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ORIGEN Data

SCALE 6.3.1



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U.S. DEPARTMENT OF ENERGY

Learning goals



Familiarize with the various SCALE data resources used by ORIGEN, including how ORIGEN uses fundamental nuclear data in depletion and decay calculations



Demonstrate how to use the Fulcrum user interface to visualize selected ORIGEN nuclear data libraries

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ORIGEN reaction and decay data



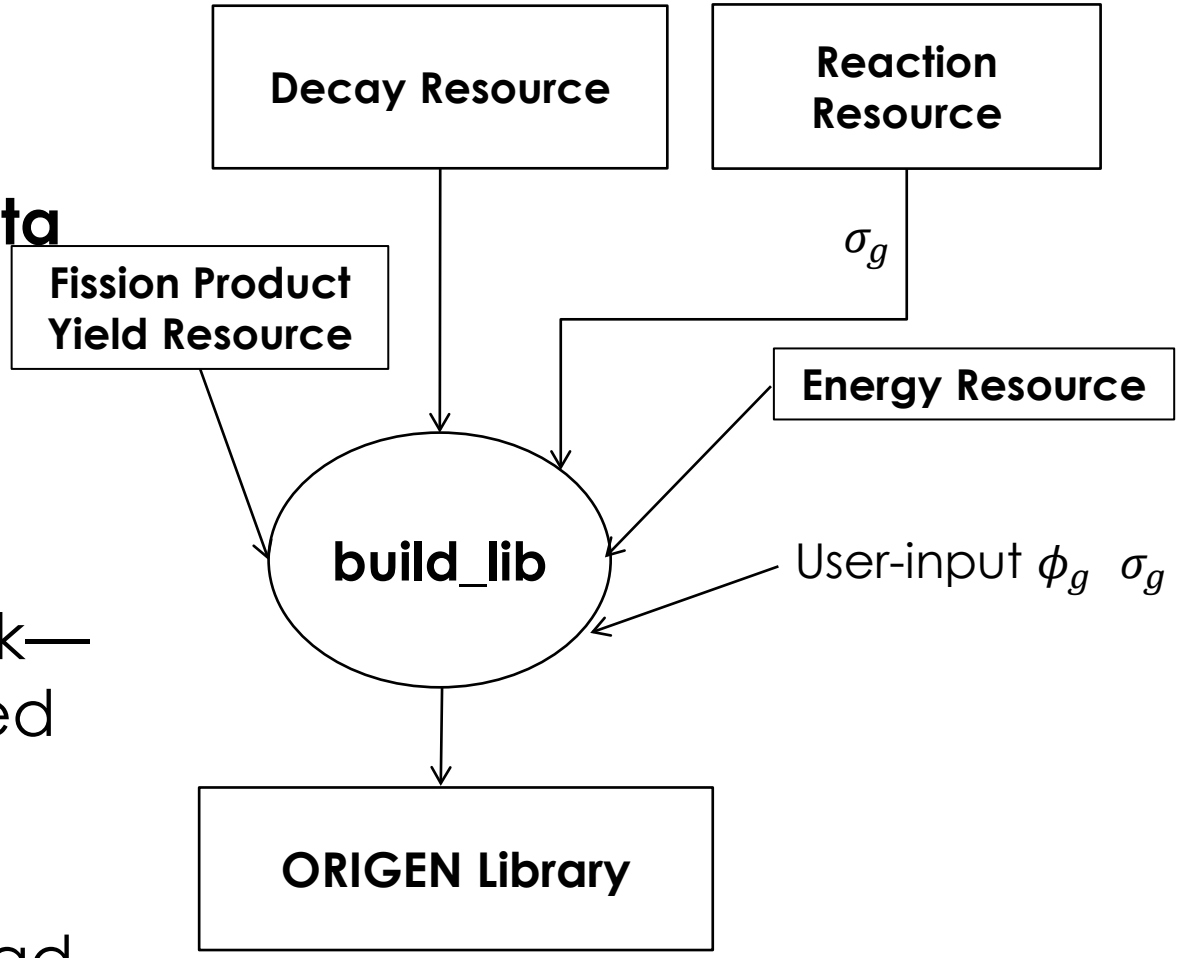
Accuracy of ORIGEN is determined by the accuracy of the nuclear data

Radioactive decay	• Half-lives • Branching fractions • Decay energy
Neutron reaction data	• Energy-dependent cross-sections
Recoverable energy	• Energy per fssion and capture
Fission product yields	• Energy-dependent data
Photon emission data	• X-ray and gamma ray emissions per decay
Neutron emission data	• Stopping powers • (a,n) yield cross sections • Spontaneous fission spectral parameters • Delayed neutron spectra
Alpha & beta emission data	• Number per decay and energy distribution

For more information:
See **Section 10.2** ("ORIGEN Data Resources") in the SCALE 6.3 manual

ORIGEN data basics

- The fundamental nuclear data mentioned on the previous slide is contained in various "resources"
- Resources plus user-input create an **ORIGEN library** which is a **portable data packet** with all the information needed for a calculation
- In SCALE 6.3
  - Users may build libraries within ORIGEN in the new "build_lib" block—in 6.2 and earlier, this was managed by COUPLE
  - Fission product yield and decay data resources may be directly read from ENDF/B formatted data files

