



FISPACT-II: basics of execution

FISPACT-II may be run in many ways, but the most common execution process takes four stages:

1. Handling the nuclear data libraries and incident spectra
 - a. Condense fission yields and decay data
 - b. Collapse (fold) cross-sections with incident spectra
 - c. Print summary of library data (optional, but often useful)
2. Setting initial conditions (material composition, etc.)
& select options (output format, uncertainty quantification)
3. Simulate irradiation phases, subsidiary calculations and output data
4. Simulate cooling phases and output summary data

FISPACT-II is run through terminal commands as:

```
machine:~ user$ fispact input files
```

Here we are assuming that `fispact` is in the user's `PATH` – otherwise it would be `/path/to/fispact`

The code will read in a file `input.i` that contains a series of commands that FISPACT-II will interpret.

A separate file (called by default `files`) lists the source (files/folders) for all the data needed to perform a simulation, i.e. cross sections, decay data, fission yields, hazard indices, etc.

The `files` file contains the mapping of all library files that FISPACT-II will use in the calculation. **Every required data must be listed** – otherwise a fatal error will be issued.

These are listed in Tables 1-3 of the User Manual in Section 3.1 p23-24

Hashed comments are OK. A `files` file could look like:

```
# Cross section data from TENDL-2015
xs_endf /path/to/tendl-2015/neutron/709-data
(in default path: /ENDFdata/TENDL2015data/tal2015-n/gx-709)
```

```
# My input spectra
fluxes /my/working/directory/my_spectra
```

```
# Decay data from ENDF/B-VII.1
dk_endf /path/to/decay2012
(default path: /ENDFdata/decay/decay_2012)
```

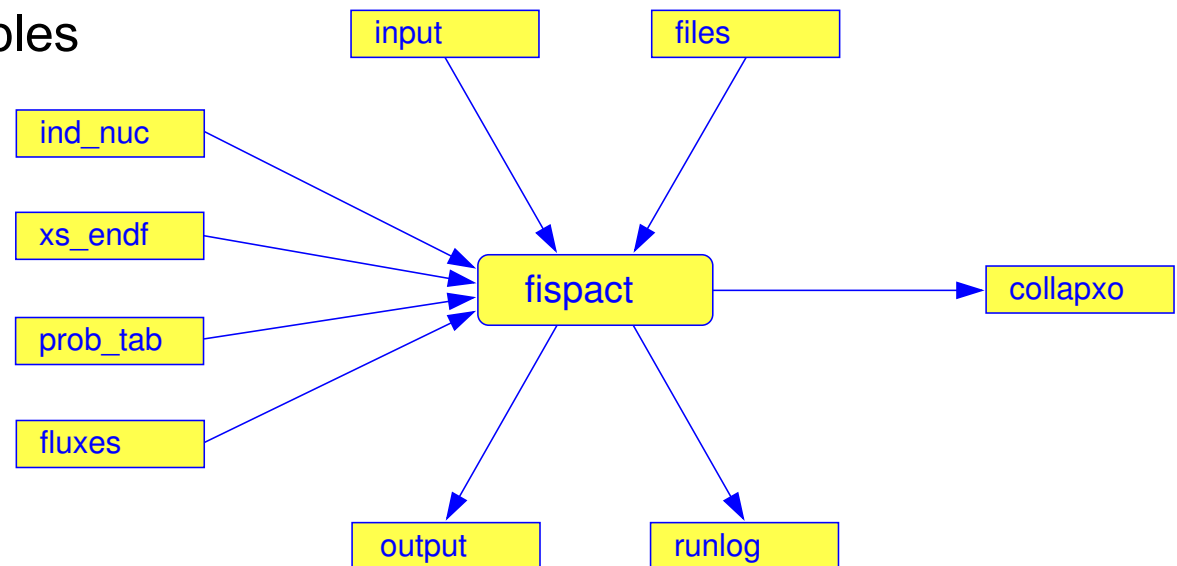
Up to 20 entries required - examples will provide guidance

- The nuclear data **condense** via `GETDECAY` produces a binary `arrayx` file from the extensive decay and fission yield data
- Key files/folders:
 - `ind_nuc` Index of nuclides; FISPACT-II will expect decay data for each nuclide listed
 - `dk_endf` decay data folder
 - `fy_endf` and `sf_endf` Induced and spontaneous fission yield data
- Additionally, a condense run may also require a irradiation spectrum (`fluxes`) to calculate spectrum-dependent fission yields, but in many cases the condense need only be run once for a particular project because `arrayx` does not change with irradiation spectrum

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`

- Key files/folders:
 - `ind_nuc` Index of nuclides
 - `xs_endf` Cross sections
 - `prob_tab` Probability tables
 - `fluxes` Incident spectra

