Oak Ridge National Laboratory

SCALE Users' Group Tutorials

ORIGEN: Activation Analysis of the Silene Experiment

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Why Do We Need COUPLE?

COUPLE creates ORIGEN libraries (f33) from fundamental data sources (and transport flux), performing two major functions

1) Converting fundamental decay data into a decay-only f33
2) Updating/adding reaction transition coefficients on an existing f33

$$\frac{d\vec{N}}{dt} = \left(\boldsymbol{A}_{\sigma,n}\mathit{\Phi}_n + \boldsymbol{A}_{\lambda}\right)\vec{N}(t) + \vec{S}_n,$$

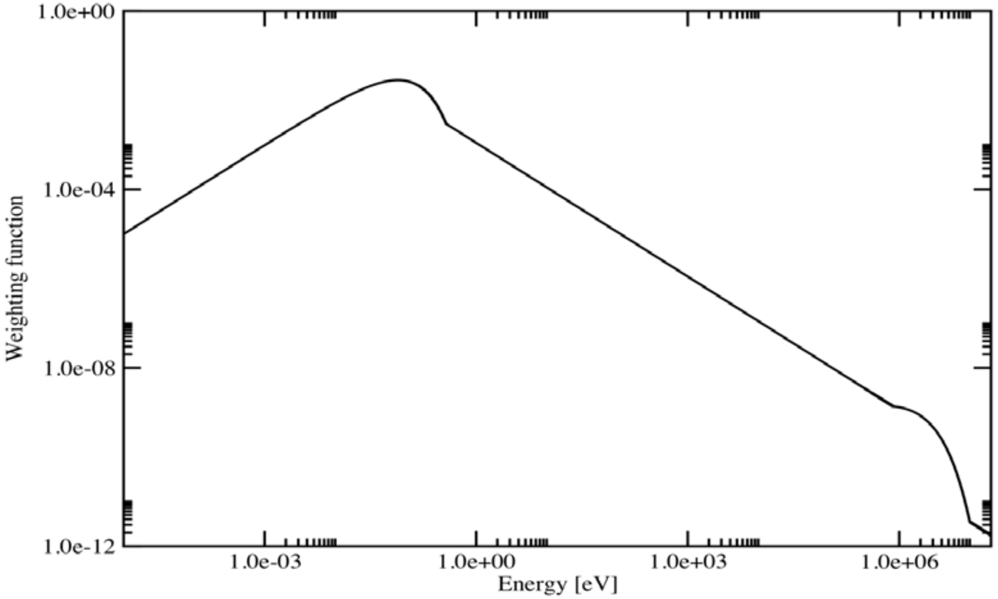
over time step $t_{n-1} \le t \le t_n$.

$$a_{ij} = \begin{cases} l_{ij}\lambda_j + f_{ij}\sigma_j\mathit{\Phi} & i \neq j \\ -\lambda_i - \sigma_i\mathit{\Phi} & otherwise \end{cases}$$