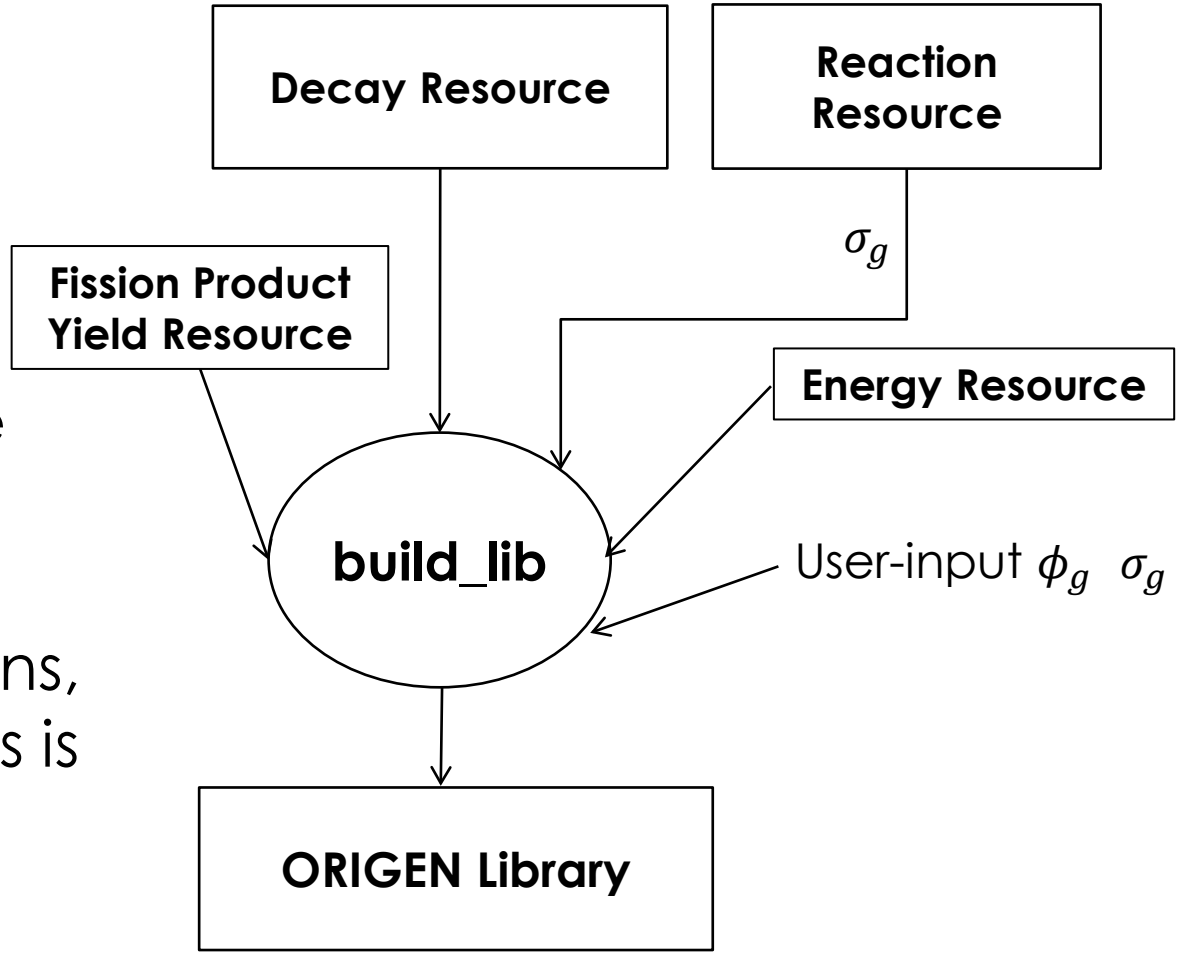


Reaction rate updates

- All reaction cross sections are collapsed using input neutron energy spectrum Φ(E) of the system
- In multi-group (MG)

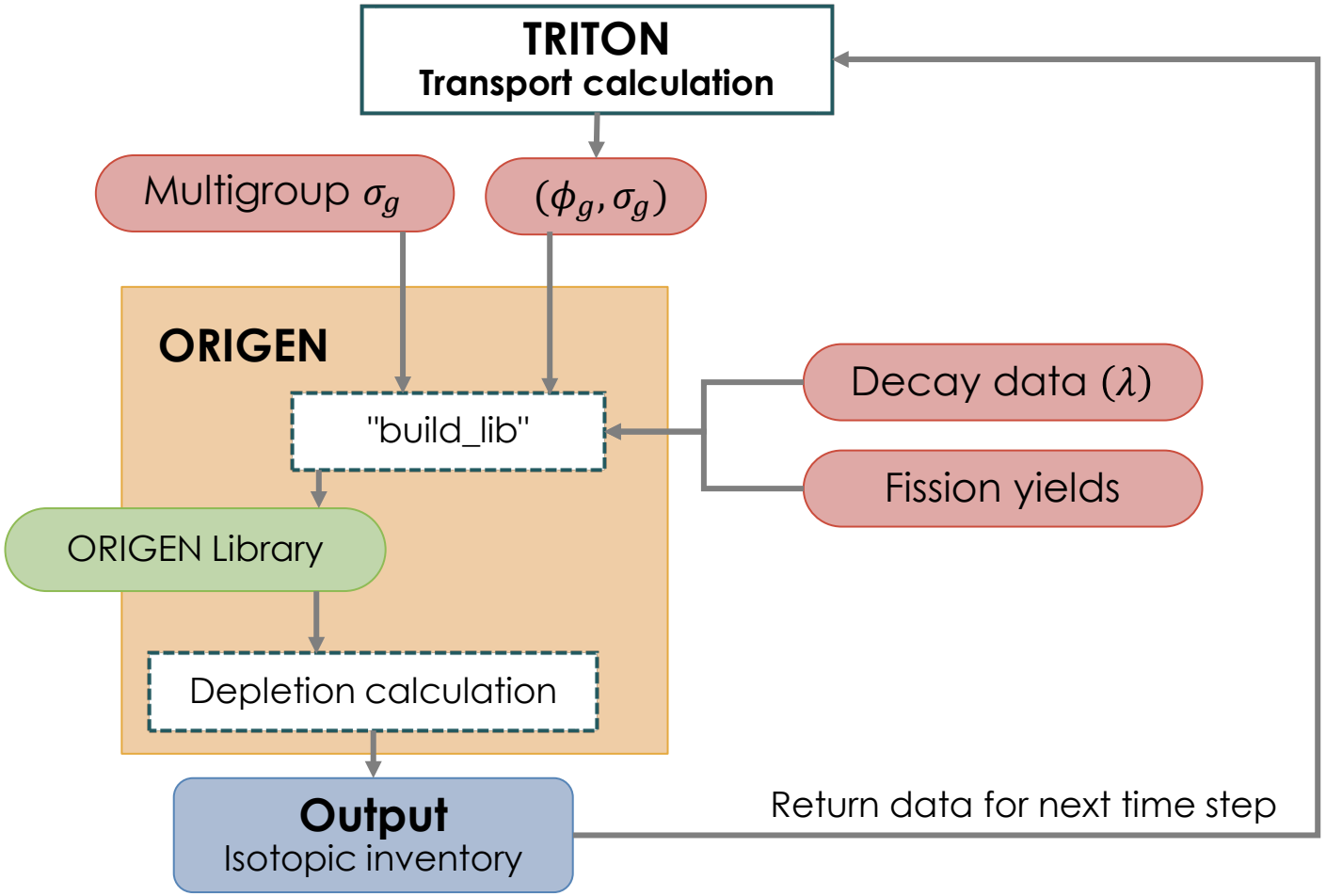
$$\bar{\sigma} = \frac{\langle \sigma(E)\phi(E) \rangle}{\langle \phi(E) \rangle} = \frac{\sum_g \sigma_g \phi_g}{\sum_g \phi_g}$$

- Note that ORIGEN's reaction resource contains infinitely dilute MG cross sections
- In many cases, for accurate simulations, self-shielded MG data is required—this is the responsibility of SCALE's XSProc module to write this data to an AMPX library

