
 (n,2n   )   H   2     10020   131   3   16     2
 (n,Xd   )               -20   131   3  204     2
```

Group Convert

FISPACT-II uses binned (group-wise) data

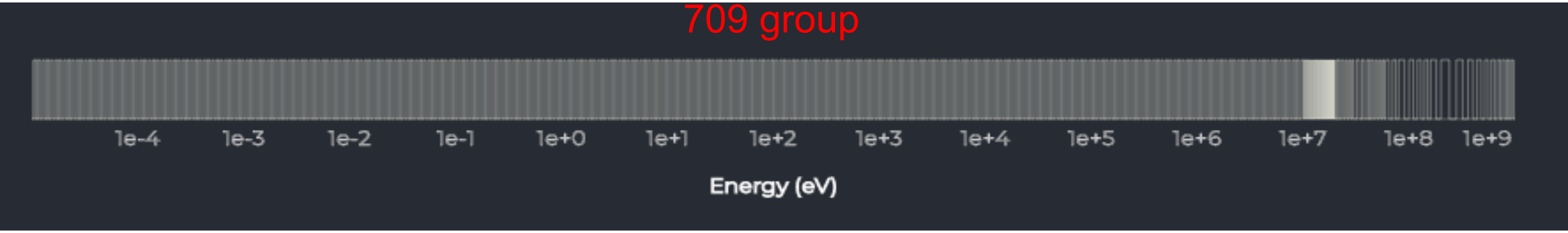
A major problem with this:

- Group structure of F-II nuclear data is usually 709 for most libraries
- Whilst 709 is generally pretty good, your flux must match this structure
- If you have a spectra in another structure how do you use it with F-II?

Two solutions:

- Make your own nuclear data for that group – use NJOY, PREPRO (not recommended)
- Use **group convert** – F-II keyword (GRPCONVERT)

709 group



Group Convert

$\mathrm{Lethargy} = u = \ln(E_0/E)$

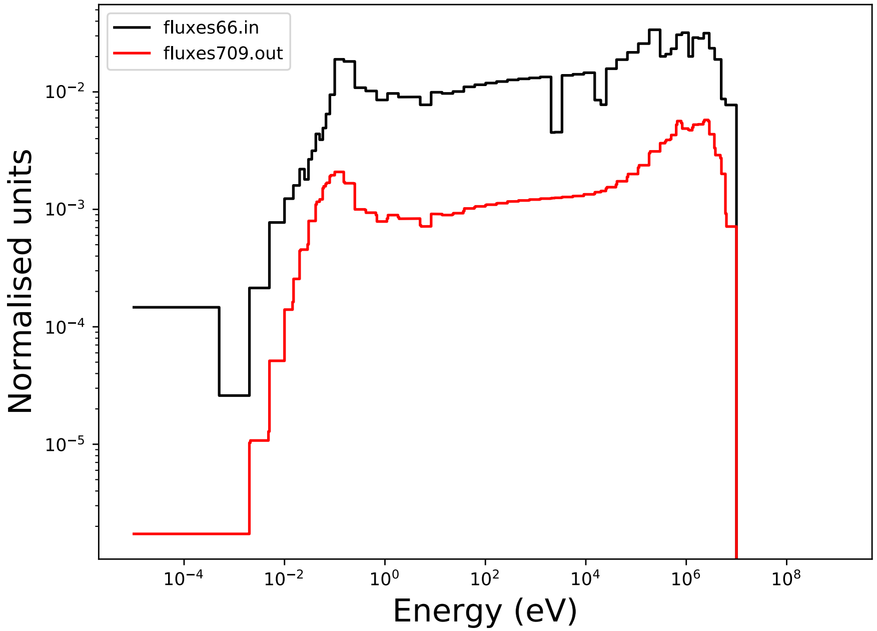
- Input arbitrary group structure
- Output F-II known group structure
- Conversion can be done using **equal lethargy** or **equal energy** per bin method (CNVTYPE)