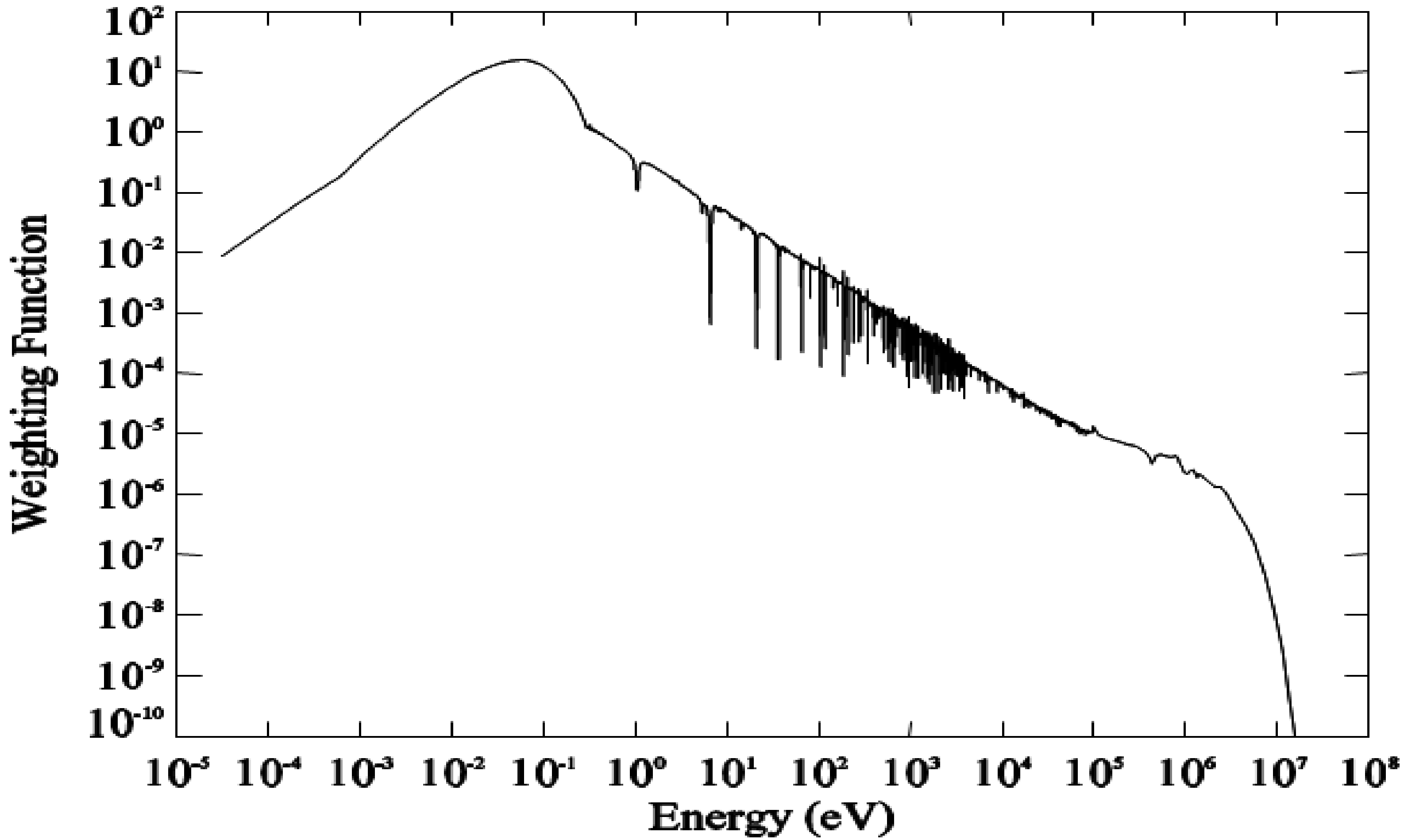
Decay and reaction pieces are stored separately in f33→later in ORIGEN, flux magnitude folded in