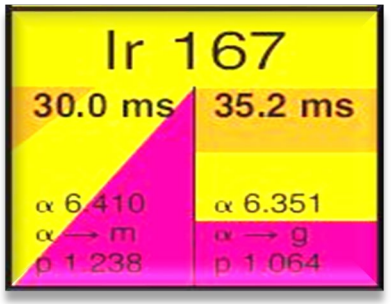


Example of coupled transport/depletion with TRITON

- TRITON uses the same resources as ORIGEN stand-alone but "automates" performing self-shielding and neutron transport for the various mixtures as the evolve
- TRITON writes ORIGEN libraries to disk which can be useful for understanding fuel evolution by "replaying" the solutions in ORIGEN



Nuclear decay data



- Data compiled entirely from ENDF/B-VII.1
  - T ½ (> 1 ms)
  - Decay branching fractions β^-, β^+, EC, a, IT, $\beta^-\beta^-$, β^-n, SF, n, β^-a
  - Transitions to ground and excited states
  - Recoverable energy from decay Q (a, *β*, *γ*)
- Other data included with nuclear decay data
  - Natural isotopic abundances (NIST data); same as used in STDCMP
  - Air and water toxicity conversion factors (EPA and ICRP 72)
- **Decay resource**: ${SCALE}/data/origen_data/origen.rev03.decay

Note: the decay-only ORIGEN library ${SCALE}/data/**origen.rev05.end7dec** Is typically used for decay calculations using the alias **end7dec**

Nuclear reaction data

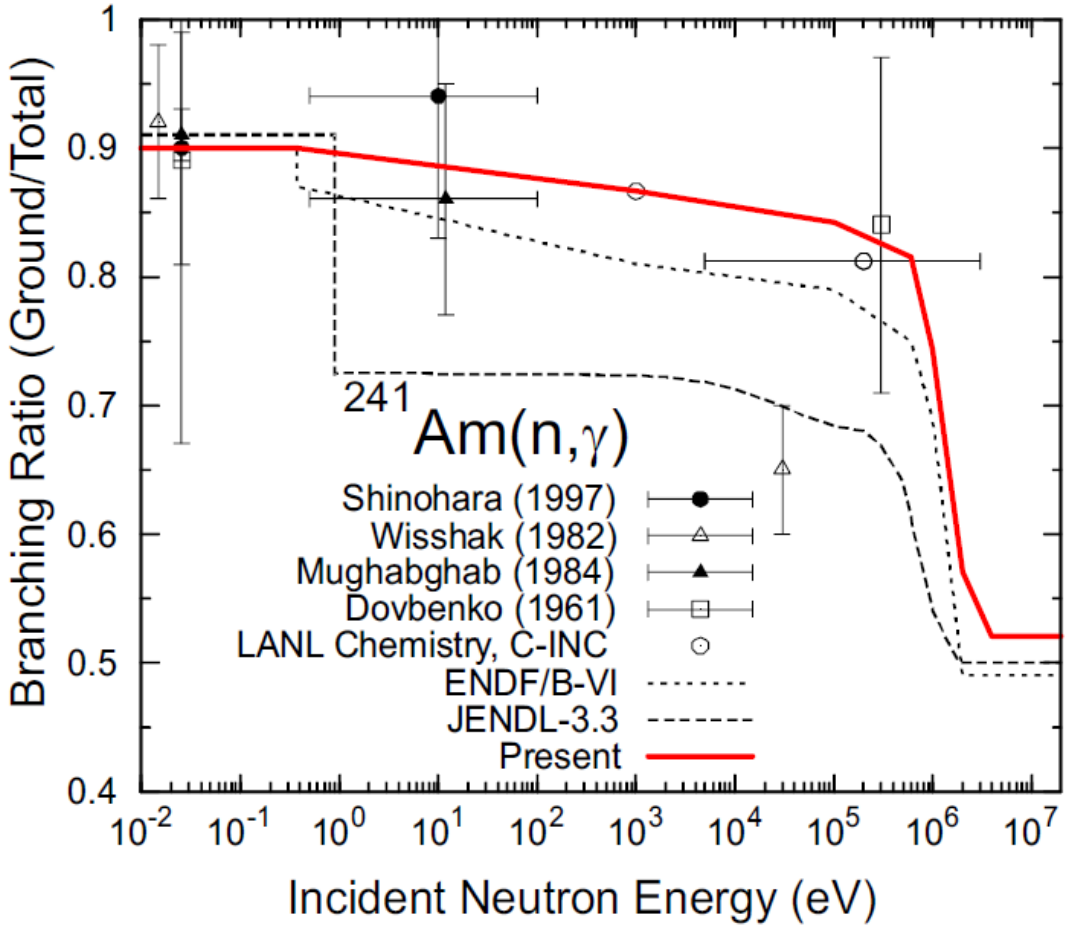
- Neutron and gamma transport libraries
  - **ENDF/B-VII.1 and –VIII.0**
  - Additional compositions defined by SCALE stdcomp, e.g. stainless steel
- Reaction Resource containing additional nuclides
  - **JEFF-3.1/A** (http://www.nea.fr/html/dbdata/JEFF/JEFF31/JEFF-3A.pdf)
  - 774 nuclides, 12,617 neutron-induced reactions
  - Expanded reaction types supported
    - (n,2n), (n,3n), (n,f), (n,na), (n,n3a), (n,2na), (n,3n a), (n,np), (n,n2a), (n,2n2a), (n,nd), (n,nt), (n,n ^{3}He), (n,nd2a), (n,nt2a), (n,4n), (n,g), (n,p), (n,d), (n,t), (n,^{3}He), (n,a), (n,2a), (n,3a), (n,2p), (n,pa), (n,t2a), (n,d2a), (n,n')
- Both transport libraries and reaction resource are stored in AMPX format and may be visualized in Fulcrum

Every reaction can produce multiple daughter nuclides

- Fission reactions produce ~1400 daughters according to the fission product yield data
- For other reactions, ORIGEN uses energy-dependent partial cross sections branching to ground and first metastable state

Data file:
${SCALE}/data/**origen.rev03.jeff200g**

^{241}Am (n,γ) → ^{242m}Am $T_{1/2}$= 114 y
^{241}Am (n,γ) → ^{242}Am $T_{1/2}$= 16 h