- Splits groups based on weighting each input and output energy group

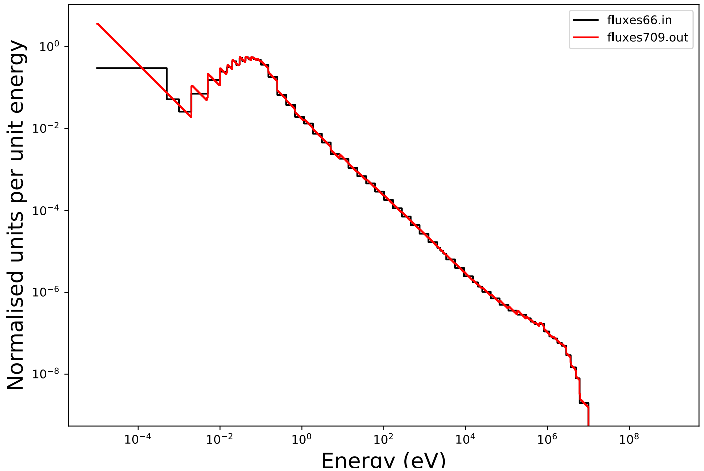
- Not a separate tool – use GRPCONVERT keyword in input file
- Requires a files file with:
  - **ind_nuc** – needed to run but not used
  - **arb_flux** – input flux file
  - **fluxes** – output flux file

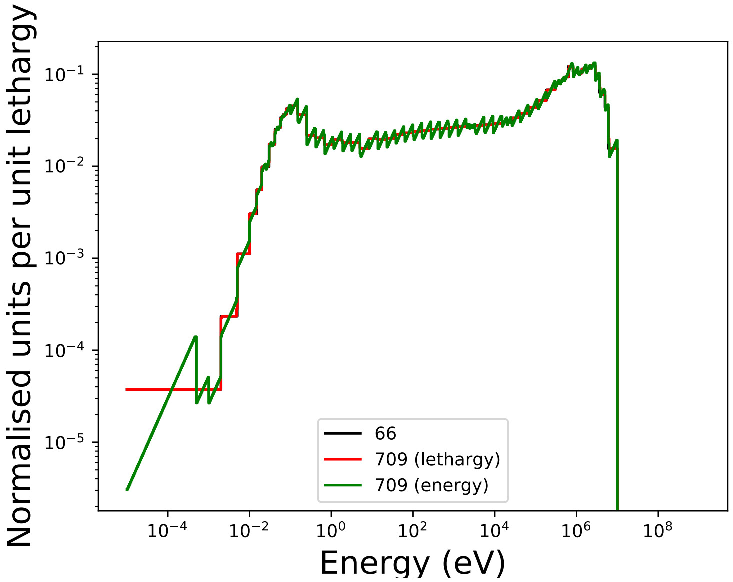
Recommended to use groups ”close” to each other. But is possible to do 66 -> 1102 if desired. Results depend on how groups “line” up.

Group Convert

Exercise ‘grpconvert’ shows conversion from group 66 to 709. Must compare using bin width (per unit energy) or unit lethargy.







Try the exercise in ‘extended’ folder.

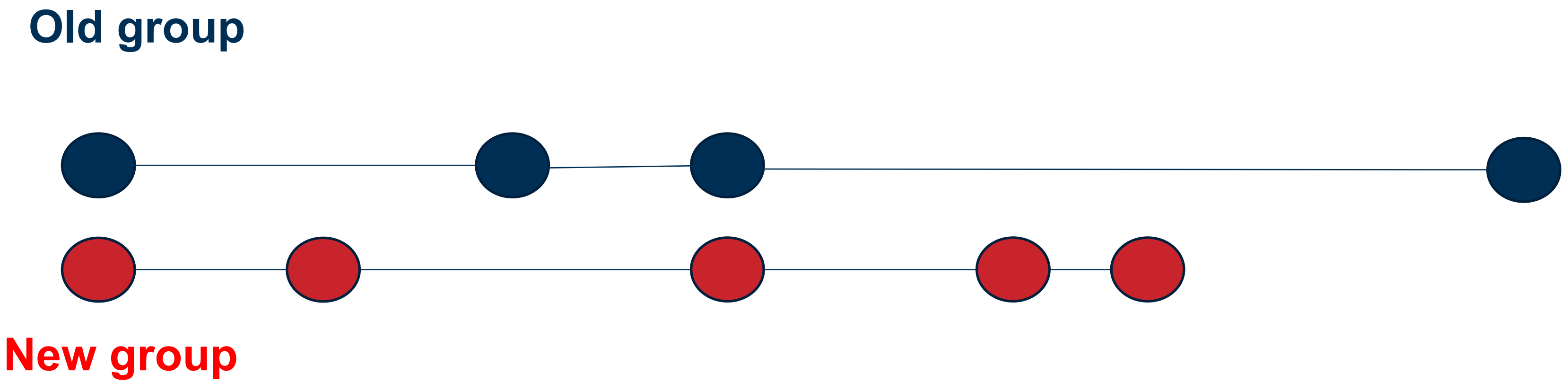
Group Convert

Also can use **Pypact** to do this (if you like Python).