Shipped JEFF Libraries

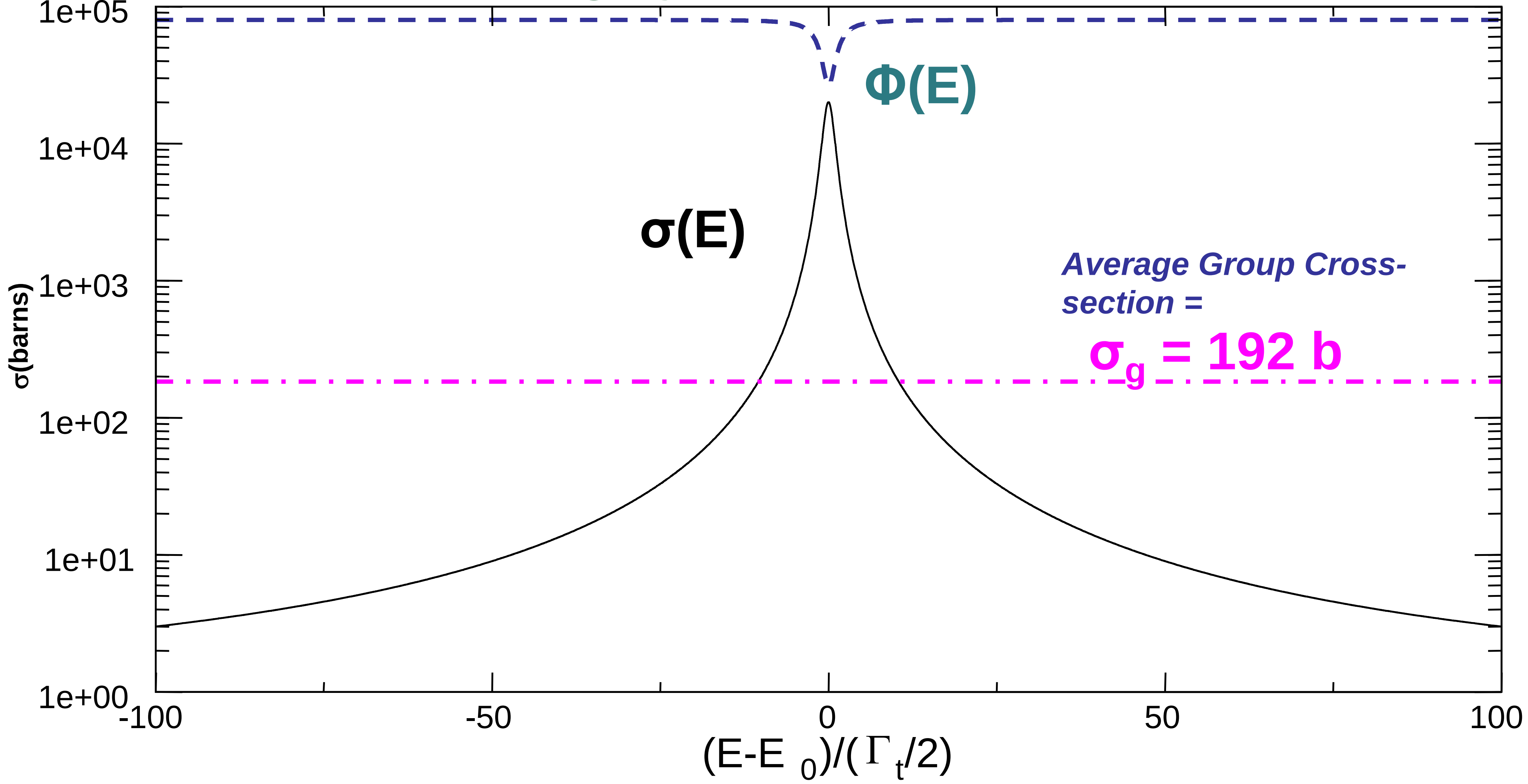
- Infinite dilution (no energy self-shielding)
- **Thermal Maxwellian + 1/E + Fission spectrum** used to create various multigroup libraries (238, 252, 56, etc.)