ENDF/B-VII & JEFF-3.1/A branching data used in ORIGEN

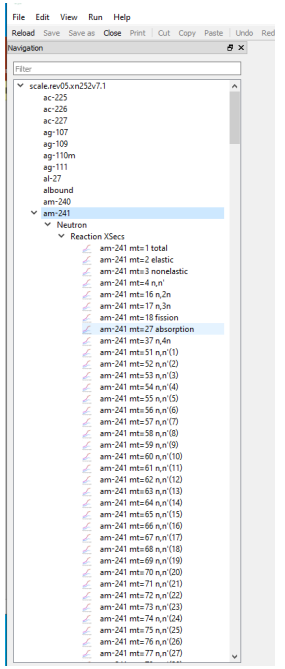
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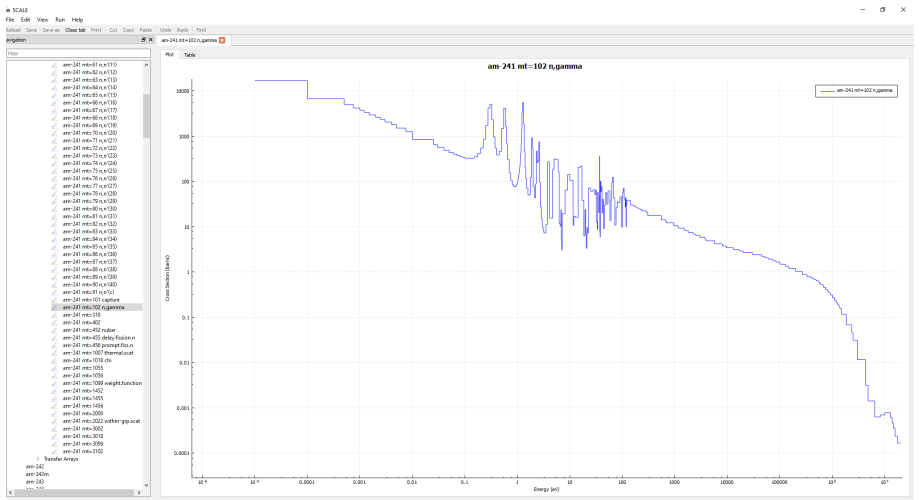
Visualizing cross section libraries data in Fulcrum



Plotting AMPX (infinitely-dilute) MG cross sections

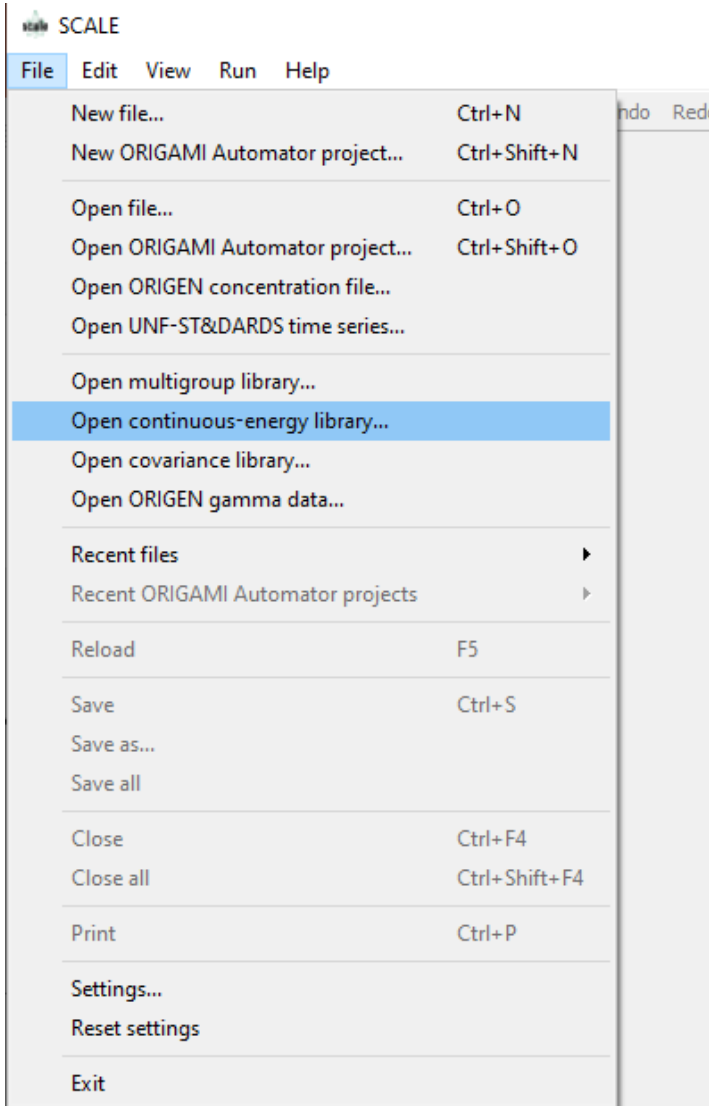
- Open multigroup library
- Navigate to data directory: **${SCALE}/data/**
  - Examples:
    - **scale.rev04.xn252v7.1** (252-group ENDF/B-VII.1)
    - **scale.rev04.xn56v7.1** (56 group ENDF/B-VII.1)
- Nuclides available to plot appear in file tree (in alphabetical order)
- Browse to desired data and double-click to plot or right click for more options





Plotting continuous energy cross sections

- Similar to plotting multigroup data, but "open continuous-energy library"
- Select xml file for desired library
  - Example: **ce_v7.1_endf.xml**



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Fission product yields in ORIGEN



