



**Nuclear  
and  
INdustrial  
EEngineering**

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## **Uncertainty quantification using SCALE 6.2 package and GPT techniques implemented in Serpent 2**

Giorgio BAIocco

Alessandro PETRUZZI

Marco CHERUBINI

- Introduction
- Codes and methods
- Test cases
- Results
  - UAM Exercise I-1
    - ✓  $k_{\text{eff}}$  sensitivity and uncertainty
    - ✓ 1 group homogenized XS sensitivity and uncertainty
- Conclusions and future work

- The main objective is to test Monte Carlo code **SERPENT-2 in S/U analysis**
- The program is tested on exercises I-1 of UAM benchmark
  - TMI fuel pin HZP
- Several cross sections (i.e. elastic & inelastic scattering, fission, capture etc.) of several isotopes (i.e.  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{16}\text{O}$  and  $^1\text{H}$ ) are perturbed
- 2 different cross section covariance libraries are used
  - 44 groups from SCALE 6.1
  - 56 groups from SCALE 6.2
- Uncertainty is assessed over different responses
  - $k_{\text{eff}}$
  - 1 group  $\sigma_{\text{capt}}$ ,  $\sigma_{\text{fiss}}$ ,  $\Sigma_{\text{capt}}$  and  $\Sigma_{\text{fiss}}$
- Results are compared with SCALE/TSUNAMI-1D

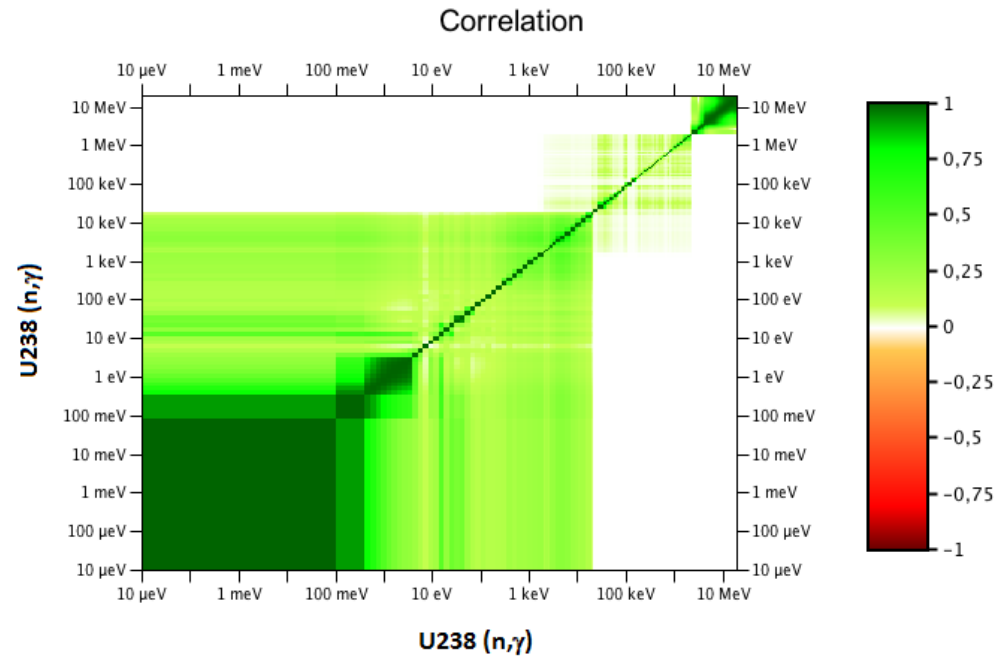
- The effect of a perturbation of a parameter  $x$  on the response  $R$  is:

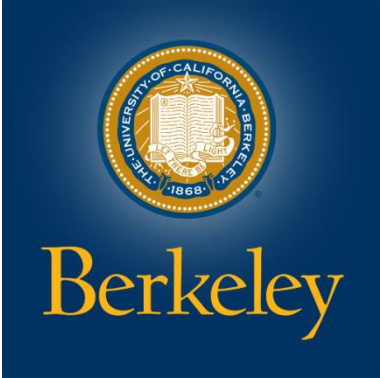
$$S_{R,x} = \frac{dR/R}{dx/x}$$

- Uncertainty can be calculated using the **sandwich rule**:

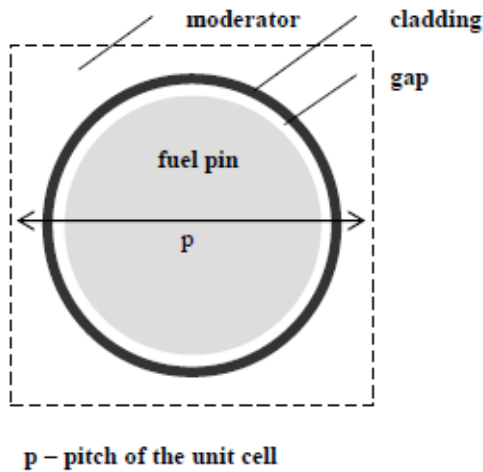
$$Var[R] = S_{R,x} Cov[x] (S_{R,x})^T$$

$$\sigma[R] = \sqrt{Var[R]}$$



- SERPENT-2 is a 3D continuous-energy Monte Carlo code for reactor physics calculation
  - In this work a modified version of SERPENT-2 (provided by UC Berkeley), with implemented GPT is used to calculate sensitivity coefficients of different response functions (i.e.  $k_{\text{eff}}$ , homogenized microscopic and macroscopic cross sections) related to the perturbation of input cross sections.
- 
- Details about this program can be found in → *M. Aufiero et al. “A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT”*
  - 2 different cross section covariance libraries are used for uncertainty quantification:
    - 44 groups from SCALE 6.1
    - 56 groups from SCALE 6.2

