

A formula for smoothing GMA results

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There is a consensus that smoothing of the cross sections that are the output of GMA code is needed before the compilation of them into an ENDF format file.

A formula proposed for such a smoothing is:

$$\sigma_i^{smoothed} = \frac{1}{2} \left(\frac{E_{i+1} - E_i}{E_{i+1} - E_{i-1}} \sigma_{i-1} + \sigma_i + \frac{E_i - E_{i-1}}{E_{i+1} - E_{i-1}} \sigma_{i+1} \right).$$

This formula is very similar to that of Pronyaev; just coefficients of σ_{i-1} and σ_{i+1} are exchanged. This corrects a strange behavior of smoothed cross sections for an unequal energy spacing case.

Derivation

A linear-linear interpolation scheme is assumed for computing cross sections at energies in between two adjacent GMA energy grids.

See Figure to understand the derivation.

From the given three pairs of energy and cross section, (E_{i-1}, σ_{i-1}) , (E_i, σ_i) , and (E_{i+1}, σ_{i+1}) ,

1) cross sections at $(E_{i-1} + E_i)/2$ and $(E_i + E_{i+1})/2$:

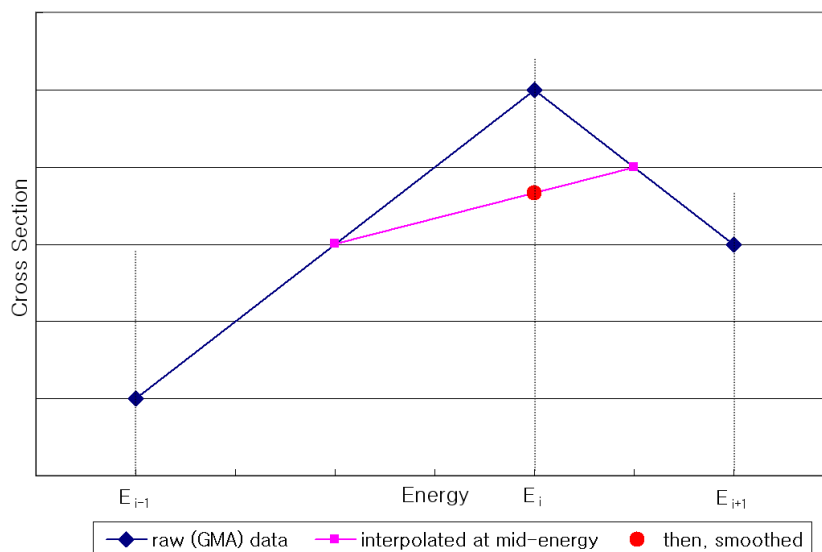
$$\sigma \left(\frac{E_{i-1} + E_i}{2} \right) = \frac{\sigma_{i-1} + \sigma_i}{2} \quad \text{and}$$

$$\sigma \left(\frac{E_i + E_{i+1}}{2} \right) = \frac{\sigma_i + \sigma_{i+1}}{2}.$$

2) From the above two interpolated cross sections, the cross section at E_i is interpolated again as

$$\sigma_i^{smoothed} = \left(\frac{\frac{\sigma_i + \sigma_{i+1}}{2} - \frac{\sigma_{i-1} + \sigma_i}{2}}{\frac{E_i + E_{i+1}}{2} - \frac{E_{i-1} + E_i}{2}} \right) \cdot \left(E_i - \frac{E_{i-1} + E_i}{2} \right) + \left(\frac{\sigma_{i-1} + \sigma_i}{2} \right)$$

i.e., interpolated = slope \times delta E + intercept



Covariance of smoothed cross sections

Applying the conventional law of error propagation, we obtain the covariance of smoothed cross sections at energy i and j such that:

$$V_{i,j}^{smoothed} = \frac{1}{4} \begin{pmatrix} C_{i,i-1} & C_{i,i} & C_{i,i+1} \end{pmatrix} \begin{pmatrix} V_{i-1,j-1} & V_{i,j-1} & V_{i+1,j-1} \\ V_{i-1,j} & V_{i,j} & V_{i+1,j} \\ V_{i-1,j+1} & V_{i,j+1} & V_{i+1,j+1} \end{pmatrix} \begin{pmatrix} C_{j,j-1} \\ C_{j,j} \\ C_{j,j+1} \end{pmatrix},$$

where

$$C_{i,i-1} = \frac{E_{i+1} - E_i}{E_{i+1} - E_{i-1}}, \quad C_{i,i} = 1, \quad \text{and} \quad C_{i,i+1} = \frac{E_i - E_{i-1}}{E_{i+1} - E_{i-1}}.$$