ORIGEN fission product yields

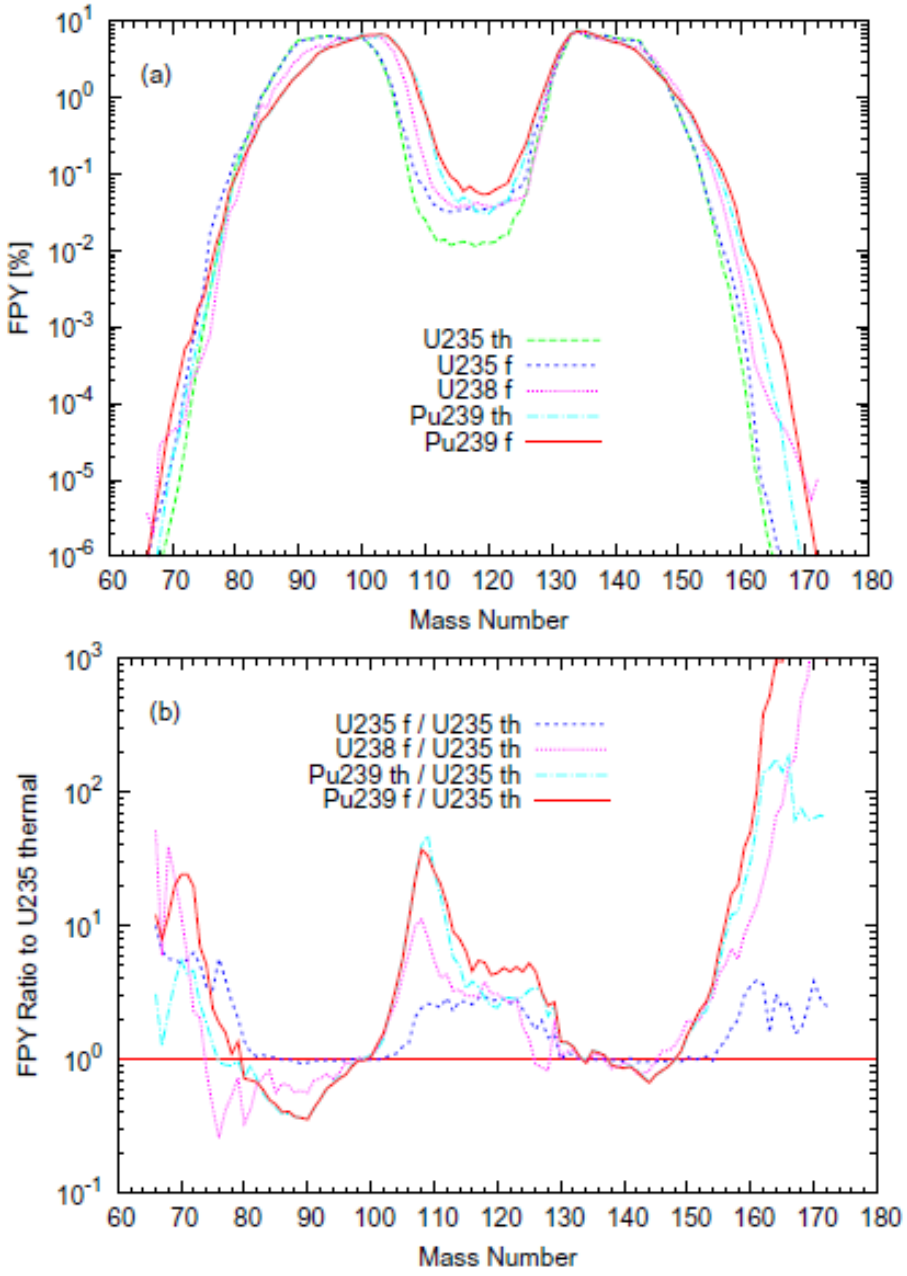
- ENDF/B-VII.1 fission yields† available for 30 actinides:
  - ^{227,228,232}Th, ^{231}Pa, $^{232\text{-}238}$U, $^{238\text{-}242}$Pu, ^{241,242m,243}Am, ^{237,238}Np, $^{242\text{-}246,248}$Cm, ^{249,252}Cf, and ^{254}Es
- Data are from England and Rider compilations
- Energy-dependent yields tabulated at:
  - **Thermal fission:** 0.0253 eV
  - **Fast fission (fission spectrum):** 2 MeV
  - **High-energy fission:** 14 MeV
- Intermediate energies interpolated using the mean energy of neutrons causing fission
- **Yield resource:** ${SCALE}/data/origen_data/**origen.rev05.yields.data**

Note: ENDF tabulates this as 500 keV; Assigned to 2 MeV in ORIGEN to more accurately reflect the average energy of the fission (Watt) spectrum (See **Sect. 10.2.6** of the SCALE manual)

† M.B. Chadwick, P. Oblozinsky, M. Herman, et. al. "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nuclear Data Sheets,* **107**, 2931-3060 (2006)

Energy dependence of fission yields

- Fission product distribution is dependent on the energy of incident neutrons causing fission
- Fission rate in each neutron energy range is calculated to obtain the effective energy of fission, and this energy is used to interpolate yields for each fissile nuclide



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Radiological emissions data used by ORIGEN

Treatment of gamma, neutron, beta, and alpha decay



Gamma emission resource data

- Following files in **${SCALE}/data/origen_data/**:
  - **mpdkxgam.data**: decay X-rays and γ-rays data for 1132 nuclides
  - **mpsfangm.data**: γ-rays accompanying spontaneous fission and (a,n) reactions
  - **mpbrh2om.data**, **mpbrh2op.data**: Bremsstrahlung spectra for decay electrons slowing down in **water** (**m** is β-, **p** is β+)
  - **mpbruo2m.data**, **mpbruo2p.data**: Bremsstrahlung spectra for decay electrons slowing down in a **UO2 fuel matrix** (**m** is β-, **p** is β+)
- **Data can be visualized in Fulcrum**
  - File > Open ORIGEN gamma data