- Considered case
  - TMI pin at HZP

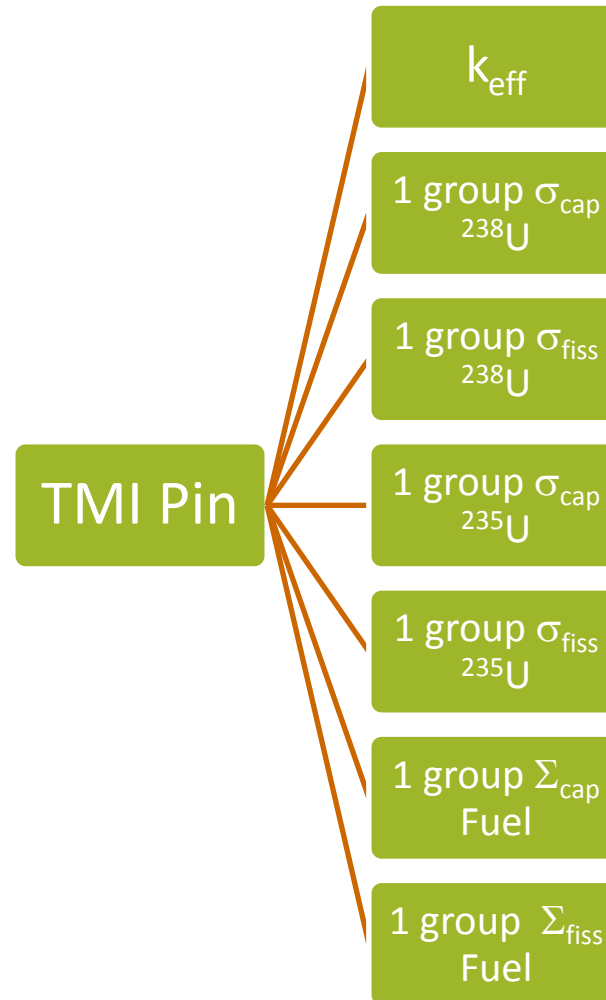


| Parameter                              | Value            |
|--|------------------|
| Unit cell pitch, [mm]                  | 14.427           |
| Fuel pellet diameter, [mm]             | 9.391            |
| Fuel pellet material                   | UO <sub>2</sub>  |
| Fuel density, [g/cm <sup>3</sup> ]     | 10.283           |
| Fuel enrichment, w/o                   | 4.85             |
| Cladding outside diameter, [mm]        | 10.928           |
| Cladding thickness, [mm]               | 0.673            |
| Cladding material                      | Zircaloy-4       |
| Cladding density, [g/cm <sup>3</sup> ] | 6.55             |
| Gap material                           | He               |
| Moderator material                     | H <sub>2</sub> O |

| Parameter / Reactor condition                     | HZP   | HFP   |
|---|-------|-------|
| Fuel temperature, [K]                             | 551   | 900   |
| Cladding temperature, [K]                         | 551   | 600   |
| Moderator (coolant) temperature, [K]              | 551   | 562   |
| Moderator (coolant) density, [kg/m <sup>3</sup> ] | 766   | 748.4 |
| Reactor power, [MWt]                              | 2.772 | 2.772 |

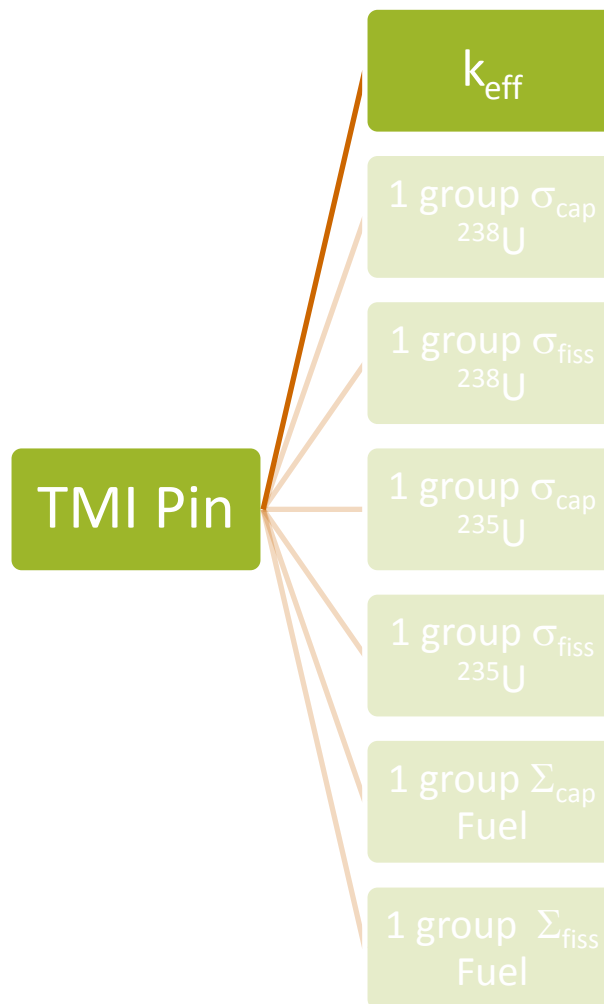
- Isotopes considered in uncertainty quantification
  - U-238
  - U-235
  - O-16
  - H-1
- Perturbed cross sections
  - (n, elastic)
  - (n, n')
  - (n, fission)
  - (n,  $\gamma$ )
  - nu-bar
  - chi-bar