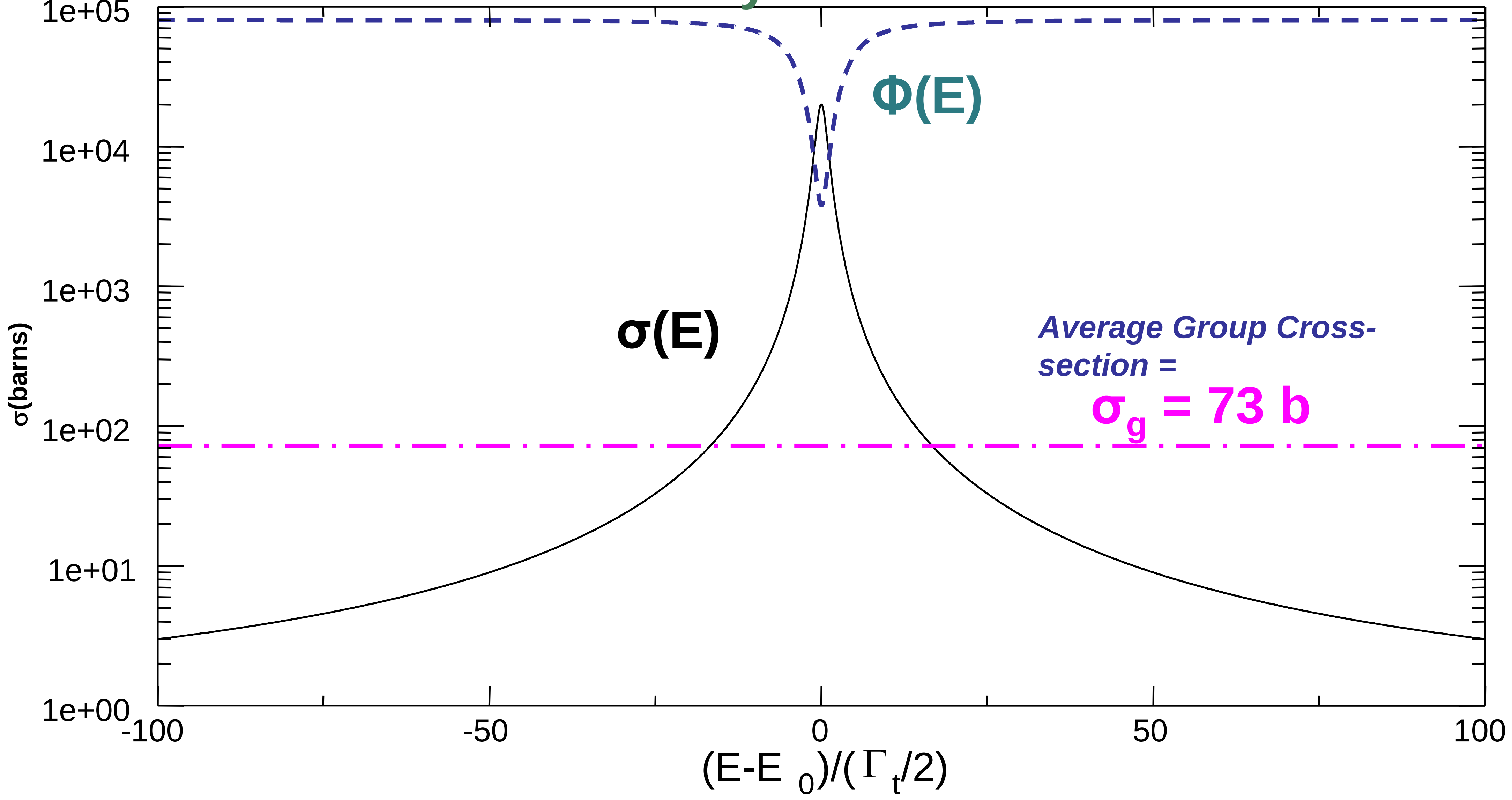
Importance of Self-Shielding



Highly Dilute Absorber



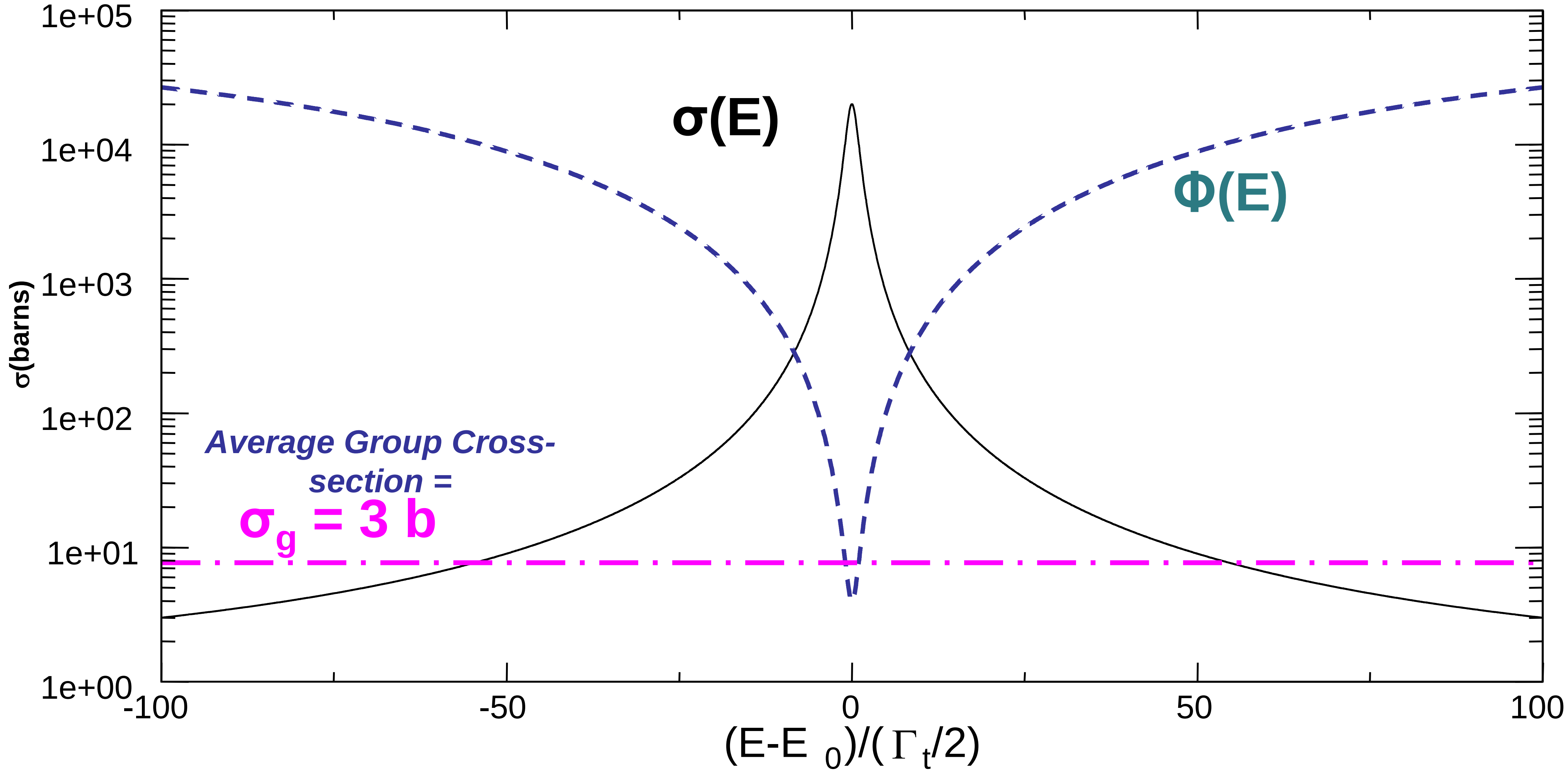
Moderately Dilute Absorber



Average Group Cross-section =

σ_g = 73 b

Undiluted Absorber (i.e., pure absorber)



One Group Cross Sections

reaction
rate

$$R = N\int_0^\infty \sigma(E)\Phi(\mathrm{E})dE$$

number density *N*

$$\approx N\sum_g \sigma^g\Phi^g$$

multi-group
approximation

$$= \frac{N\Phi\sum_g \sigma^g w^g}{\sum_g w^g}$$

multi-group
weighting
function w^g

flux magnitude
Φ (n/cm^{2}s)

$$= N\Phi\sigma$$

COUPLE Input Format (FIDO)

- Define neutron flux spectrum to weight cross sections
- Specify fission nuclides with yields
- Print all weighted cross section values
- User can specify their own cross section values via input

COUPLE Input Cont’d

The first blank line terminates the title input.

