UK Atomic Energy Authority

FISPACT-II

Advanced Usage

Thomas Stainer, Mark Gilbert, Greg Bailey
United Kingdom Atomic Energy Authority

FISPACT-II workshop

June 19-21, 2019, OECD/NEA, Paris

This work was funded by the RCUK Energy Programme
[Grant number EP/P012450/1]

Research Councils UK Energy For a Low Carbon Future

CCFE CULHAM CENTRE FOR FUSION ENERGY

Additional tools

UK Atomic Energy Authority

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:

- **Pypact** – python3 package to parse output file and other functions
  - GitHub - https://github.com/fispact
- **Docker** – premade container environments with nuclear data included
  - DockerHub - https://hub.docker.com/u/fispact/

GitHub

CCFE CULHAM CENTRE FOR FUSION ENERGY

Compress_xs_endf

UK Atomic Energy Authority

Large nuclear data libraries can take a while to read…

- TENDL 2017 can take up to 2 minutes to read and process in it's entirety
- This can be improved by up to **60%** when using compress_xs_endf

Command line tool just like FISPACT-II

- Needs a lightweight files file
- No input file, just command line args
- Only works on ENDF-6 format, not EAF
- Only compresses reaction data, not decay data
- Binary files are platform and complier dependent (non-transferable)
- **Reduce the size from 9GB to > 2GB!**

Note: if we use binary files, we use GETXS -1 in input file and key xs_endfb must point to path of binary file

Try the exercise in 'extended' folder, to understand how to use it and create the libraries.