## Uncertainty quantification

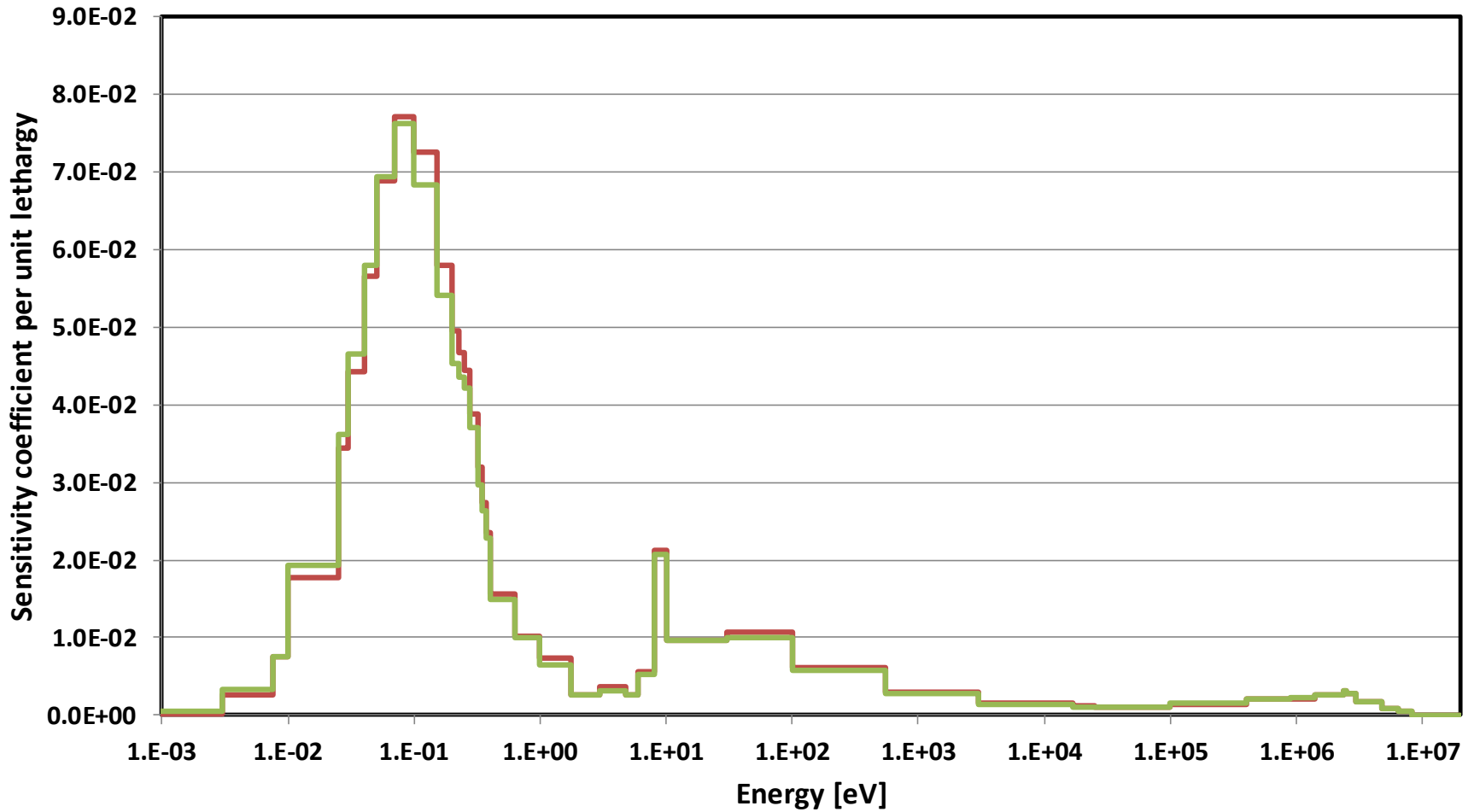




## Uncertainty quantification

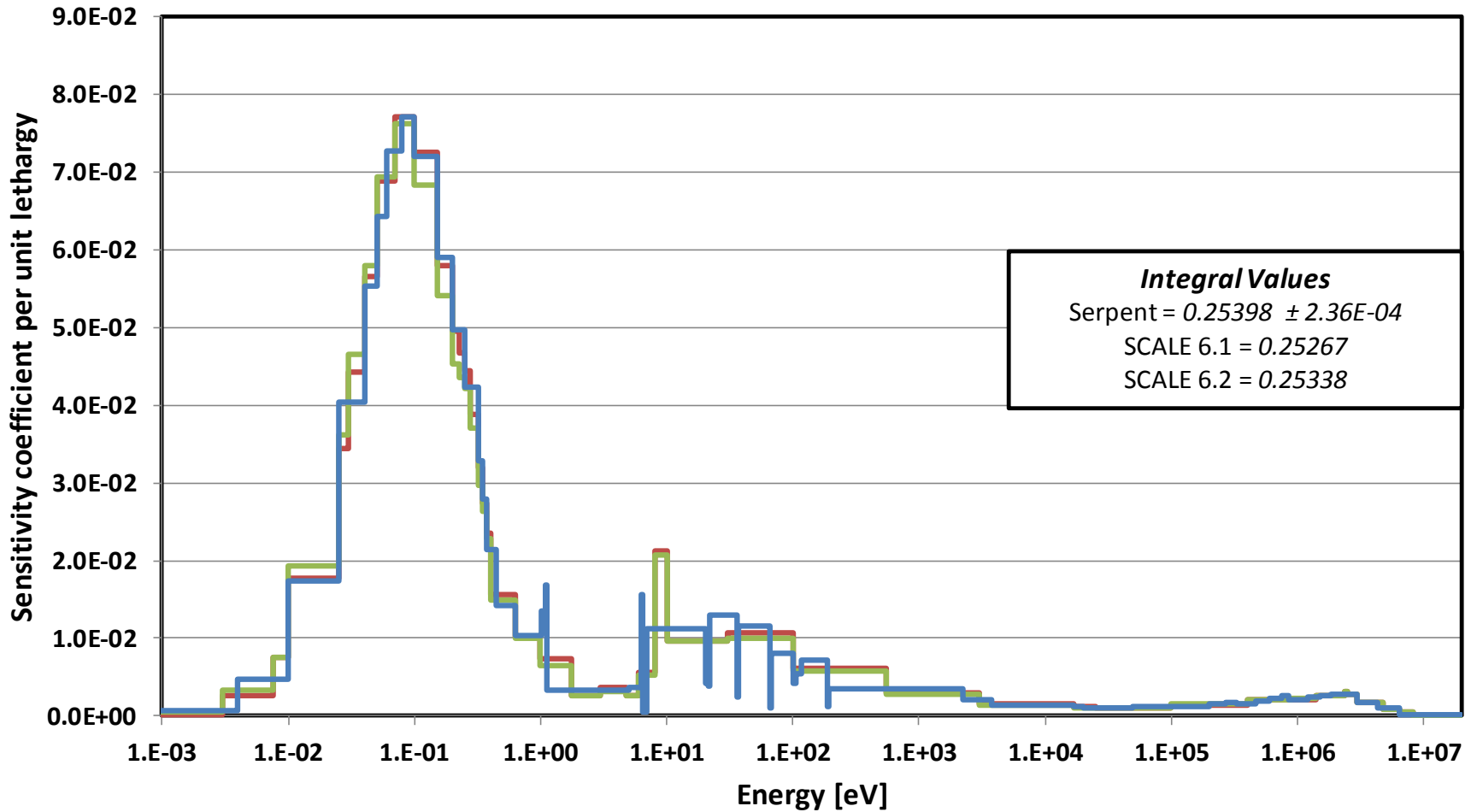


## TMI Pin - $k_{\text{eff}}$ - $^{235}\text{U}$ (n,fission)



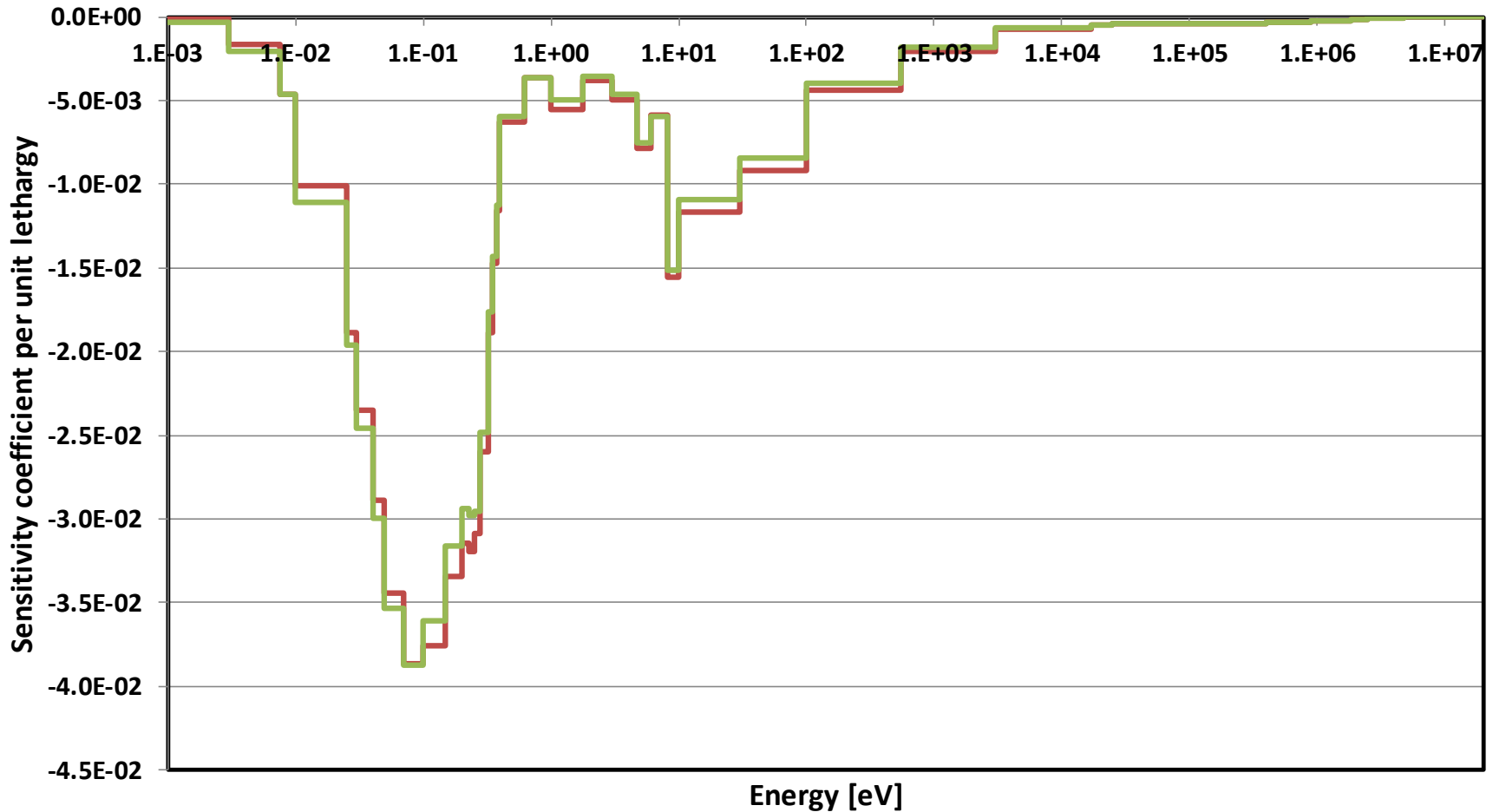