The same algorithm is implemented in pypact with all FISPACT-II groups.

See example here:

https://github.com/fispact/pypact/blob/master/examples/groupconvert/66_to_709_compare.py

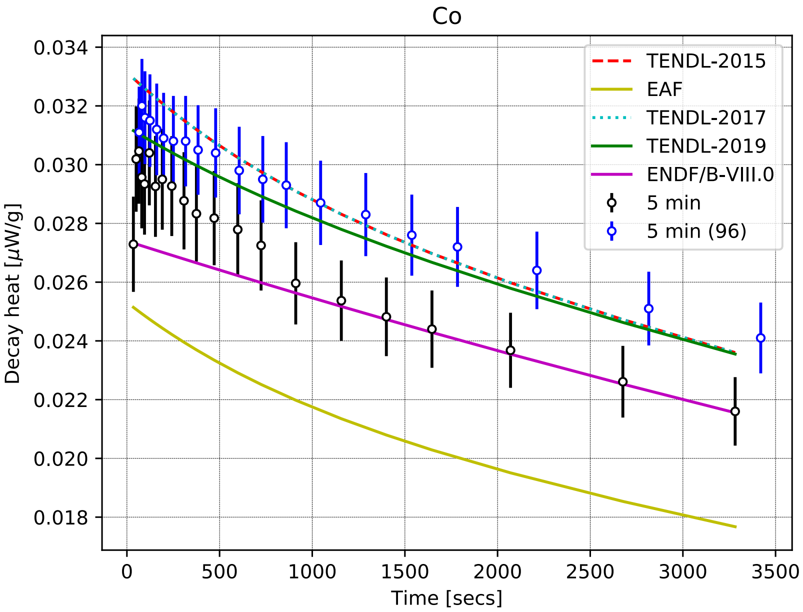


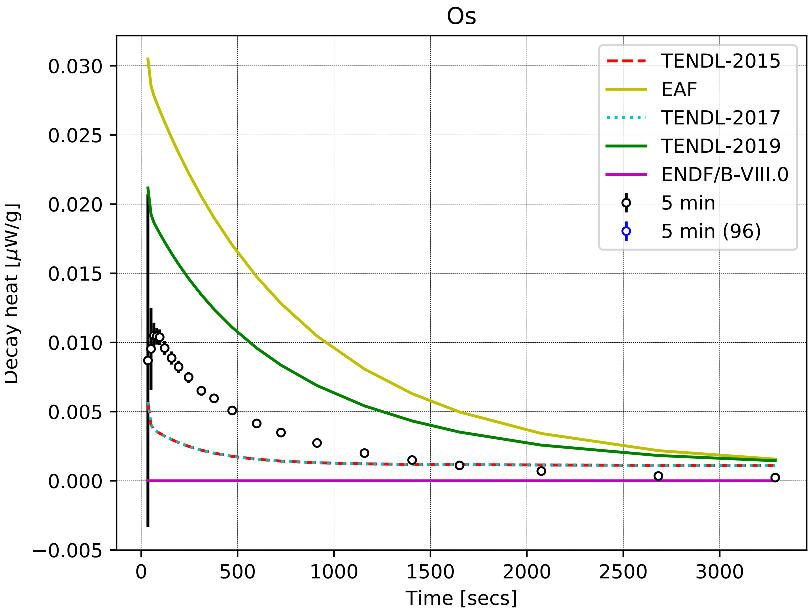
Algorithm here: https://github.com/fispact/pypact/blob/master/pypact/input/groupconvert.py

Library variations

- Can get dramatically different results depending on which nuclear data library you use.
- Nuclides and reactions not consistent in all libraries
- Always good to compare with at least another library
- Typically domain specific – fusion, fission, spallation, waste, gamma spec…..