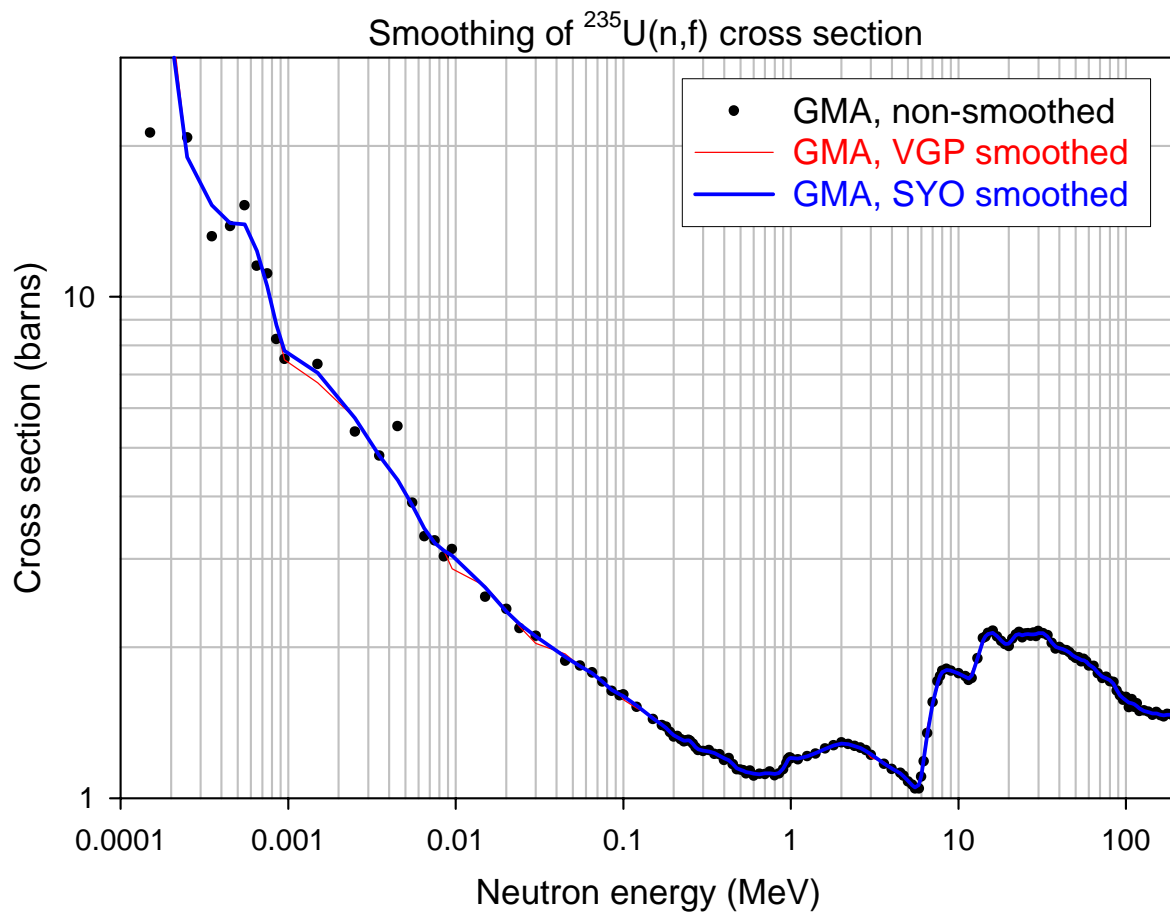


Fig.1.