— SERPENT 44 groups    — SCALE 6.1 - 44 groups

## TMI Pin - $k_{\text{eff}}$ - $^{235}\text{U}$ (n,fission)



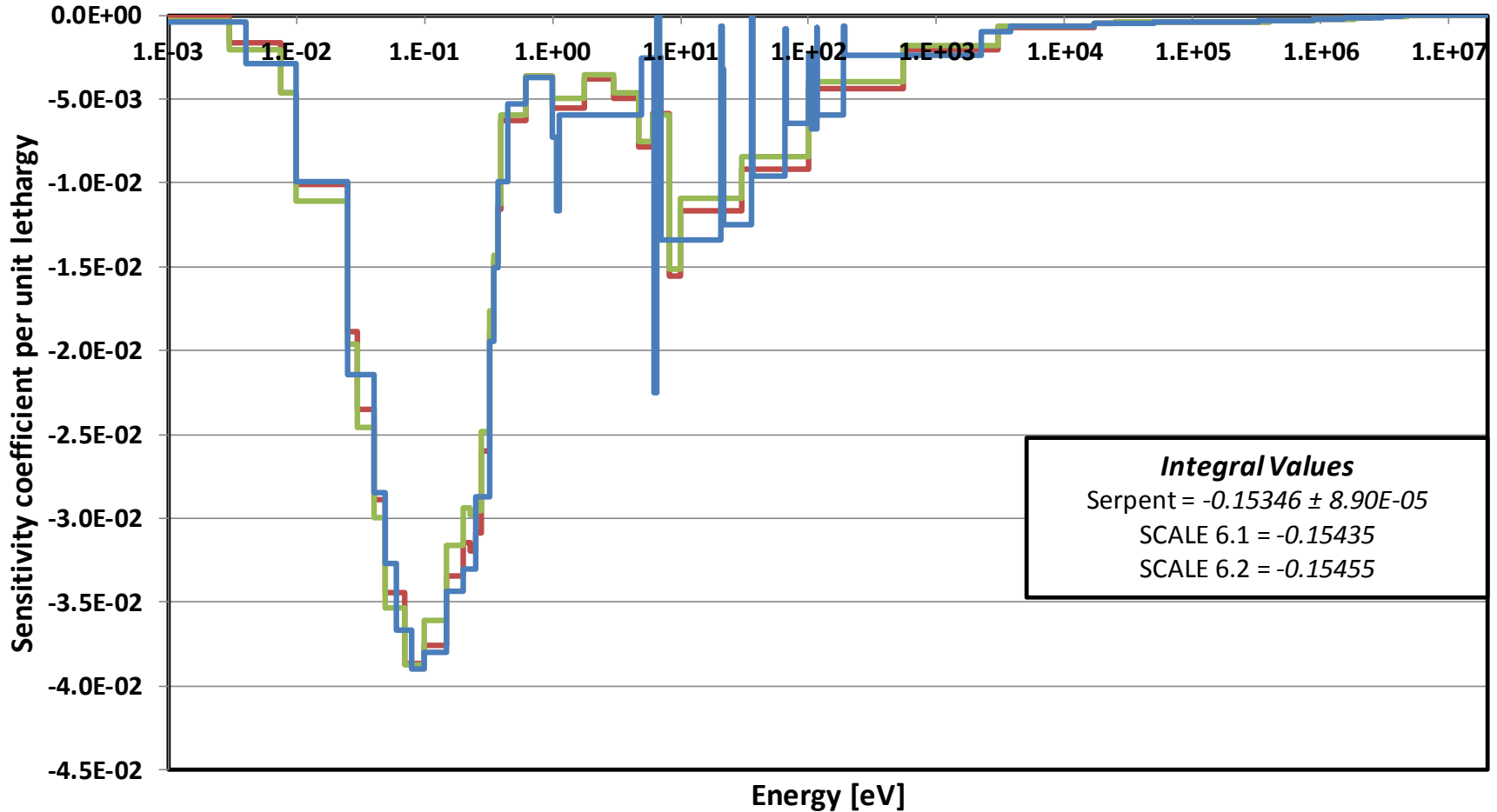
— SERPENT 44 groups    — SCALE 6.1 - 44 groups    — SCALE 6.2 - 56 groups