- More than just neutron: **proton, alpha, triton, deuteron, gamma** incident particles

Try the exercise in 'extended' folder on 'library variations' to get a feel for doing this.

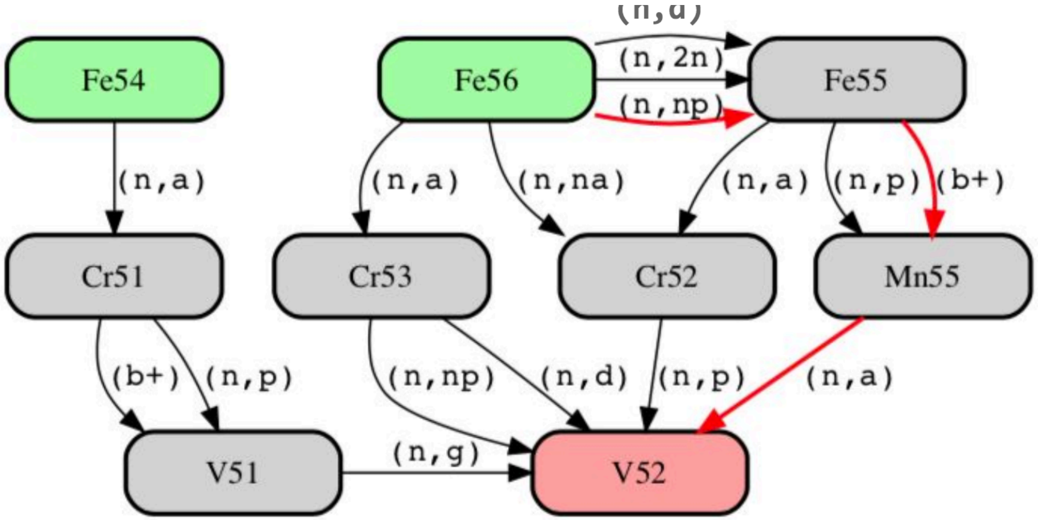




Pathways

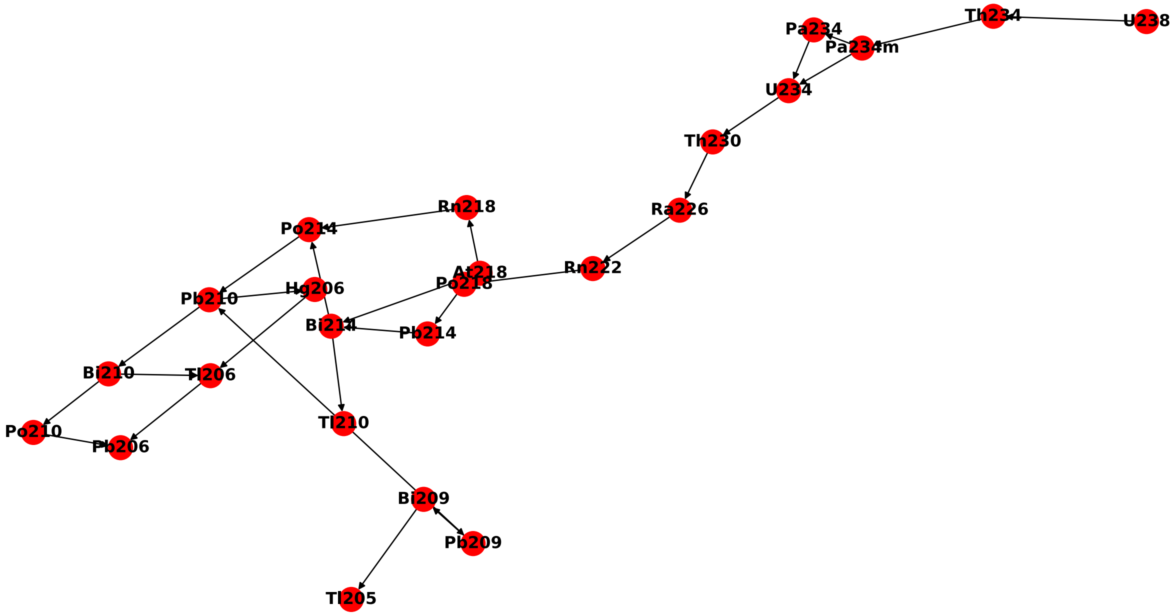
- Nuclear data represents a major contributor to uncertainties in nuclear simulations
- There are known knowns, known unknowns, and unknown unknowns
- We can estimate the known unknowns via pathways analysis built into FISPACT-II
- Pathways also provides information on the path from parent to child
  - How much of X comes from Y?