CCFE CULHAM CENTRE FOR FUSION ENERGY

Extract_xs_endf

UK Atomic Energy Authority

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

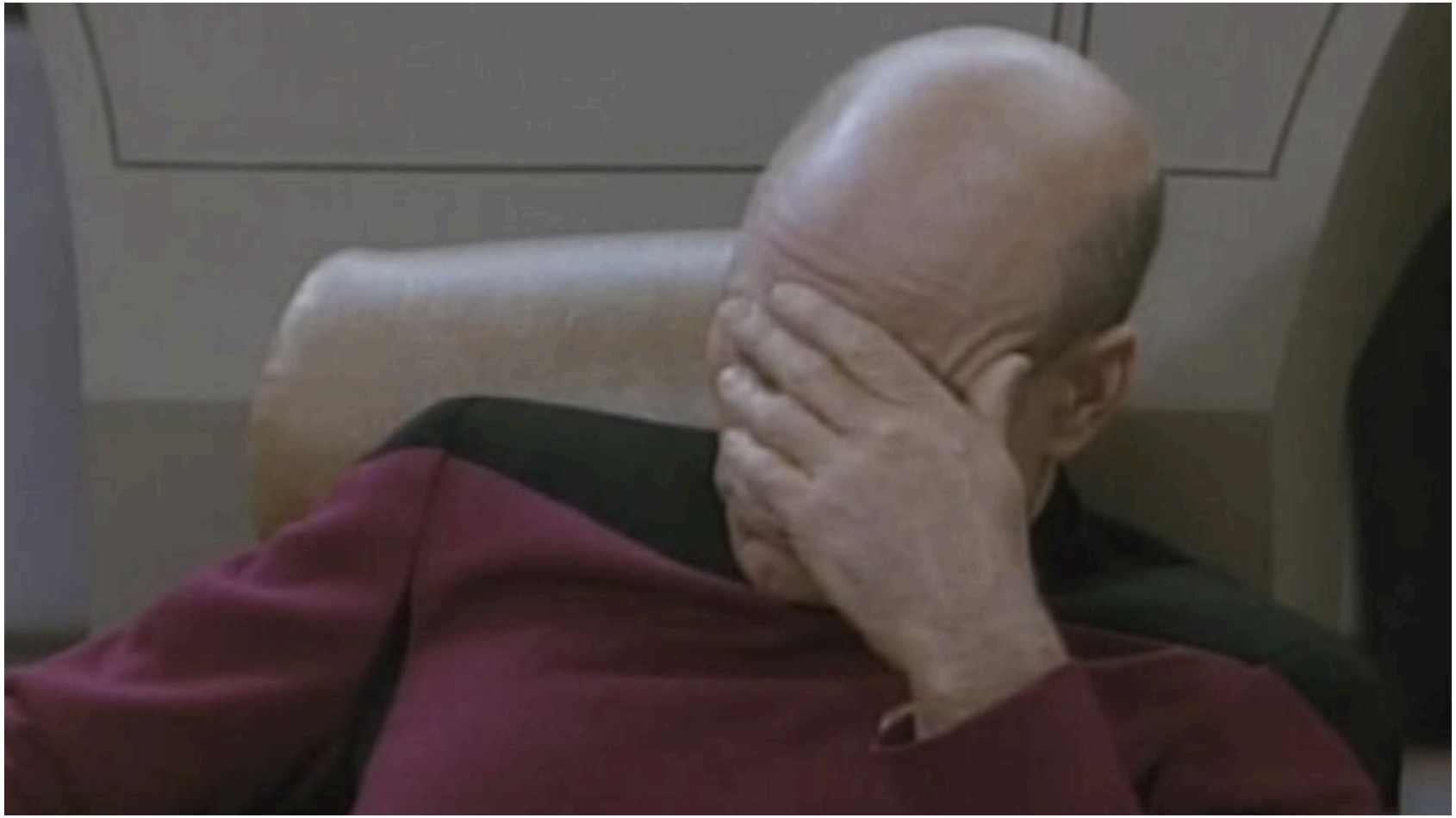
First argument is really redundant, since you can give it a proton file and input “g”, but for correctness use the correct particle for that file.

```
[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

UK Atomic Energy Authority

My nuclear data is in group 709 but my flux is in group 175!



CCFE CULHAM CENTRE FOR FUSION ENERGY

Group Convert

UK Atomic Energy Authority

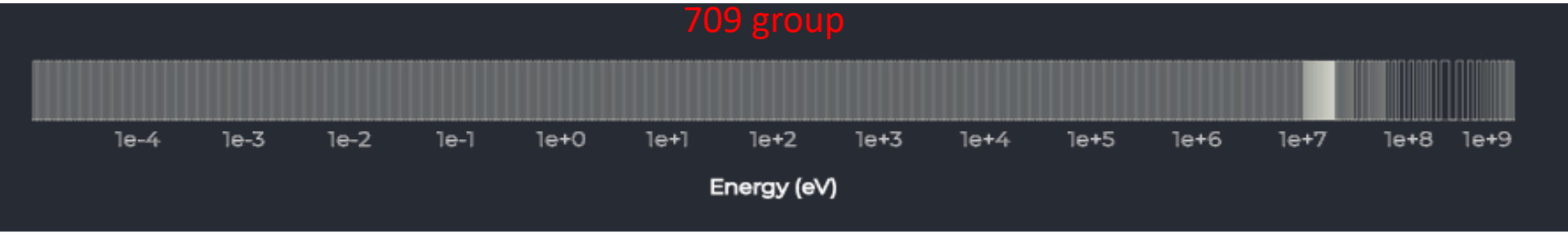
FISPACT-II uses binned (group-wise) data

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)



CCFE CULHAM CENTRE FOR FUSION ENERGY

Group Convert

UK Atomic Energy Authority

- Input arbitrary group structure
- Output F-II known group structure

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

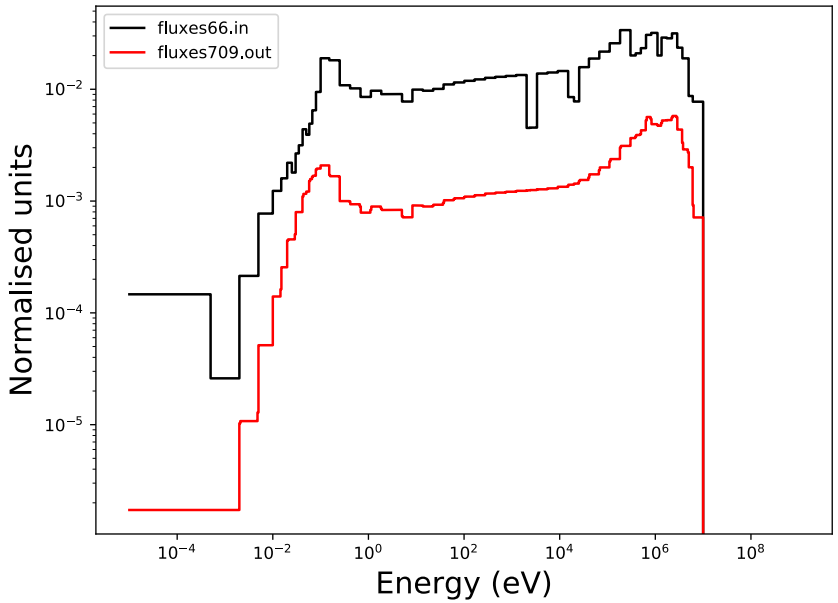
- Conversion can be done using **equal lethargy** or **equal energy** per bin method (CNVTYPE)
- Splits groups based on weighting each input and output energy group