## TMI Pin - $k_{\text{eff}}$ - $^{235}\text{U}$ (n, $\gamma$ )



— SERPENT 44 groups    — SCALE 6.1 - 44 groups

## TMI Pin - $k_{\text{eff}}$ - $^{235}\text{U}$ (n, $\gamma$ )

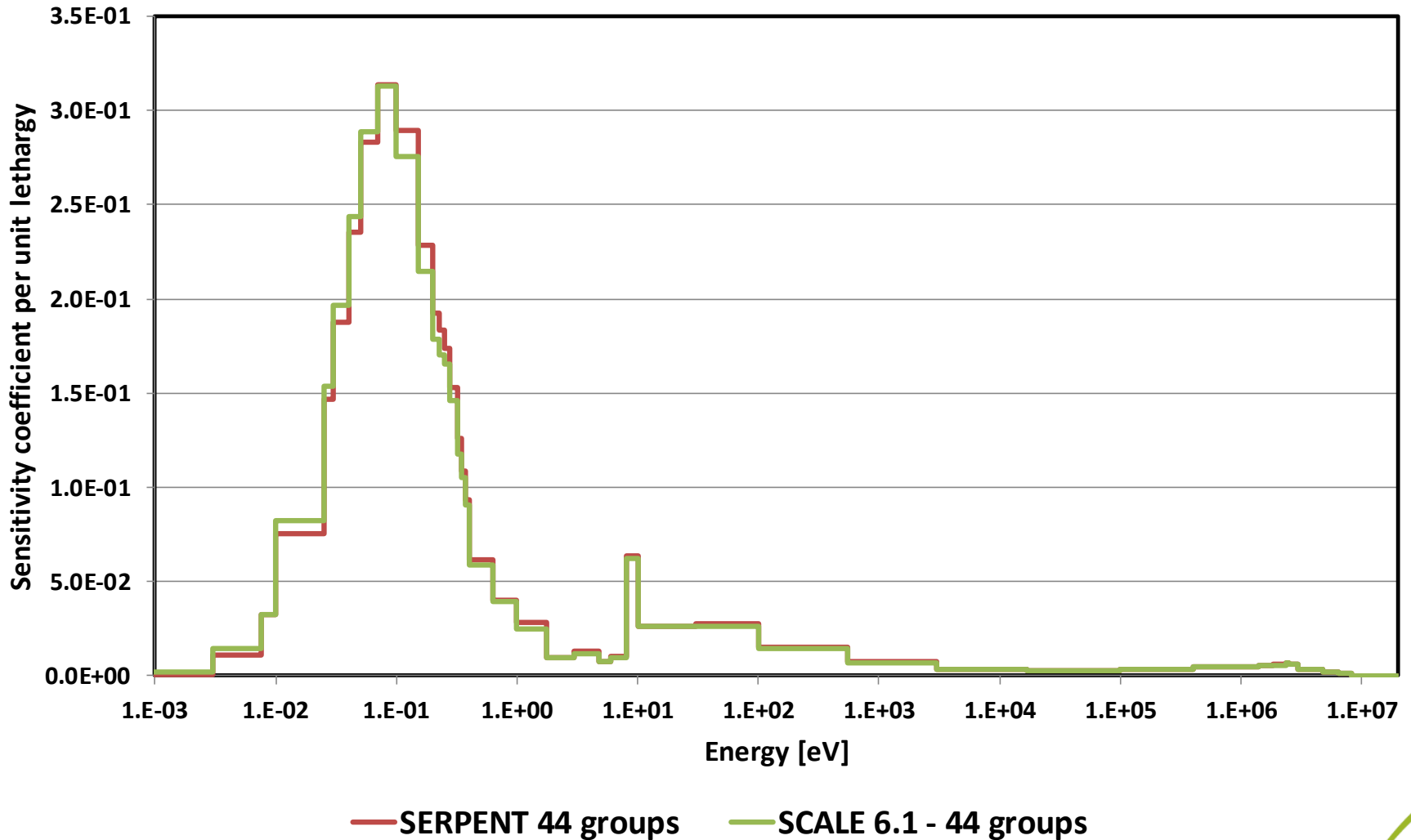