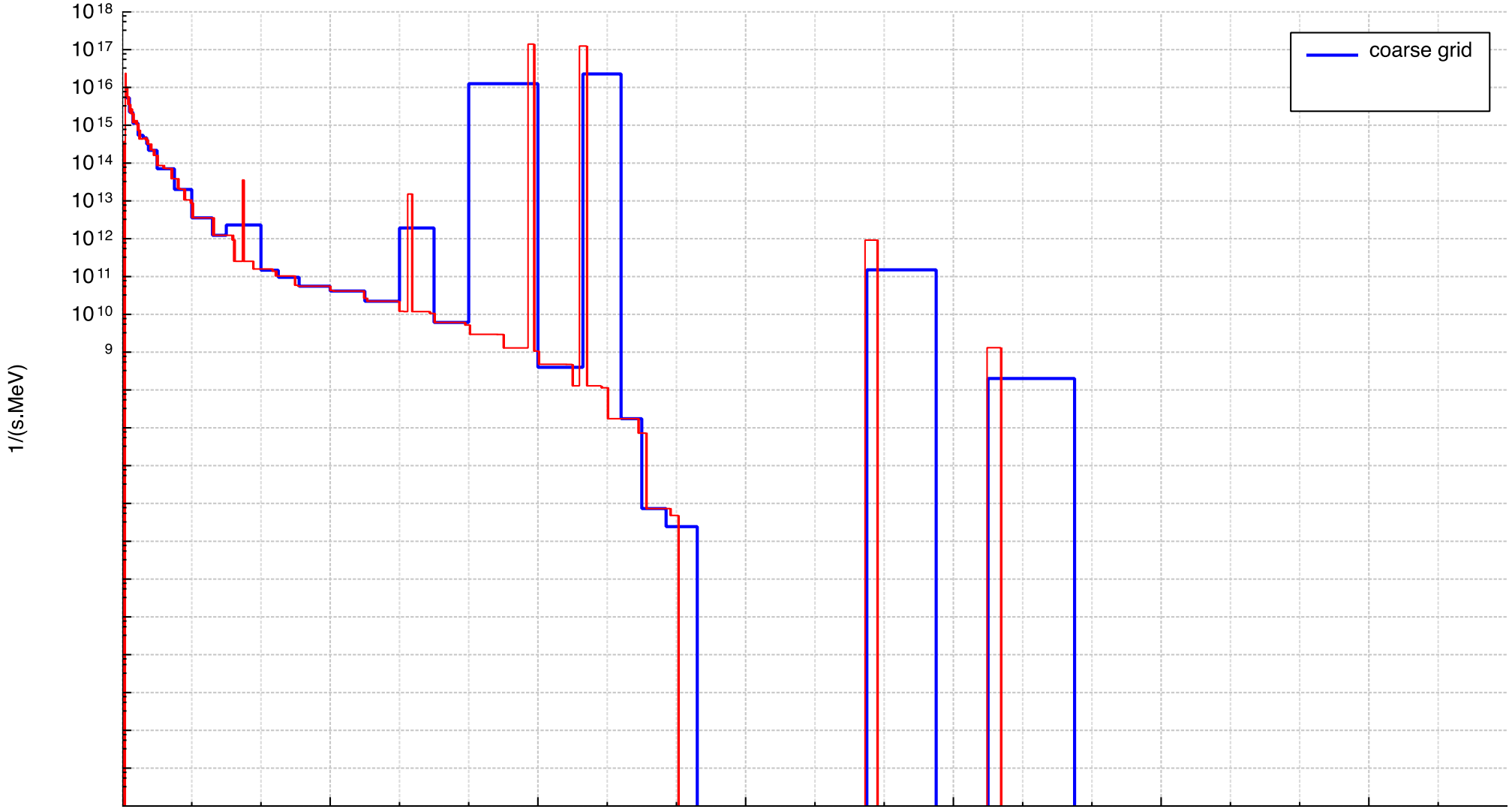
Gamma emission calculation

- Photon libraries contain discrete gamma and X-ray energies and the yield per decay (data stored as energy-yield pairs)
  - Continuous energy Bremsstrahlung is represented with a series of narrowly-spaced discrete energies
- Binning of discrete gamma line data by ORIGEN
  - ORIGEN bins each discrete gamma line within specified group bins
  - Any gamma energy group structure may be defined
  - Binned spectrum can conserve **particles** or **energy**

$$I_{group} = I_{\gamma} \cdot \frac{E_{\gamma}}{E_{avg}}$$

  - If gamma line energy falls near energy bin boundary, particle may be split into both adjacent energy bins

Fine vs. broad-group gamma spectra (^{60}Co Decay)

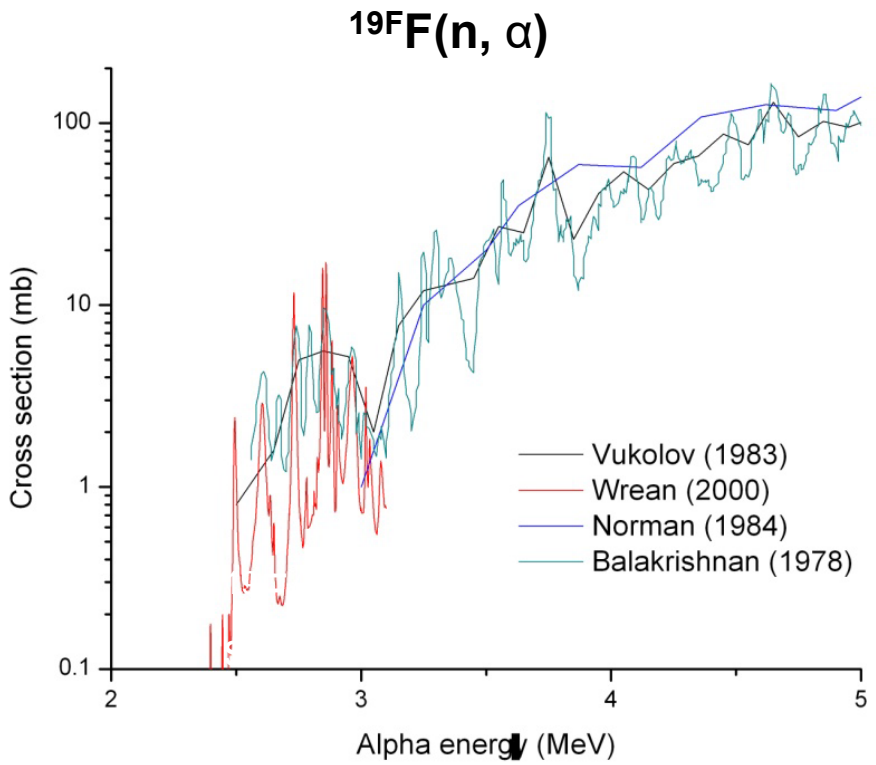


Neutron emission calculation

- Neutron source methods and data adapted from LANL code SOURCES-4C
  - **Spontaneous fission:** Watt fission spectrum parameters for 41 actinides
    - $N(E) = C\, e^{-E/A} \sinh (B\, E)^{1/2}$
    - ν values and SF branching fractions
  - **(alpha,n) neutrons:**
    - 89 alpha-emitting actinides and 7 alpha-emitting fission products
    - 19 light target nuclides: **^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O, ^{19}F, ^{21}Ne, ^{22}Ne, ^{23}Na, ^{25}Mg, ^{26}Mg, ^{27}Al, ^{29}Si, ^{30}Si, ^{31}P, and ^{37}Cl**

Neutron emission resource data

- Following files in **${SCALE}/data/origen_data**:
  - **alphdec.data**: neutron decay library, spontaneous fission nubar and Watt spectrum parameters for 49 actinides, alpha particle energies and intensities, delayed neutron branching fractions and spectra for 105 fission products
  - **stcoeff.data**: a-particle stopping power library
  - **alphaxs.data**: target (a,n) cross section library
  - **alphyld.data**: target (a,n) product level branching library, available for 19 target nuclides



(alpha,n) Neutron emission calculation

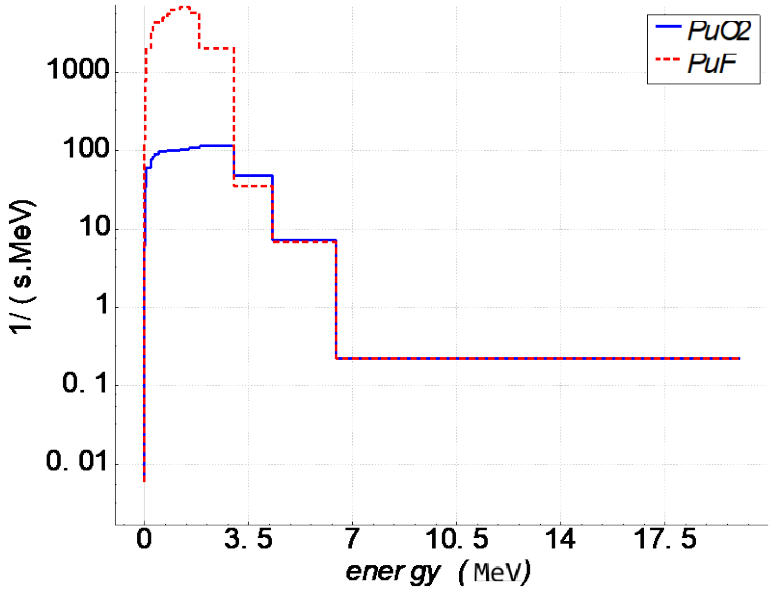
- Neutron yield Y and spectra Y(E) determined for all source α-particle energies E_α and target nuclides (i)

$$Y_i = \frac{N_i}{N} \int_0^{E_\alpha} \frac{\sigma_i(E)}{S(E)} dE$$

  - N = total atomic number density
  - S(E) = atomic stopping power (cm^2/atom) $= -\frac{1}{N}\frac{dE}{dx}$
  - σ(E) = alpha interaction cross section (cm^2)

