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FISPACT-II Worked example

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Introduction

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FISPACT-II is a nuclear inventory simulation code .

Exercise: Irradiation of Cobalt for 3 days

1. Configure FISPACT-II to irradiate 1kg of Cobalt and produce a plot of its activity and heat output
2. Use Tendl 17, GEFY 6.1 and the fluxes from the FNS getting started example
3. Configure one input file (to show a different approach)

Step by step example: Please proceed at your own pace - I will proceed slowly to keep things moving. Prerequisite: *Previously ran the FNS example in getting started.*

Step zero

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All at the same place

1. Make a new folder called Cobalt_Workshop

   ```
   $mkdir  Cobalt_Workshop
   ```

2. Move into Cobalt_Workshop

   ```
   $cd  Cobalt_Workshop
   ```

Step one

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Configure the **files** file: *The files file tells FISPACT-II the location of required inputs for a simulation (page 30 of the 2018 users manual)*

- We need to point FISPACT-II to the correct Tendl-17 and GEFY files
- ind_nuc, xs_endf need to point at TENDL2017data within nuclear data
- fy_endf, sf_endf need to point at GEFY61data
- we also need to point the decay data, dk_endf, to decay
- Point fluxes at fluxes

Try doing this. Hint: look at the getting_started examples

Step one

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files settings	
ind_nuc	index of nuclides to be included in simulation
xs_endf	Binary compressed cross-section and covariance data
fluxes	Projectile spectrum and wall loading for a standard group structure
dk_endf	Decay and its uncertainty data
fy_endf	Induced fission yield data
sf_endf	Spontaneous fission yield data
collapxi	Input collapsed cross-section library
collapxo	Output collapsed cross-section library
arrayx	Input and output condensed decay library

Point these to the required locations; i.e. ind_nuc /Pathto/nuclear_data/TENDL2017data/tendl17_decay12_index

Hint: Look at FNS example

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```
# index of nuclides to be included
ind_nuc  /Users/fosterd/nuclear_data/TENDL2017data/tendl17_decay12_index

# Library cross section data
xs_endf /Users/fosterd/nuclear_data/TENDL2017data/tal2017-n/gxs-709

#fluxes
fluxes  fluxes

# Library decay data
dk_endf /Users/fosterd/nuclear_data/decay/decay_2012

# Library fission  data
fy_endf /Users/fosterd/nuclear_data/GEFY61data/gefy61_nfy
sf_endf /Users/fosterd/nuclear_data/GEFY61data/gefy61_sfy

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

# condensed decay and fission data (in and out)
arrayx  ARRAYX
```

Step two: input file

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Your files file should look like mine

The input file tells FISPACT-II what to do.

In the getting started examples we see that the input files are separated into four separate *files*, *collapse*, *condense*, *print_lib*, inventory.

Here we are making one file to do it all, called **combine.i**

Step two: input file

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We now need to configure the input file:

Initial settings	
CLOBBER	Allows Fispact-II to overwrite output files
GETXS 1 709	(1) tells Fispact to collapse the cross sections from the ENDF library, (709) states that the 709 group energy multi-group should be used
GETDECAY 1	causes the decay data to be read from the decay library files connected to dk endf
FISPACT	separates the library input from the initial conditions
* Cobalt	key word information about the particular run - used in graph titles

Step two: input file

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We now need to configure the input file:

Material definition	
MASS 1.0E-3 4	total mass (kg) and the number of elements in the material to be irradiated
CO 100.0	100% Cobalt

Step two: input file

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We now need to configure the input file:

Output settings	
GRAPH 2 2 1 1 3	Graph output settings. (2) plots, (2) use gnuplot, (1) include uncertainty data, (1) activity, (3) Heat output
UNCERTAINTY 2	Uncertainty settings, (2) both estimates of uncertainty and the pathway information are output
HALF	include half-life of each nuclide in output

Step two: input file

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We now need to configure the input file:

Output settings	
Irradiation phase	
FLUX 10.116E+20	total energy-integrated projectile flux (in $cm^{-2}s^{-1}$)
ATOMS	starts the initial solution of the inventory equations
TIME 2 DAYS	sets the first time interval for the inventory calculation and terminates the initial conditions section
ATOMS	restarts the solution of the inventory equations

Step two: input file

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We now need to configure the input file:

cooling phase	
FLUX 0.	total energy-integrated projectile flux (in $cm^{-2}s^{-1}$) for this time period
ZERO	reset the time value to zero after an irradiation
TIME 36 ATOMS	Inventories after 36s are output
END	terminates the input of data for a particular run. Must be preceded by the * with a title.