— SERPENT 44 groups

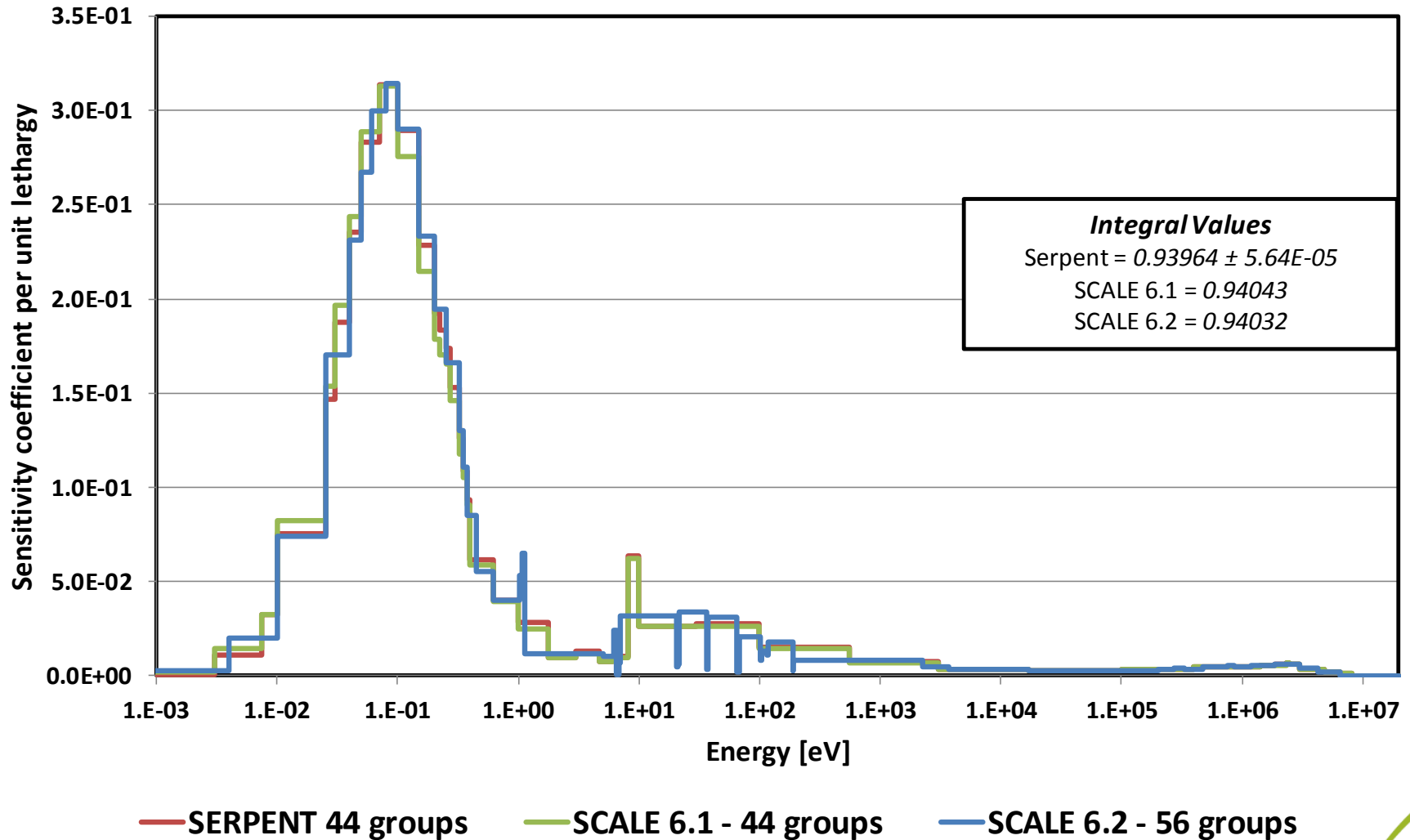
— SCALE 6.1 - 44 groups

— SCALE 6.2 - 56 groups

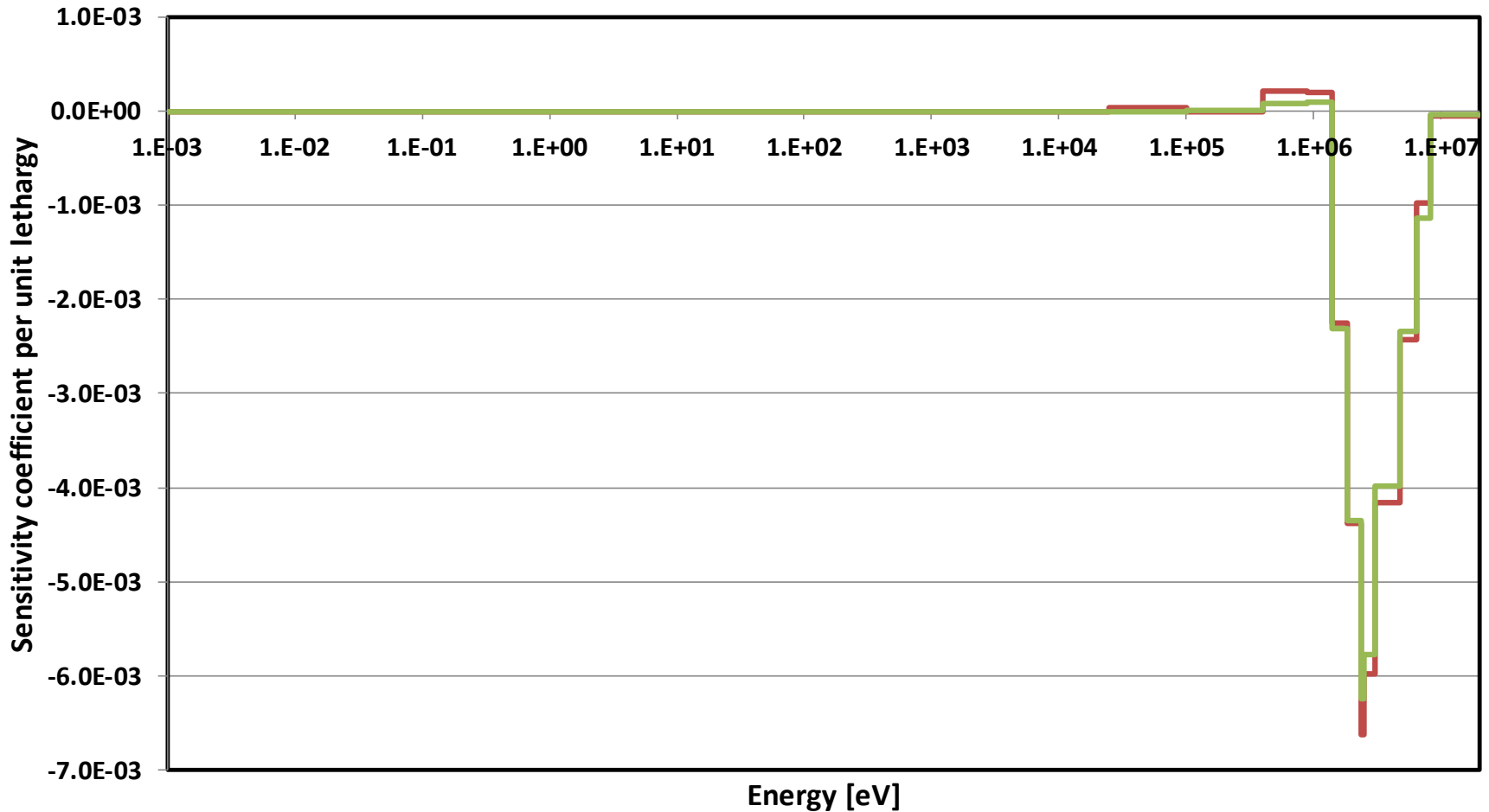
## TMI Pin - $k_{\text{eff}}$ - $^{235}\text{U}$ nubar