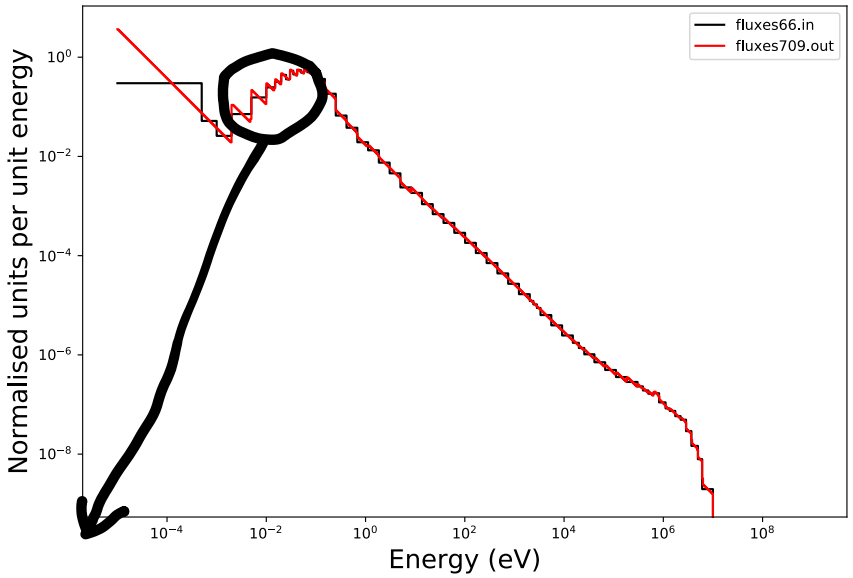
- Not a separate tool – use GRPCONVERT keyword in input file
- Requires a files file with:
  - **ind_nuc** – needed to run but not used
  - **arb_flux** – input flux file
  - **fluxes** – output flux file

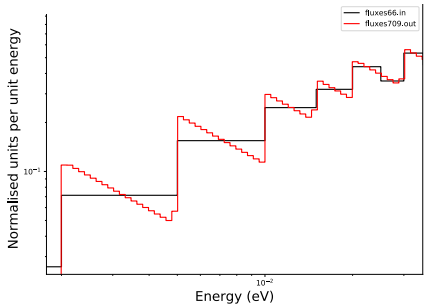
Recommended to use groups ”close” to each other. But is possible to do 66 -> 1102 if desired. Results depend on how groups “line” up.

Group Convert

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







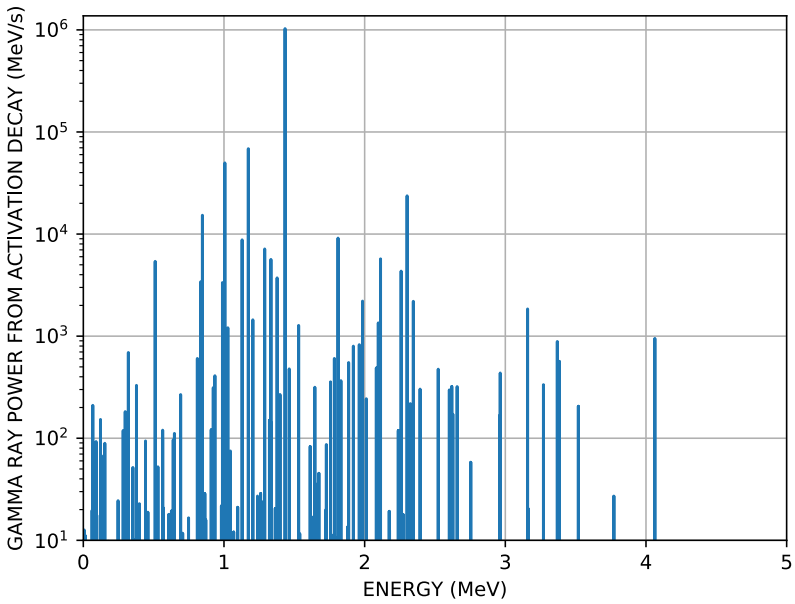
Try the exercise in ‘extended’ folder.

Gamma spectrum

UK Atomic Energy Authority

FISPACT-II also outputs the gamma spectrum 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.

CCFE CULHAM CENTRE FOR FUSION ENERGY

FISPACT-II Output Format

UK Atomic Energy Authority

- 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

CCFE CULHAM CENTRE FOR FUSION ENERGY

Multiflux

UK Atomic Energy Authority

- 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

CCFE CULHAM CENTRE FOR FUSION ENERGY

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
```