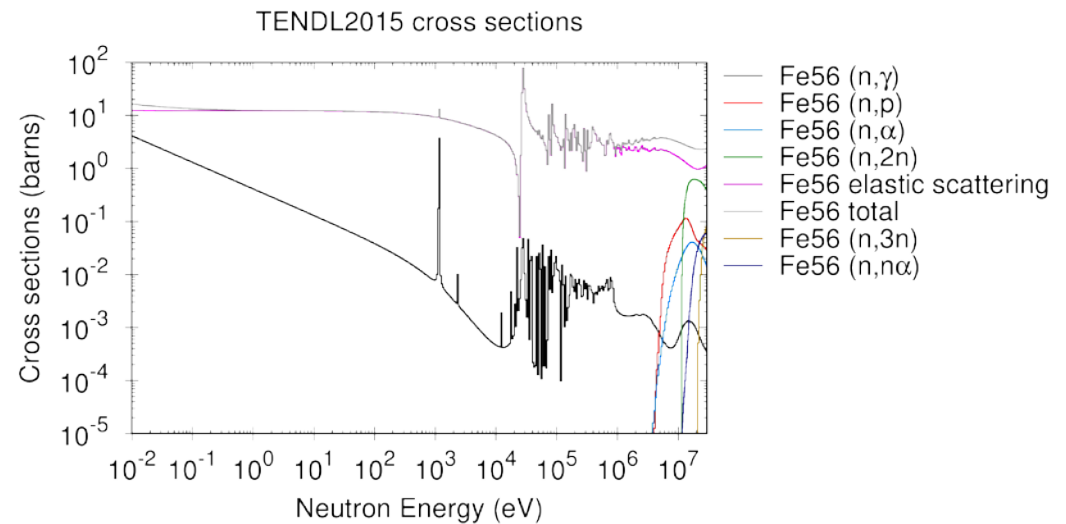
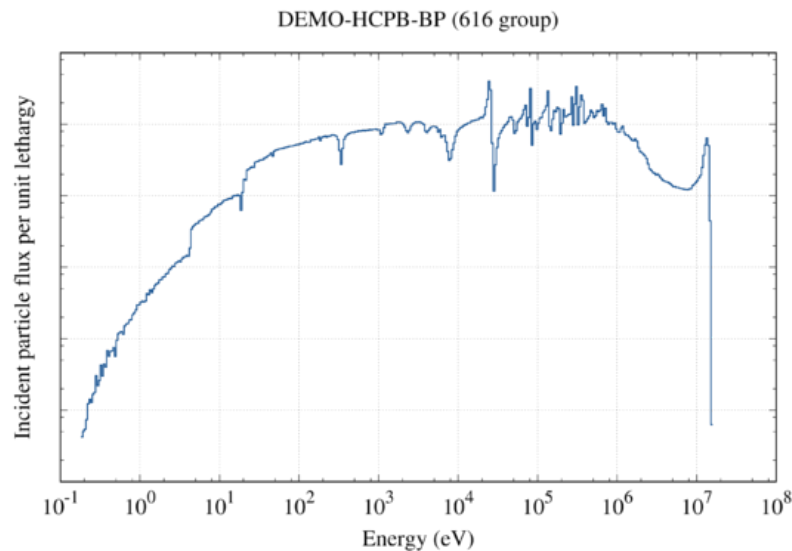
Produces a binary `collapx` file of 1-group data with uncertainties



- Nuclear data collapse is the generation of one-group 'effective' cross-sections for all allowable reactions with a given incident particle spectrum:

$$\bar{\sigma} = \sum_i^N W_i \sigma_i, \text{ using weights } W_i,$$

$$W_i = \phi_i / \sum_i^N \phi_i.$$

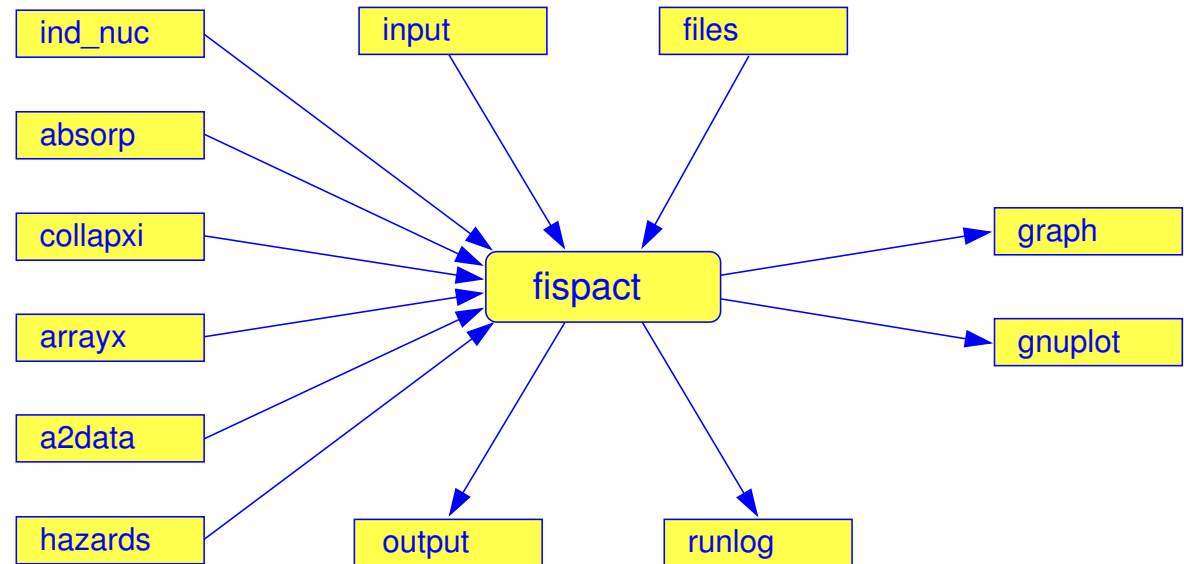


Fe 56	(n, a)	Cr 53	9.30007E-03+-	1.87183E+02	Fe 56	(n, h)	Cr 54	1.43520E-11+-	5.52180E+02
Fe 56	(n, 2p)	Cr 55	1.89736E-12+-	0.00000E+00	Fe 56	(n, t)	Mn 54	2.71346E-08+-	4.06438E+02
Fe 56	(n, np)	Mn 55	1.09412E-02+-	1.71659E+01	Fe 56	(n, d)	Mn 55	9.78951E-04+-	2.52961E+02
Fe 56	(n, p)	Mn 56	3.09369E-02+-	6.14934E+00	Fe 56	(n, 2n)	Fe 55	1.10279E-01+-	1.43515E+01
Fe 56	(n, E)	Fe 56	3.39432E+00+-	8.08801E-01	Fe 56	(n, n)	Fe 56	3.59211E-01+-	1.13654E+01
Fe 56	(n, g)	Fe 57	1.11989E-02+-	3.18853E+00					

...

- FISPACT-II can calculate and output many derived radiological quantities in the inventory stage

- `absorp`, `a2data`, `hazards` are data files for gamma absorption, transport A2 values and hazard indices




- The binary `arrayx` and `collapxi` are required

- Results of the inventory simulation can be output in a variety of different files, in addition to the main `.o` file
 - “tab” files with specific data output in a convenient format
 - Plotting (with gnuplot) ready output files and scripts

- FISPACT-II uses input files with a required sequence of **keywords**
 - Different choices of keywords and/or options on keywords allow users to control calculations
 - Many options are selected by default, but can be overwritten by user

Basic scheme (<...> are optional comments):

```
< -- Control phase -- >  
GETXS option_1 option_2  
GETDECAY option_3  
FISPACT  
* Description of calculation  
< -- Initial phase -- >  
...  
< -- Inventory phase -- >  
...
```



- Setup the nuclear data handling**
- These lines separate the initial ND handling**
- Select calculation options**
- Define inventory simulation**

- The most recent (Dec 2016) 3-20 version of FISPACT-II available through the NEA Data Bank has ~100 keywords, see:

http://fispact.ukaea.uk/wiki/FISPACT-II_keywords

- Many have options, e.g.

```
GETXS option_1 option_2
```

```
option_1 = 0 (read from pre-compiled binary file)
```

```
1 (read from library and collapse)
```

```
option_2 if option_1 = 1 specify the energy group  
else do not include option_2
```

E.g. “GETXS 0” or “GETXS 1 709” would be valid commands

- Some keywords must be used, some are almost always used and some are for specific scenarios

FISPACT	Required to start simulation
GETXS/GETDECAY	Required to process/read-in nuclear data
END	Required to end input
TIME	Used to specify time intervals
ATOMS/STEP	Used to instruct the code to solve
HAZARD/DOSE	Used to request standard outputs
MASS/FUEL	Used to specify input material
USEFISSION	Used to turn on fission (default is off)
FLUX/POWER	Used to set flux normalisation
PRINTLIB	Used to print nuclear data
ZERO	Used to zero the clock for cooling
SSFCHOOSE/ SSFMASS/SSFFUEL	Used to include resonance self-shielding

- Some can be used multiple times, for example re-collapse data in burn-up with spectral shift or change the flux/power normalisation
 - See the wiki for all details or the User Manual

- Both the manual and wiki have getting started tutorials
- This is the best place to start:
 - see `/getting_started/ examples`

Steps:

1. Open a terminal and move to the FISPACT-II install location
2. Move to the `/getting_started/FNS_Inconel` folder
3. Open the user manual to Section 3 'Getting Started'
 - See `/doc/CCFE-R(11)11.pdf`