0$$ Array – Logical Unit Assignments

1.	NOUT	Printed output unit number (6).
2.	LIBDEC	ORIGEN Decay Resource {if LBIN = 1} (1$ array) (27).
3.	JD	ORIGEN Reaction Resource MG XS library (80=238-group) {always required} (80).
4.	ND	Input ORIGEN Library {if LBIN = 0} (21).
5.	LD	(optional) Self-Shielded AMPX Library (0).
6.	MD	Output ORIGEN Library (33).

COUPLE Input Cont’d

1$ Array – Control Constants [19 entries]

1. LBIN 1/0 – Input library in formatted / binary mode (0).
2. PRT 1/0 – Suppress informational output / print informational output (0).
3. LBUP 1/0 – Update with user input cross sections (Data Block 8) / no user update (0).

12.IDREF – Nuclide ID number of the isotope in AMPX library on unit LD that contains the neutron flux

13.NZONE – The zone of the nuclides with which to add/update the library (0).

14.IEDOU 1/0 – Request edit of data on the output working library on MD (0).

15.NFISW – Number of fissile nuclides in output library entered in 7$ array {JADD = 1} (-1 automatically adds 30 nuclides).

18.NWGT – Defining source of weighting flux spectrum data (0).
/0/N= AMPX working library on IDREF/ input N-group flux in 9* array

T – Data Block 1 terminator

COUPLE Input Cont’d

7$ Array – Nuclide ID numbers for nuclides with fission yields [NFISW entries].

9* Array – User input cross section weighting function [NWGT entries].

T – Data Block 2 terminator

DONE

COUPLE Input Simple Example

```
=couple
ORIGEN Decay Library Revision 3
Prepared by Johnny B. Good on 2015-10-18

1$$ a1 1 e
1t
3$$ a1 0 e
3t
done
end

'Save a copy of the ORIGEN library.
=shell
cp ft33f001 "${OUTDIR}/my_dk.f33"
end
```

COUPLE Input – Things to Remember

- **Formatting**
  - COUPLE uses FIDO→max. line length of 72
  - "done" is required to terminate
  - empty line after title is required to terminate title
- **Group Structures**
  - Reaction Resource (JEFF) and optional AMPX library must have same group structure
  - ${DATA}/origen_filenames gives mapping of "unit number" to name
- **Output**
  - ORIGEN library (f33) is output to working directory as ft33f001
  - Usually a good idea to rename:

```
=shell
cp ft33f001 "${OUTDIR}/my.f33”
end
```

```
=couple

0$$ a2 27 a6 25 e
1$$ 1 0 0 e t
3$$ 0 e 3t
done
end
```

no title still needs a blank/empty line!

ORIGEN Input

- between `=origen` and `end` in SCALE
- syntax is Scale Object Notation (SON)
  - key/value pairs, e.g. `print_xs=yes`
  - arrays, e.g. `power=[40 45 60 20]`
  - blocks, e.g. `lib{ file="end7dec" pos=1 }`
- for backwards compatibility, can still read SCALE 6.1 FIDO syntax

Overview

```
'SCALE comment
=origen

     % ORIGEN comment %

bounds{ … }
solver{ … }
options{ … }

case(A){
    time=[31 365] % days
    …
}

case(B){
    …
}

% more cases?

end
```

- comments
  - inside ORIGEN, SON uses **%** *(anywhere)*
  - outside ORIGEN, SCALE uses **'** *(beginning of line only)*
- "root" level
  - *one of*: bounds, solver, options
  - *sequence of*: case
- main problem specification in cases
  - can have optional id, case(ID)
- hierarchical

Input Component: case

```
=origen
…
case(ID){
    title="my title"

    lib{ … }
    mat{ … }
    time{ … }
    flux{ … } % or power{ … }

    print{ … }
    save{ … }

    gamma{ … }
    neutron{ … }
}
…
end
```