FISPACT-II JSON

UK Atomic Energy Authority

Why JSON?

- Human readable
- Light weight
- Easy to parse
- Very popular format
- Supported by many languages – Python, C++, Fortran, js, …
- Web friendly (more on this later)
- Full double precision

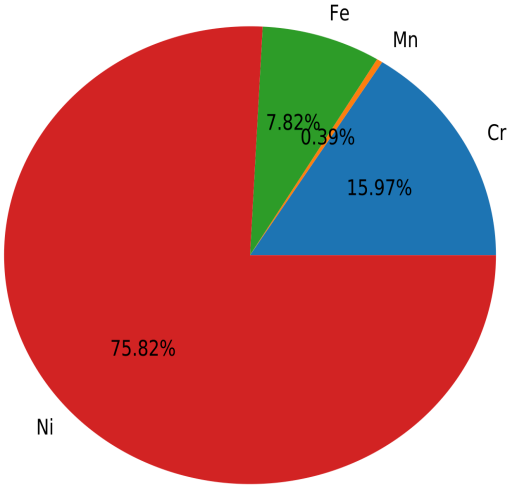
FISPACT-II JSON

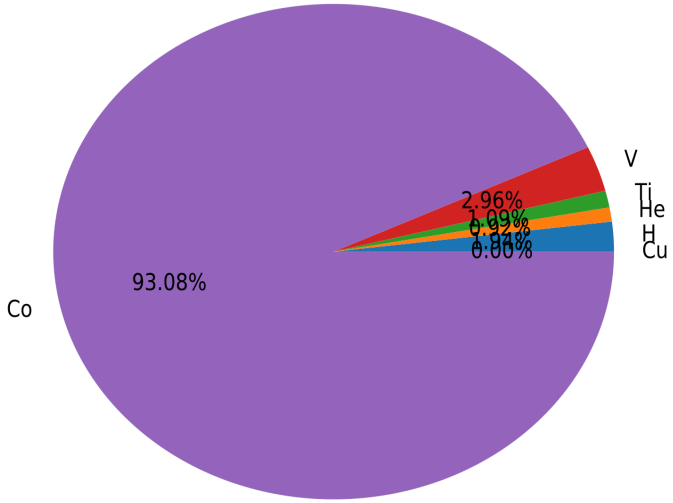
Supports most common output data

- Run data - timestamp, run name, flux name
- Inventory data - list of timesteps, each containing
  - Irradiation and cooling time
  - Flux amplitude
  - Heat - alpha, beta, gamma
  - Ingestion and inhalation
  - Dose
  - Nuclides → the inventory (activity, grams, heats,…)