  - What if we isotopically tailored X?

Where did my ^{52}V come from?



Pathways

- Use the **PATH** keyword to specify a path of interest
- Use **ROUTES** keyword to specify a parent and child to find all routes
- Other keywords to related to pathways analysis
  - **PATHRESET**
  - **LOOKAHEAD**
  - **UNCERTAINTY**
  - **ZERO**
  - **FISCHOSE**
  - **GENERIC**



Exercise pathways (extended) shows how to use it

Pulse

The PULSE keyword is useful if doing repetitive irradiations, periodic time intervals over a long period.

For example, in an operational fusion reactor we could have:

- **2 shifts of 8 hours per day**, repeating pulsed flux
  - 300 seconds of irradiation (1e14 n/cm2/s)
  - 1500 seconds off (decay only)
- **1 shift off** (another 8 hours)
- Repeats **5 days a week** (weekends off)
- For **10 years** (if we are lucky)

PULSE will save us a lot of lines in the input file and makes it much more readable.

Of course, we can script this too.

Try the exercise in ‘extended’

More advanced....

Gamma spectrum

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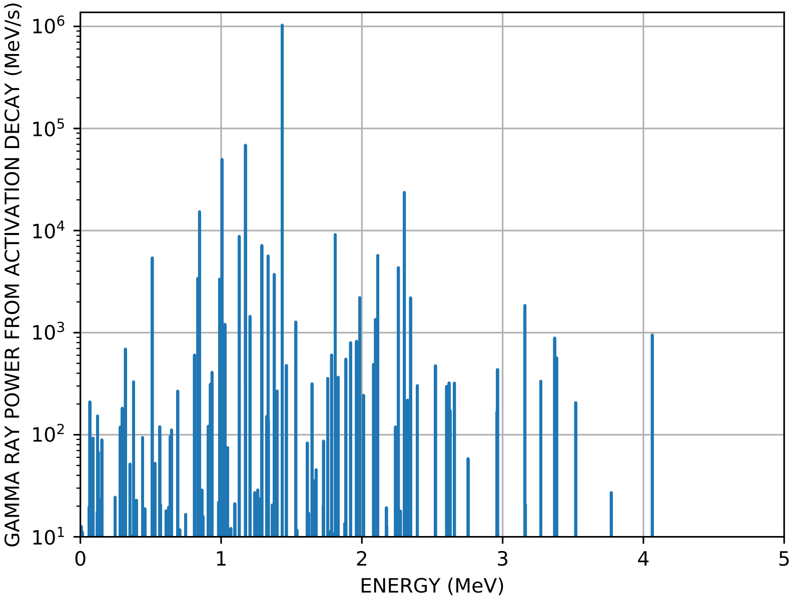
FISPACT-II also outputs the gamma spectrum rate (power) at each timestep.

- If you use **ATOMS** or **SPECTRUM** the data will be in the output file
- Default gamma group is 24-energy group structure
- Use **GROUP 1** to use 22-group 'Steiner' structure
- If this is too coarse you can input custom bin boundaries with **READGG**



20,000 bins

Try the exercise in ‘advanced’ folder, to understand how to use it and plot cross sections.