- Energy spectra calculated assuming emitted (α,n) neutrons are isotropic in CM system
- Slowing down integral solved by divided E_α into discrete energy bins (user specified) to approximate continuous slowing down

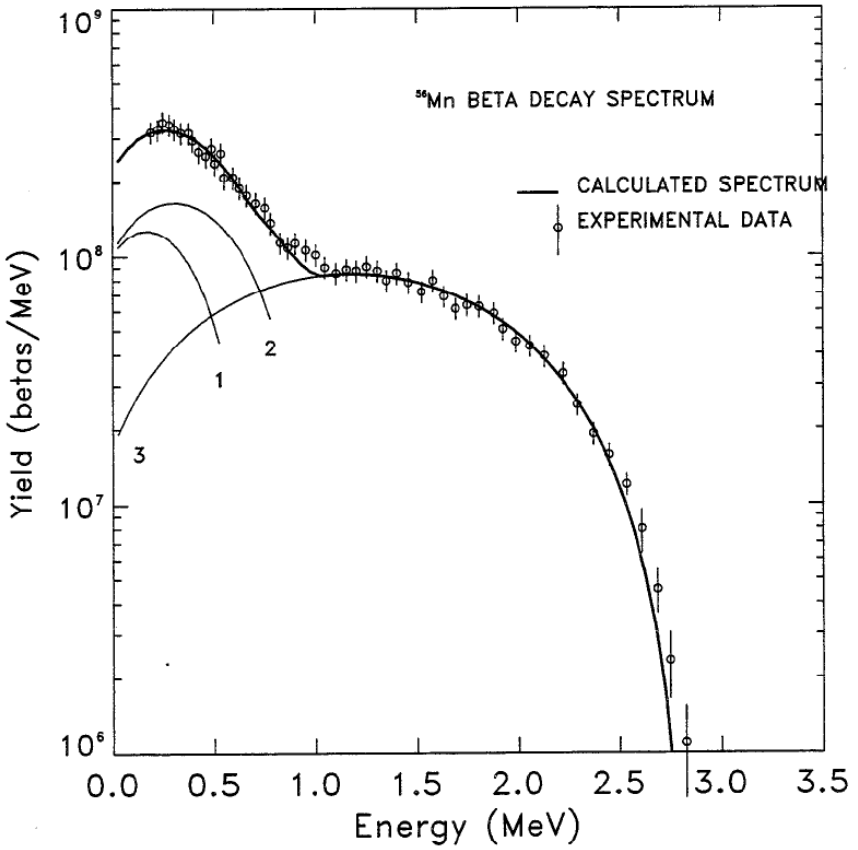
Neutron emission options



- (alpha,n) options available for matrix of
  - UO_2
  - Borosilicate glass
  - Problem-specific (user input) matrix
- Output as yields (n/s) by isotope
- Energy spectra calculated for spontaneous fission, (alpha,n) source, and delayed neutrons
- Any energy group structure may be defined

Beta emission data

- Beta decay data from the Evaluated Nuclear Structure Data File (ENSDF)
  - 715 nuclides and 8486 beta transitions
- Beta emission data in ${SCALE}/**data/origen_data**
  ensdf95beta.data
  - Nuclide ID
  - Branching fractions
  - Maximum beta endpoint energy
  - Transition type
    - 0 = allowed type
    - 1 = First forbidden
    - 2 = Second forbidden
    - 3 = Third forbidden

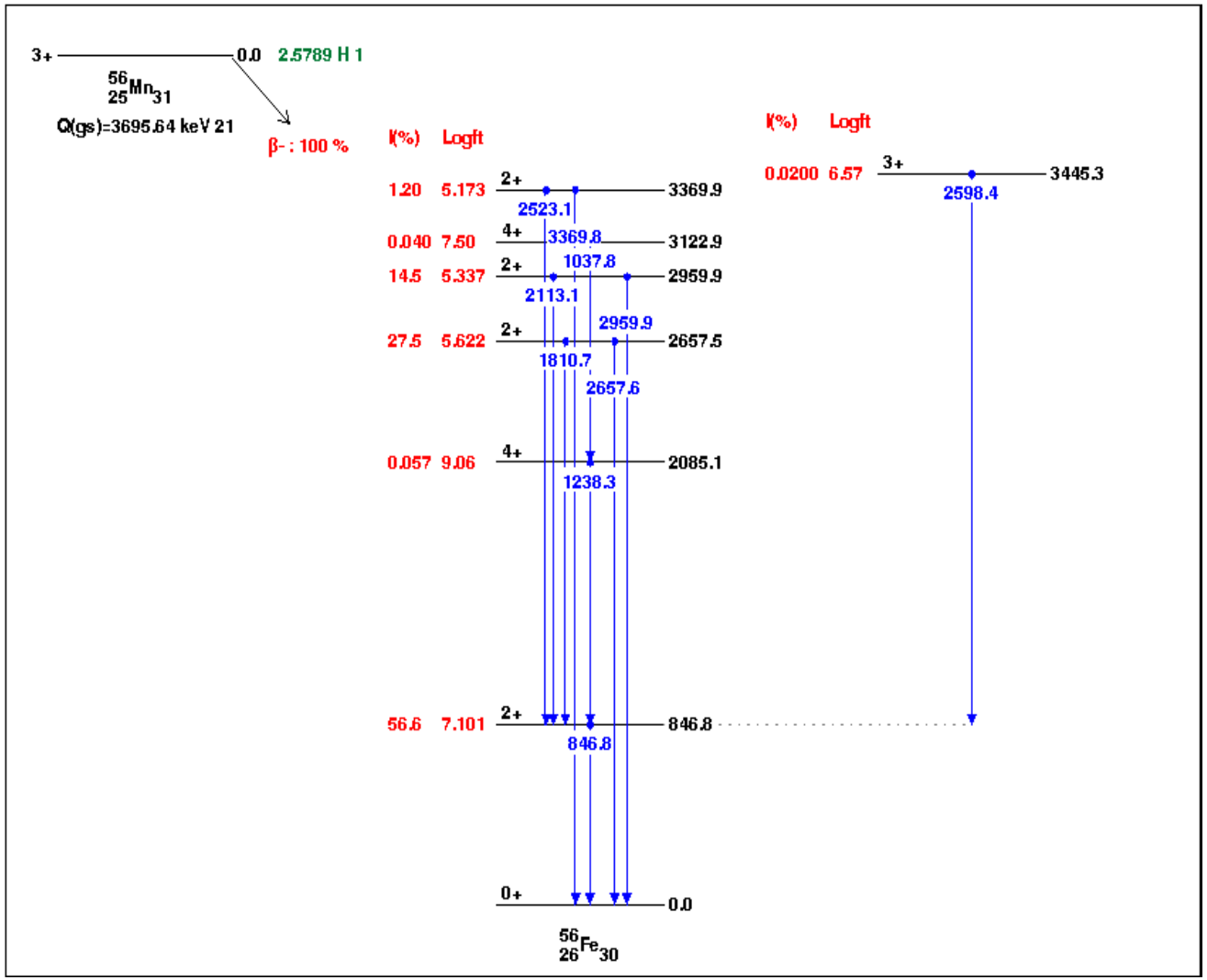


^{56}Mn beta decay calculation

Beta emission calculation

- Beta emission spectrum calculations require:
  - Beta decay branch
  - Branching probability to each excited level of daughter
  - Transition type of each branch based on spin & parity
  - Maximum endpoint beta energy