Exercise JSON (advanced) shows how to do this

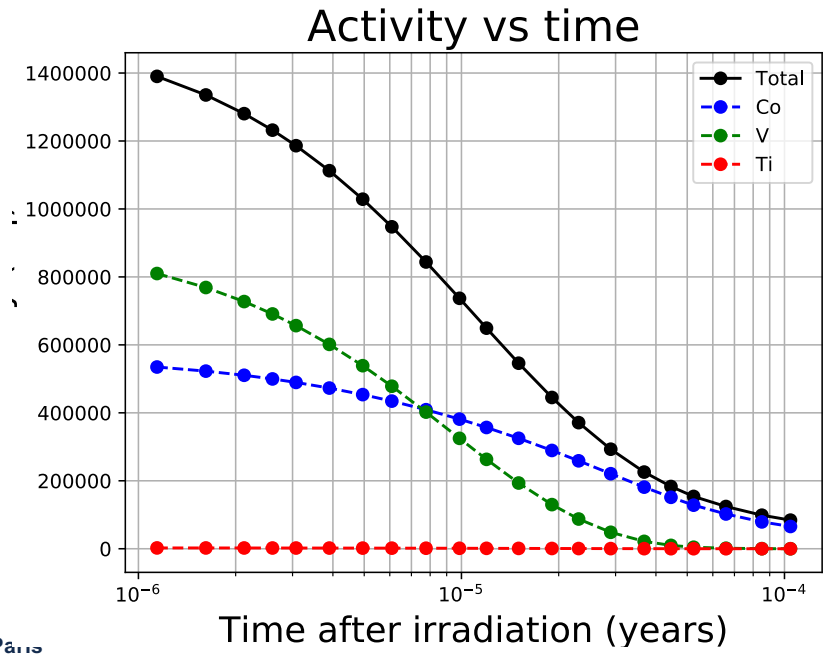
Exercise JSON





Left: initial

Right: final (excluding initial)



Alternative options

UK Atomic Energy Authority

Could alternatively have used **TAB1** keyword to get this data

Contains columns of nuclide with atoms and grams only!

Alternatively, we can use pypact

CCFE CULHAM CENTRE FOR FUSION ENERGY

Pypact

UK Atomic Energy Authority

Python package to parse fispact output files

Advisable to use JSON - but pypact works on standard output file (*.out) also

Will work on FISPACT-II files pre version 4.0

Makes scripting easier and analyse FISPACT-II outputs

Easy to install via pip (python package management system)

```
pip3 install pypact
```


CCFE CULHAM CENTRE FOR FUSION ENERGY

Pypact

First let's do a very simple example with pypact

```
# import the library
import pypact as pp

# read the output file
with pp.Reader('inventory.out') as output:
    print(output.run_data.timestamp)
    print(output.run_data.run_name)
```

Pypact

UK Atomic Energy Authority

Another more interesting example

```
import pypact as pp
import matplotlib.pyplot as plt

time = []
data = []

with pp.Reader('inventory.out') as output:
    for t in output.inventory_data:
        if t.flux == 0.0:
            time.append(t.currenttime)
            data.append(t.gamma_heat)

plt.loglog(time, values, 'k', alpha=0.6)
plt.xlabel("Cooling time [s]", fontsize=18)
plt.ylabel("Gamma heat (kW)", fontsize=18)
plt.show()
```


CCFE CULHAM CENTRE FOR FUSION ENERGY

Pypact

UK Atomic Energy Authority

Can also use the JSON file

```
import json
import matplotlib.pyplot as plt

time = []
values = []
with open('inventory.json') as f:
    data = json.loads(f.read())
    for t in data['inventory_data']:
        if t['flux'] == 0.0:
            time.append(t['cooling_time'])
            values.append(t['gamma_heat'])

plt.loglog(time, values, 'k', alpha=0.6)
plt.xlabel("Cooling time [s]", fontsize=18)
plt.ylabel("Gamma heat (kW)", fontsize=18)
plt.show()
```