- setup
  - lib – load transition matrix data from library
  - mat – define initial composition
- operating history
  - time – define time steps
  - flux/power – define flux or power level
- archival
  - print – results to output file
  - save – results to f71 binary file
- emission calcs
  - gamma (beta), neutron (alpha)

Input Component: lib

```
=origen
…
case(initial){
    lib{ file="my.f33" pos=1 }
    mat{ … }
    …
}
case(continuation){
    lib{ pos=2 }
    …
}
…
end
```

- library files can contain multiple (usually burnup-dependent) "positions"
- default is pos=1 (will always exist on any library)
- file="end7dec" is a special decay library
- ORIGEN libraries can be created by
  - COUPLE
  - ARP
- position/data set fixed for each case

Input component: mat

```
% from iso
mat{
    iso=[ u235=1.0 u238=9.0 ] %id(sublib)=amount
    units=GRAMS               %units in iso array
}

% from iso with number density input
mat{
    iso=[ u235=1e-2 u238=1e-1 ] %id(sublib)=amount
    units=ATOMS-PER-BARN-CM     %units in iso array
    volume=200                  %cm^3
}

% from position on f71 file
mat{
    load{ file="origen.f71" pos=11 }
}

% from previous case
mat{
    previous=4 %step index from previous case
}
```

- iso array
  - list of id=amount
  - units in:
    - GRAMS
    - MOLES or GRAM-ATOMS
    - ATOMS-PER-BARN-CM
    - CURIES
  - ATOMS-PER-BARN-CM requires volume
- load from position on the binary concentrations file f71
  - not the same as library (f33)!
- load from previous case

Input Component: time

```
% simple decay case (two steps 0→31 and 31→365 days)
time = [ 31 365 ]

% flux irradiation (decay if flux=0)
time = [ 31   365  396 ]
flux = [ 2e14 1e14 0 ]

% power irradiation (decay if power=0)
time = [ 31 365 396 ]
power= [ 50 45  0 ] %50 MW, 45 MW, then decay

% changing units using time block
time{
    t = [ 5 15 300 ]
    units = HOURS
    % available units:
    % SECONDS, MINUTES, HOURS, DAYS, YEARS, CUSTOM
}

% custom units
time{
    t = [ 1 2 3 ]
    units = CUSTOM
    custom_name = "MONTH"
    custom_length = 2678400 %seconds per "MONTH"
}
```

- operating history
  - **time – define time steps**
  - flux/power – define flux or power level
- time can be

  a simple array [] of time steps with default units of days

  OR

  a block with a t=[] array and units=
  - SECONDS
  - MINUTES
  - HOURS
  - DAYS
  - YEARS
  - CUSTOM!

Input Component: flux/power

```
% simple decay case (two steps 0→31 and 31→365 days)
time = [ 31 365 ]

% flux irradiation (decay if flux=0)
time = [ 31   365  396 ]
flux = [ 2e14 1e14 0 ]

% power irradiation (decay if power=0)
time = [ 31 365 396 ]
power= [ 50 45  0 ] %50 MW, 45 MW, then decay

% changing units using time block
time{
    t = [ 5 15 300 ]
    units = HOURS
    % available units:
    % SECONDS, MINUTES, HOURS, DAYS, YEARS, CUSTOM
}

% custom units
time{
    t = [ 1 2 3 ]
    units = CUSTOM
    custom_name = "MONTH"
    custom_length = 2678400 %seconds per "MONTH"
}
```

- operating history
  - time – define time steps
  - **flux/power – define flux or power level**
- either flux or power (not both)
- total flux (neutrons/cm^{2}s) is required to solve depletion equations
- power (MW) can be provided
  - converted internally to flux
- must have same number of time and flux/power entries

Note: for fuel, it is convenient to specify 1e6 total grams of heavy metal so power is MW/MTIHM