## TMI Pin - $k_{\text{eff}}$ - $^{235}\text{U}$ nubar



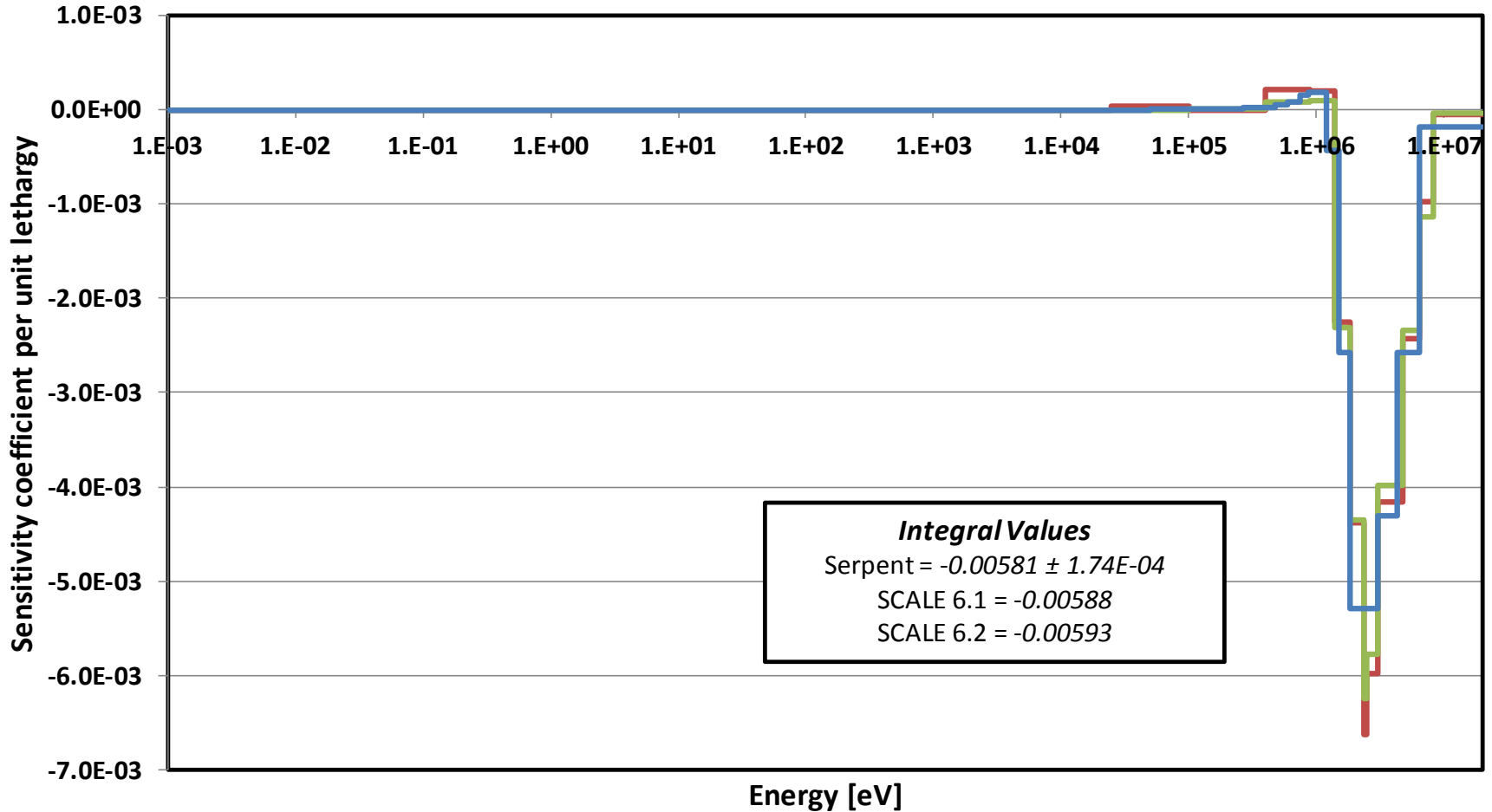
## TMI Pin - $k_{\text{eff}}$ - $^{238}\text{U}$ (n,n')