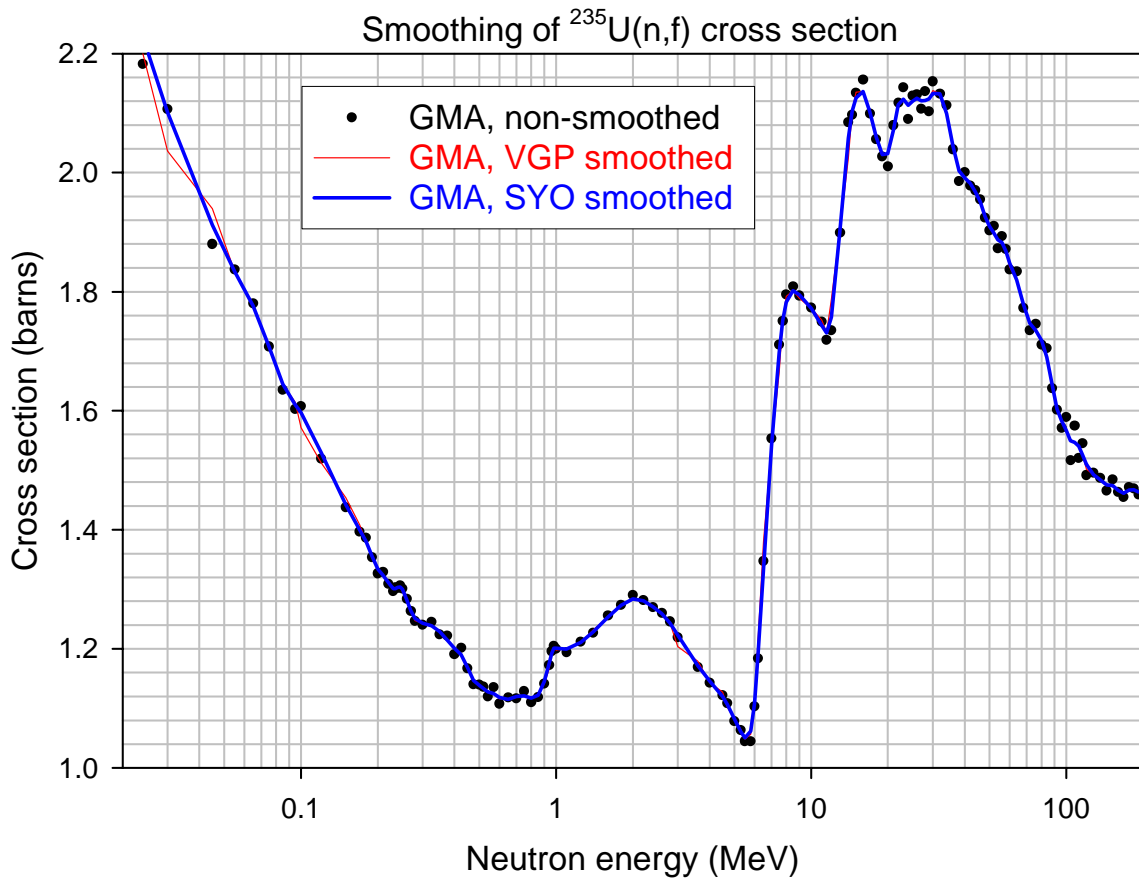


Fig. 2.