Input Component: save

```
case{
    mat{ … }
    time=[ 1 10 100 1000 ] % 4 steps
    save{
        file="my.f71"      % file name
        steps=[0 2 4]      % save initial (0) isotopics
                           % end-of-step 2 (10 days)
                           % end-of-step 4 (1000 days)
    }
}
```

```
=origen
case{
    % use ENDF/VII-based decay library
    lib{ file="end7dec" }
    % create a material with 1 gram U-238
    mat{
        units=grams
        iso=[u238=1.0]
    }
    time=[20L 1.0 1e9] %default units are days

    % save to f71
    save{
        file="u238.f71"
        steps=ALL
    } %save=yes is shortcut for ALL, ${OUTPUTBASENAME}.f71
}
end
```

- save block requires
  - file name, file="xyz.f71"
  - array of step indices, steps=[]
- each value in the time array indicates a "step" from the previous time
  - the first step is from 0 days to 1 day
  - second is from 1 day to 10 days
  - etc.
- using log interpolation L and linear interpolation `I` is convenient for time and steps, respectively
  - for *x*L A B logarithmic spacing, total number of steps is x+2

Input Component: save (2)

```
=origen
case(irrad){
    lib{
        file="mylib" pos=1
    }
    % 1 MT of enriched uranium
    mat{
        units=GRAMS
        iso=[u234=356 u235=40000 u236=184 u238=959460]
    }
    time=[ 50 100 150 200 ] %time in default days
    power=[ 15 15 15 15 ] %power in MW
}
case(decay){
    time{
        units=YEARS
        start=0
        t=[0.1 0.3 0.9 1 2 3 4 5]
    }
    save{ file="discharge" steps=[0 LAST] }
    %only save begin and end in this case
}
end

'must copy back f71 explicitly because doesn’t match *.f71
=shell
cp discharge ${INPDIR}/discharge
end
```

- f71 file is ORIGEN's "results" file
  - binary ☹
  - can post-process with OPUS ☺
  - initialize ORIGEN material with it ☺
  - view in Fulcrum ☺☺
  - also called "concentrations" file
  - contains concentrations *and* spectra
- SCALE rule: all files with extension ".f71" or ".f33" will be copied out of the working directory back to the user directory
- to avoid automatic copy back of either type of file, can use filenames ft71f001 and ft33f001 (legacy SCALE names)
- shortcuts
  - LAST for last step index
  - steps=ALL for everything

Tutorial Problem – SILENE Experiment

- CEA Valduc experimental facility, France
- Critical pulse 93% ^{235}U uranyl nitrate solution
- Threshold activation foil measurements

Measurements

- Aluminum holders have 3 foil cavities containing Fe, Ni, and Mg foils with > 99% elemental purity
  - Nickel, 1 mm thick, 2.807 g
  - Iron, 3 mm thick, 7.292 g
  - Magnesium, 2 mm thick, 1.089 g
- Activation from fast (*n,p*) reactions were measured
- Measured activities per unit mass and relative uncertainties (2 sigma)
  - ^{54}Fe(n,p)^{54}Mn, ^{54}Mn activity 0.1961 Bq/g ± 4.1%
  - ^{58}Ni(n,p)^{58}Co, ^{58}Co activity 12.99 Bq/g ± 3.2%
  - ^{24}Mg(n,p)^{24}Na, ^{24}Na activity 59.10 Bq/g ± 4.1%

Description

Assumptions

- neutron energy spectrum provided
- natural isotopic abundance of foil elements
- total fluence of 1.6351×10^{11} n/cm^2

Goals

- calculate the specific activity (Bq/g) for each foil
- observe time-dependence post-irradiation
- compare to experiment plus uncertainty

Procedure

- Begin with silene.starter.inp
- Copy/paste in flux.txt to finish COUPLE library setup.
- Create an ORIGEN activation input with 3 cases, 1 for each sample
  - Note that starter has outline and follow-on OPUS post-processing
  - Make 'iron' case work first
  - Then copy/paste/modify for the 'nickel' and 'magnesium' cases
  - Uncomment the OPUS inputs for 'nickel' and 'magnesium'
- *Alternatively, you could open each .f71 in Fulcrum and use OPUS F71 Viewer*