Pypact

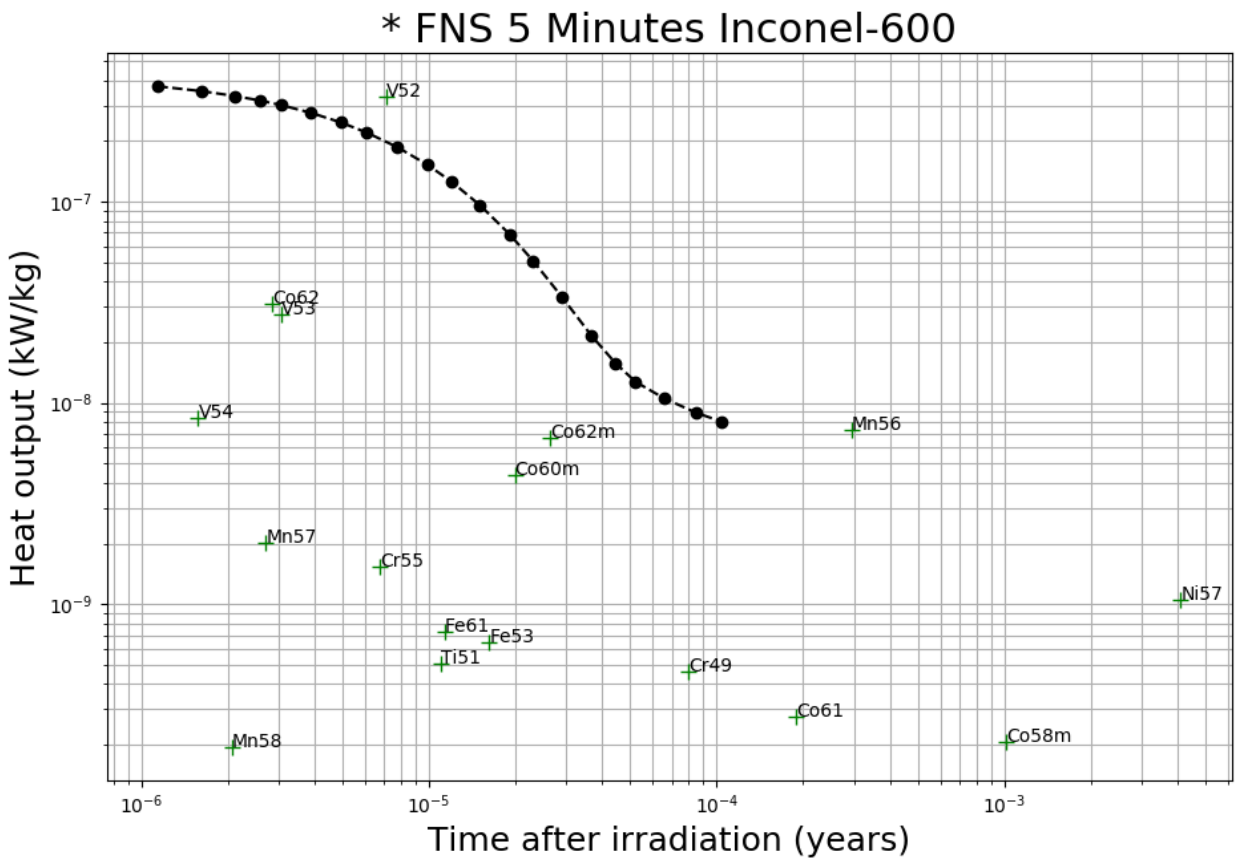
Use pypact to get all the output times from the output file

It can be done in 3 lines!!

```
import pypact as pp

with pp.Reader('inventory.out') as o:
    [print("Time {} (secs)".format(t.currenttime)) for t in
o.inventory_data]
```

We will do another analysis using pypact to produce a similar plot as in FNS Inconel for gnuplot

Exercise Pypact



Pypact Summary

UK Atomic Energy Authority

Status

- Handle legacy FISPACT-II output files and JSON files
- Process nuclides, doses, ingestion, burnup, ..
- Create and read files files
- Contains all fispact keywords and group structures built in - 66, 69, ..., 709, 1102
- Simple plotting with analysis extension

Future

- Pathways and uncertainties
- Gamma spectrum
- Optimizations and API improvements

Feedback welcome!

CCFE CULHAM CENTRE FOR FUSION ENERGY

Docker

UK Atomic Energy Authority

Engine for running containers...

A container image is a lightweight, stand-alone, executable package of a piece of software that includes everything needed to run it

Can be thought of as a lightweight Virtual Machine.

FISPACT-II with Docker

UK Atomic Energy Authority

We utilise Docker to bundle all dependencies in a single image

Including nuclear data (in binary format) - faster!

To read binary data we use GETXS -1

Docker not installed on your machines, but you can run it with

```
docker run -it -v
/opt/fispact/bin/ubuntu/16.04/ifort18/fispact:/fispact
fispact/ubuntu:16.04_gfortran_5_data bash
```


CCFE CULHAM CENTRE FOR FUSION ENERGY

FISPACT-II with Docker

UK Atomic Energy Authority

Then we have ubuntu with nuclear data!

```
root@580a028b793c:/# ./fispact
FATAL ERROR: unable to find FILES file
               also unable to find input file
RUN TERMINATED
Either provide the FILES name as a second argument, or
provide a file named 'files', 'Files' or 'FILES'
in the present working directory, or
provide input file .i
in the present working directory.
```


CCFE CULHAM CENTRE FOR FUSION ENERGY

FISPACT-II Advanced Summary

UK Atomic Energy Authority

- 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
  - Supports both JSON and standard output file formats
  - Very easy to script plots and analysis
  - Can read and plot flux file
  - Contains tool to create files file
  - Contains all keywords for FISPACT-II
- Docker
  - Many images ready made with nuclear data inside
  - Self contained environment to run fispact easily
  - Nuclear data in binary format – performance improvement