```
CLOBBER
GETXS 1 709
GETDECAY 1
FISPACT
* Cobalt
MASS 1.0 1
CO  100.0
GRAPH 2 2 1 1 3
UNCERTAINTY 2
HALF
<< -----irradiation phase----- >>
FLUX 10.116E+20
ATOMS
TIME 2 DAYS
ATOMS
<< -----cooling phase----- >>
FLUX 0.
ZERO
TIME    36 ATOMS
TIME    15 ATOMS
TIME    16 ATOMS
TIME    15 ATOMS
TIME    15 ATOMS
TIME    26 ATOMS
TIME    33 ATOMS
TIME    36 ATOMS
TIME    53 ATOMS
TIME    66 ATOMS
TIME    66 ATOMS
TIME    97 ATOMS
TIME   127 ATOMS
TIME   126 ATOMS
TIME   187 ATOMS
TIME   246 ATOMS
TIME   244 ATOMS
TIME   246 ATOMS
TIME   428 ATOMS
TIME   606 ATOMS
TIME   607 ATOMS
TIME   707 ATOMS
END
* END
```

Step three: Run FISPACT-II

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Now we have the input files we simply type:

```
$/Pathto/fispact combine
```

this will produce a print out like:

```
combine:  cpu time =  530.     secs.  1196 errors/warnings, for details see log file.
```

and a file called **combine.gra**.

Step three: Output, combine.gra

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```
# Run timestamp = 11:16:22 19 November 2020
#  Cobalt
# Time after irradiation (years)
#          Activity (Bq/k
# index    0
#   time          value         uncert
  0.00000E+00  1.01669E+19  0.00000E+00
  1.14077E-06  2.49546E+16  0.00000E+00
  1.61609E-06  1.20301E+16  0.00000E+00
  2.12310E-06  5.68792E+15  0.00000E+00
  2.59842E-06  2.96459E+15  0.00000E+00
  3.07374E-06  1.66735E+15  0.00000E+00
  3.89763E-06  8.38871E+14  0.00000E+00
  4.94334E-06  5.98039E+14  0.00000E+00
  6.08411E-06  5.45864E+14  0.00000E+00
  7.76358E-06  5.37935E+14  0.00000E+00
  9.85500E-06  5.37059E+14  0.00000E+00
  1.19464E-05  5.36596E+14  0.00000E+00
  1.50202E-05  5.35989E+14  0.00000E+00
  1.90445E-05  5.35291E+14  0.00000E+00
  2.30372E-05  5.34703E+14  0.00000E+00
  2.89629E-05  5.33999E+14  0.00000E+00
  3.67582E-05  5.33222E+14  0.00000E+00
  4.44901E-05  5.32638E+14  0.00000E+00
  5.22853E-05  5.32201E+14  0.00000E+00
  6.58478E-05  5.31680E+14  0.00000E+00
```