Multiflux

- In most practical scenarios, energy spectra changes with time and space
- Important for burn-up calculations
- Need to allow for different spectra in inventory calculations, but…
  - One simulation/run = one collapse

⇒ When the spectra is changing, we must re-collapse

- Chain input1, output1 => input2, output2 =>…
- Can be difficult to parse output file
  - As mentioned before, a few options - TAB, JSON, PYPACT
- We will use the **TAB1** file to help automate this, since the input just needs to know the number of atoms

Exercise multiflux (advanced) shows how to do this

FISPACT-II Output Format

- Fairly easy to look inside and read a value
- Hard to script and parse values
- Output files can be quite large (often > 5MB)
- Grep will only take you so far

Solutions:

- Write your own parser (not recommended)
- Use **TAB** files for easier parsing (limited output, limited precision)
- Use **JSON** output (standardised format, high precision, since v4 only)
- Use **pypact** (python3 package designed for parsing output)

Exercise on each in advanced section

FISPACT-II JSON

FISPACT-II 4.0 now has a JSON output

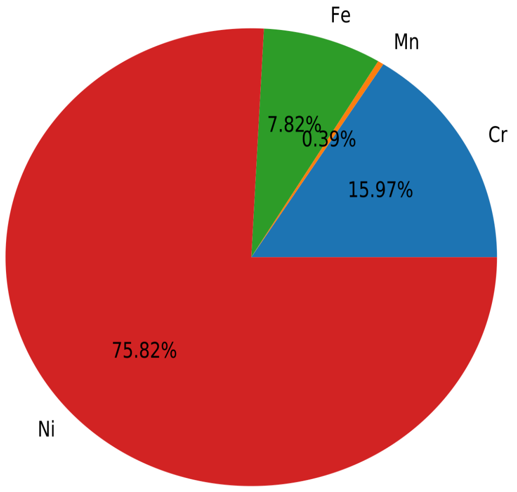
```
{
    "name" : "json",
    "description" : "I am JSON",
    "id" : 4,
    "value" : 4.3e+9
}
```

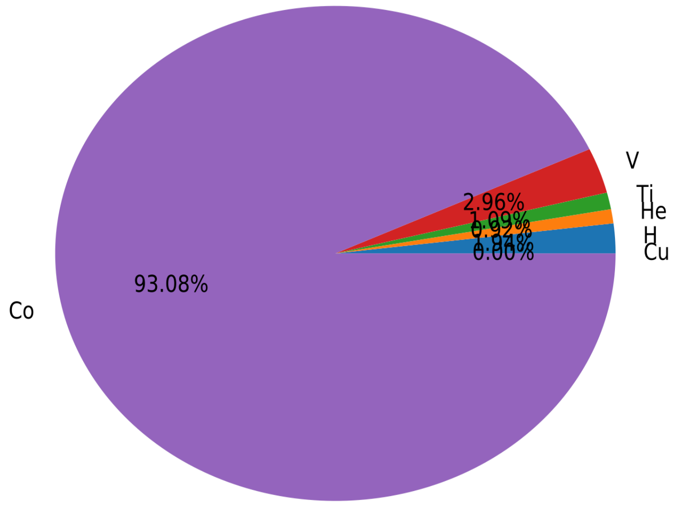
Simply use JSON keyword in control section

We did this in FNS Inconel example

```
<< -----set initial switches and get nuclear data----- >>
CLOBBER
JSON
GETXS 0
GETDECAY 0
FISPACT
* FNS 5 Minutes Inconel-600
```

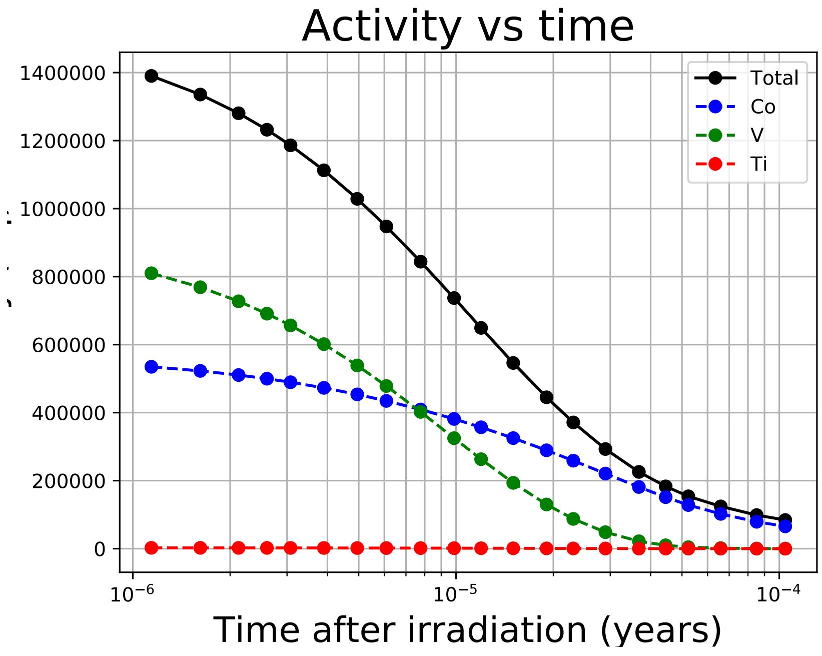
Exercise JSON





Left: initial

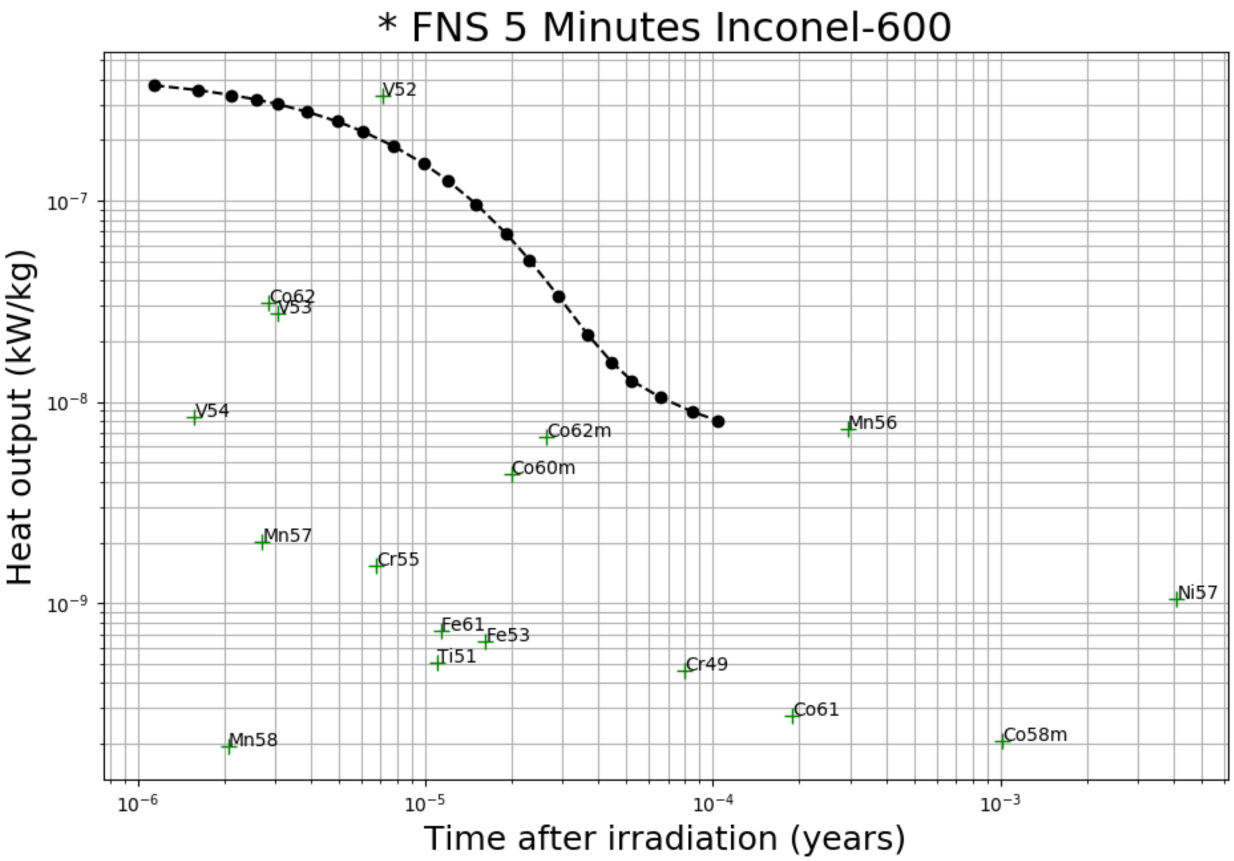
Right: final (excluding initial)



Exercise JSON (advanced) shows how to do this

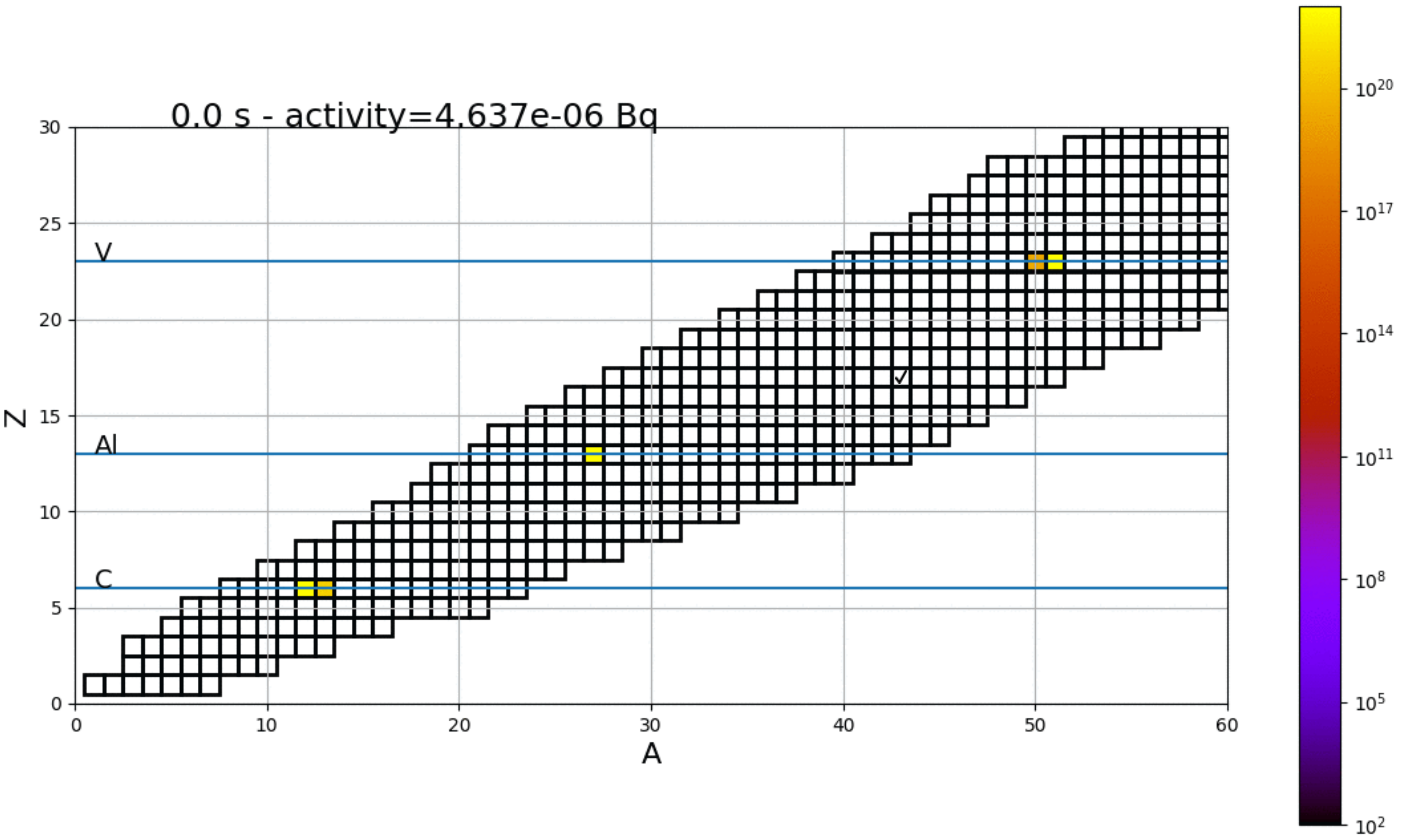
Exercise Pypact

Use pypact to make simple plots vs time



Exercise Pypact

Chart of nuclides animation – less than 70 lines of code!



Summary and more

- **FISPACT-II is an advanced multigroup Multiphysics code** capable of:
  - Providing radio properties per nuclide at times from **1e-20 to 1e20 seconds**!
  - Associated **gamma spectrum** at time interval
  - **Extract** + plot XS data
  - **Uncertainty** analysis
  - **Pathways** analysis
- **Open source tools** – in active development
- Many ways to analyse FISPACT-II output
  - **GNU plotting** built in
  - **TAB** files can make life easier but difficult hard to script
  - **JSON** output has many parsers ready - C++, Fortran, Python, js, …
  - **Pypact**
- **Docker**
  - Many images ready made with nuclear data inside
  - Self contained environment to run fispact easily
  - Nuclear data in binary format – performance improvement