^{56}Mn beta decay scheme and branching levels



Beta emission calculation

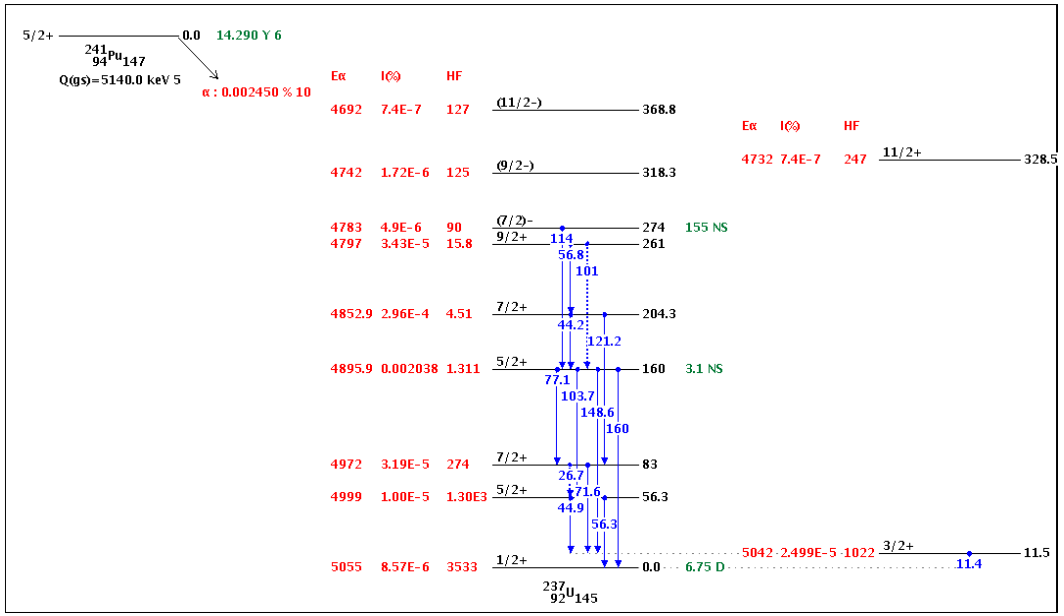
- Beta emission rates and energy spectrum are calculated using analytic expression for the kinetic energy of β- particles
- Based on the Beta-S code (available from RSICC)

$$N(Z,W) = \frac{g^2}{2\pi^3} F(Z,W)\rho\, W(W_0 - W)^2 S_n(W) dW$$

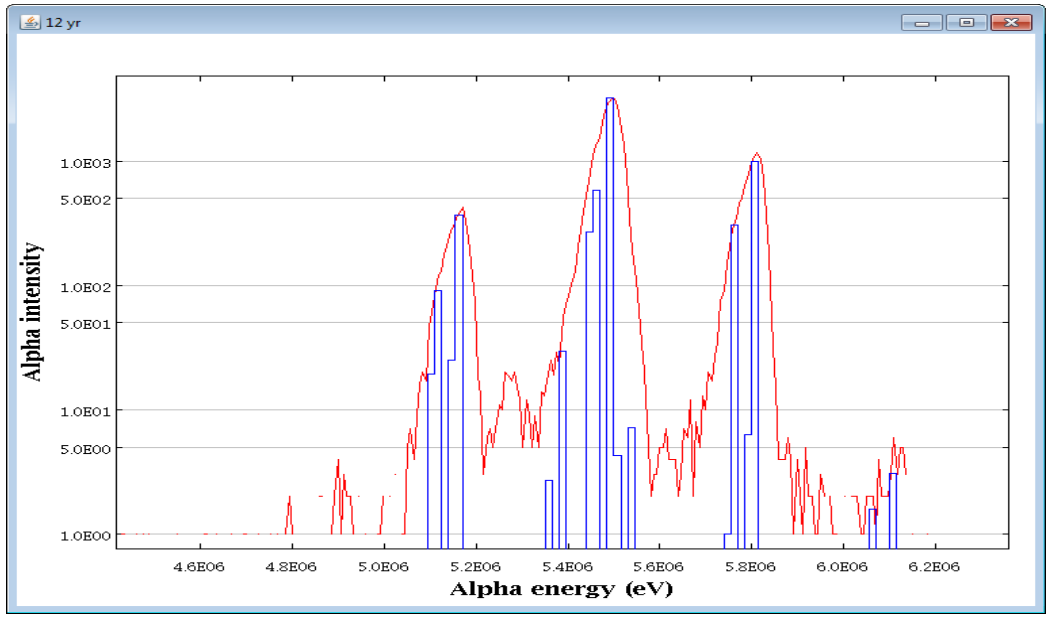
$F(Z,W) =$ Fermi function
$W =$ Kinetic energy ($\mathrm{m_e c^2}$ units)
$W_0 =$ Endpoint beta energy
$\rho = \sqrt{W^2 - 1} =$ momentum
$S_n(W) =$ spectral shape factor based on transition type

Alpha emission data

- Alpha emission rates and energy spectrum can be calculated using the alpha branching fractions and a-particle energies developed for the (a,n) neutron source calculation
- Text file **alphdec.data** has alpha decay data for 85 actinides and contains 607 discrete alpha particle emission energies



^{241}Pu alpha decay scheme



Measured and calculated alpha spectrum (spent fuel)

Summary of sources of ORIGEN nuclear data

Decay data

- ENDF/B-VII.1
- Natural isotopic abundances (NIST database)
- ICRP 72 inhalation dose coefficients, EPA Report 12 external exposure

Neutron reaction cross section data

- JEFF 3.1/A special purpose activation file
- ENDF/B-VII.1, -VIII.0

Fission product yields

- ENDF/B-VII.1

Photon emission line-energy data

- Evaluated Nuclear Structure Data Files (ENSDF)
- ENDF/B-VII.1

Neutron emission libraries

- SOURCES 4C code
- Spontaneous fission decay and delayed neutron data
- Alphas stopping powers, (a,n) cross sections, excitation levels

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Backup



How SCALE & ORIGEN use nuclear data