Step three: Plotting

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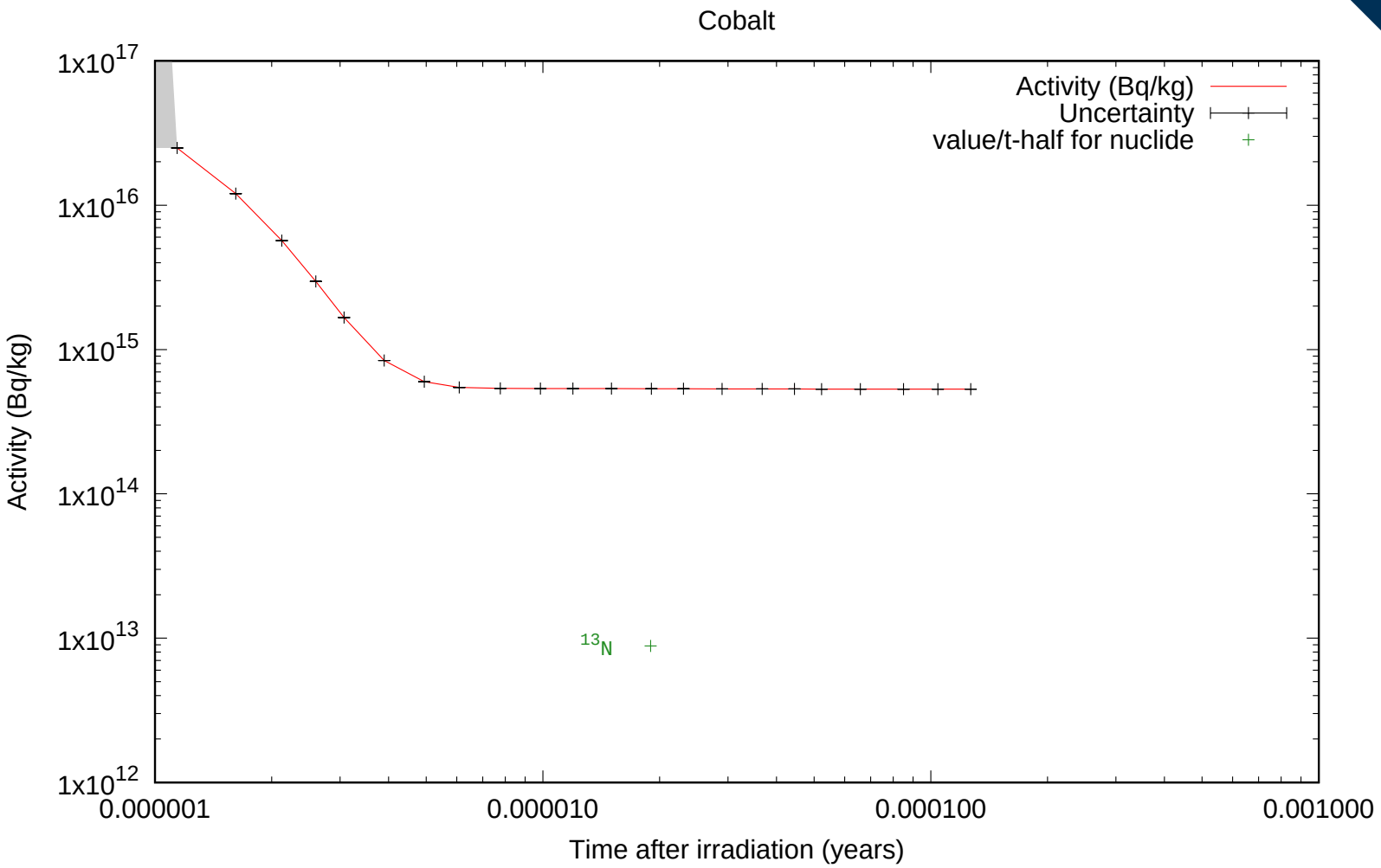
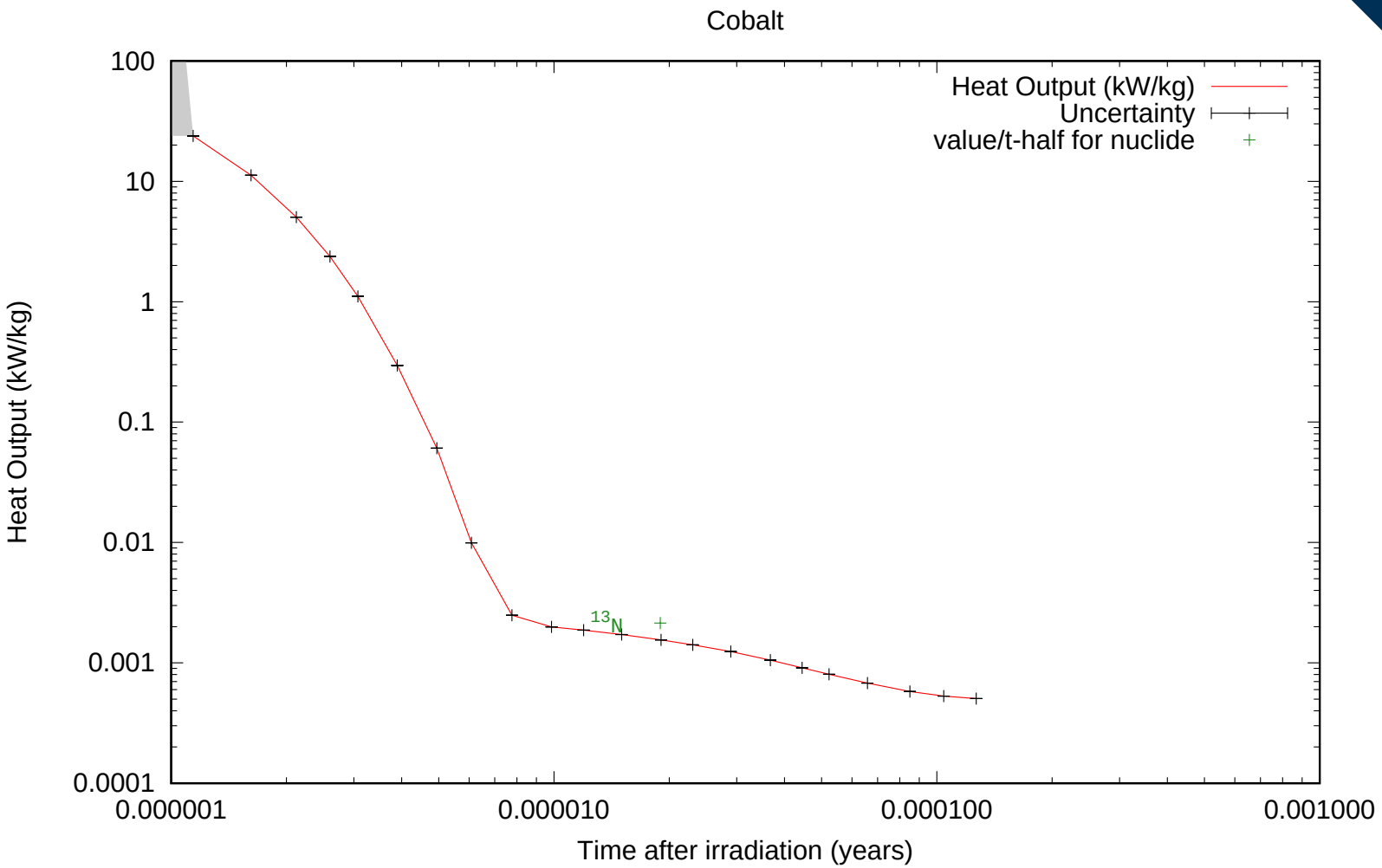
Now we have the **.gra** file we can extract the two columns and plot.
On Linux and Mac (if installed) we can simply type:

```
$gnuplot combine.plt
```

(if installed).
(Or copy the two columns into a plotting program (such as Excel)).
Producing, a file called **combine.gra.ps**



file name = combine.gra run timestamp = 11:16:22 19 November 2020



file name = combine.gra run timestamp = 11:16:22 19 November 2020

Conclusion

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- We now have the Activation and Heat output

Extensions

- Change the irradiation time, and then adding those new curves to the plots. How does the activity change with increased irradiation time?
- Change the neutron flux.
- Did we need to include the GEFY fission data?