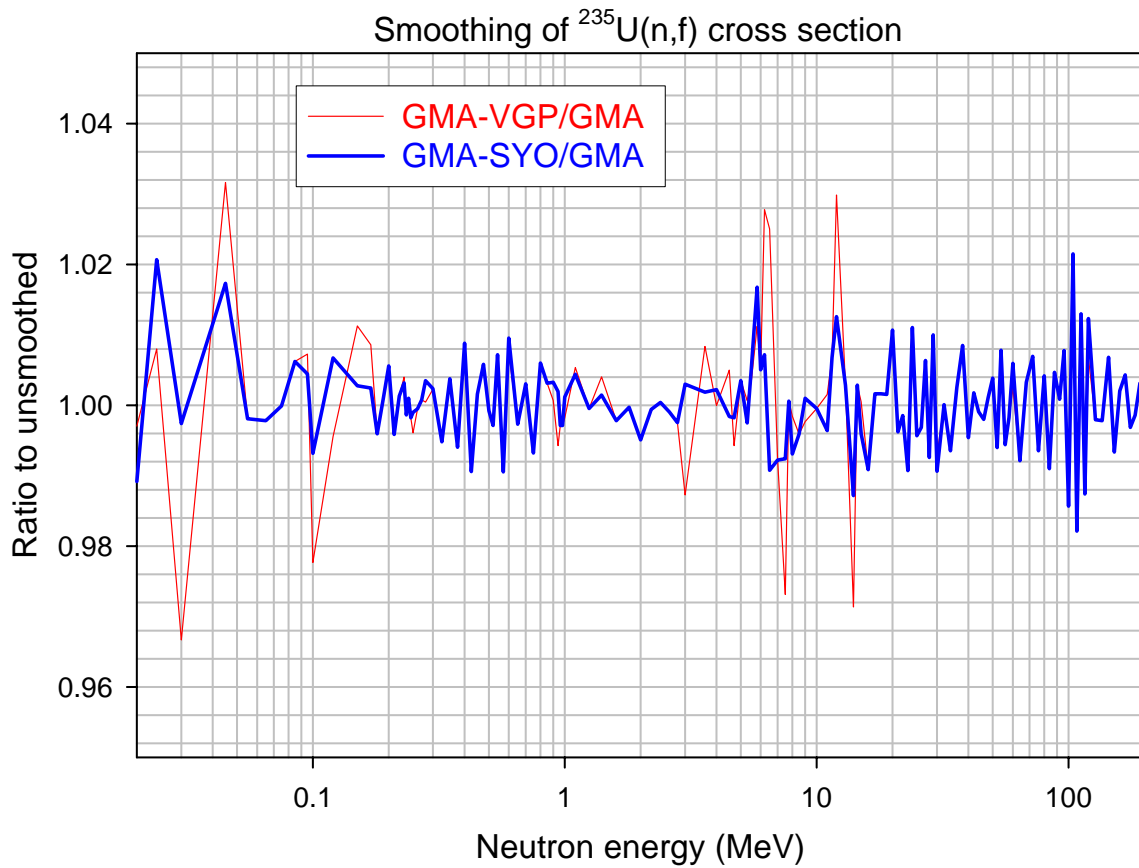


Fig. 3.

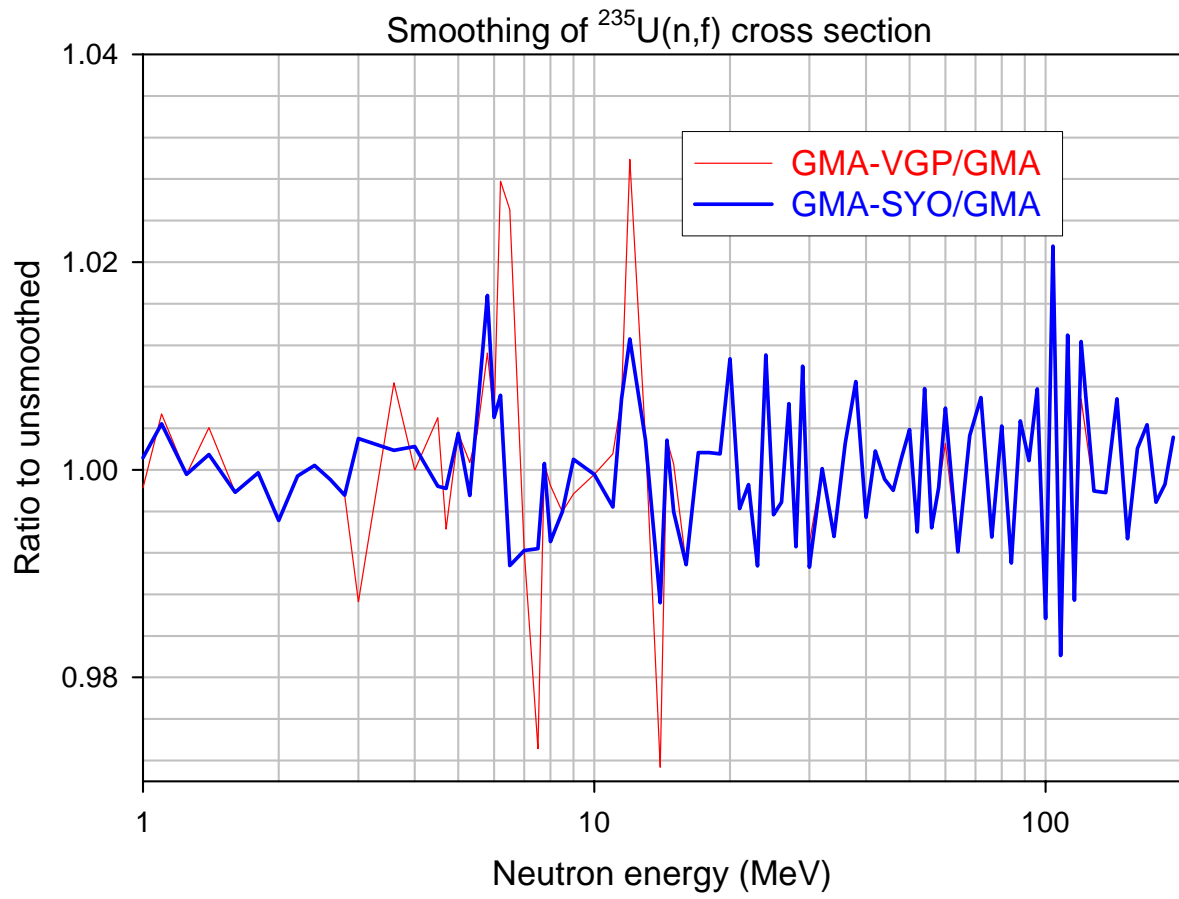


Fig. 4.