— SERPENT 44 groups    — SCALE 6.1 - 44 groups



## TMI Pin - $k_{\text{eff}}$ - $^{238}\text{U}$ (n,n')

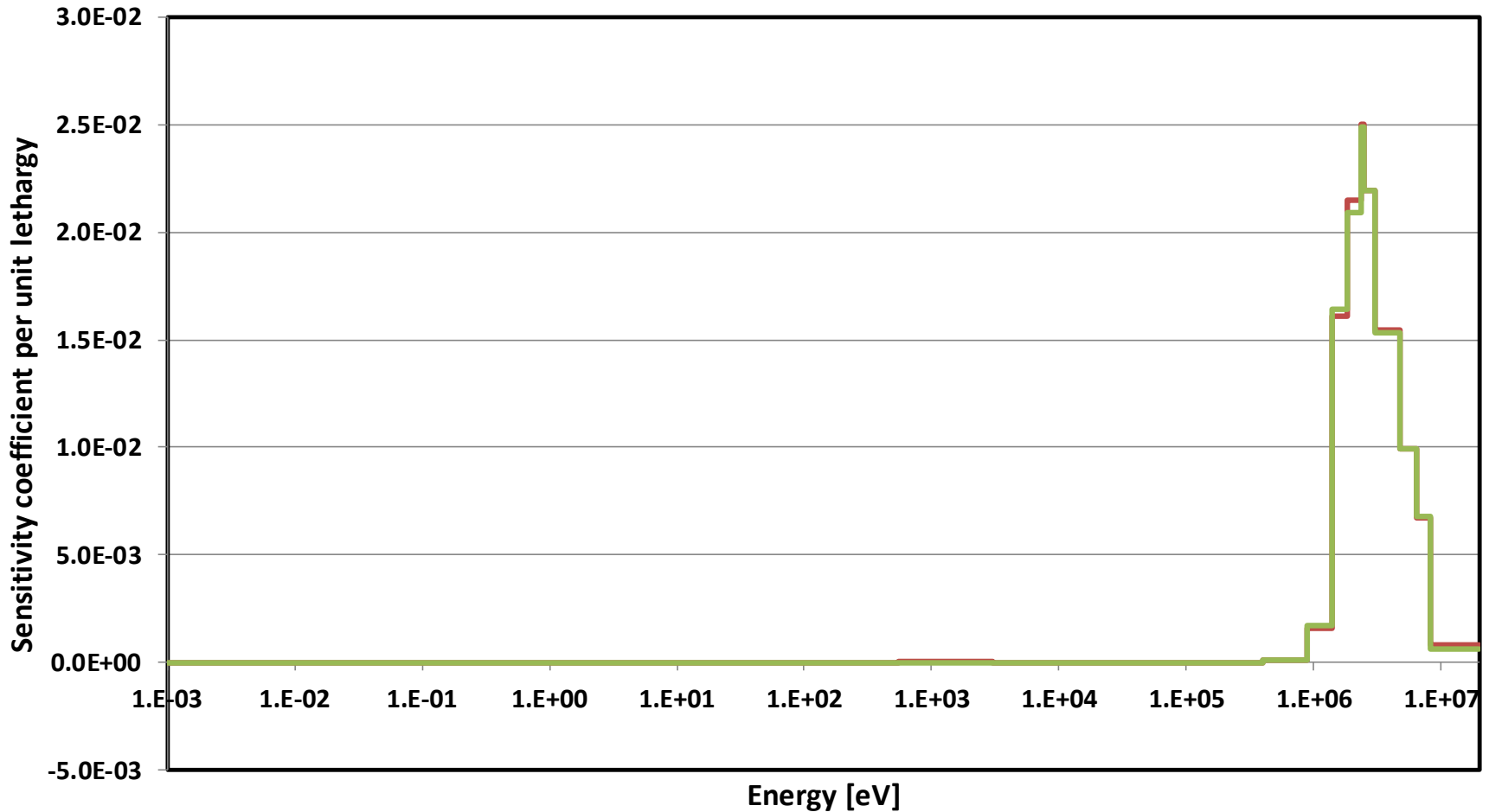


— SERPENT 44 groups

— SCALE 6.1 - 44 groups

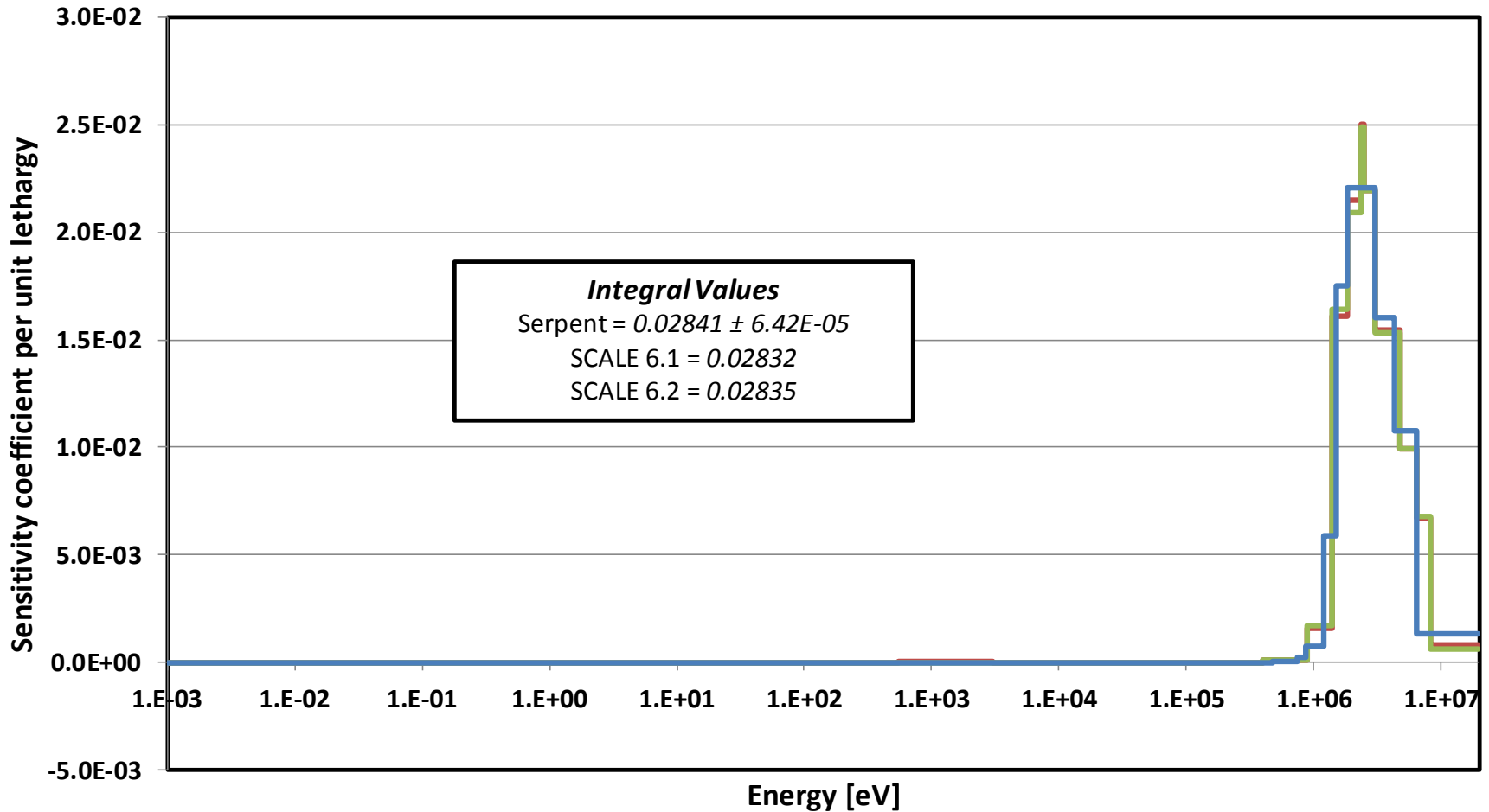
— SCALE 6.2 - 56 groups

## TMI Pin - $k_{\text{eff}}$ - $^{238}\text{U}$ (n,fission)



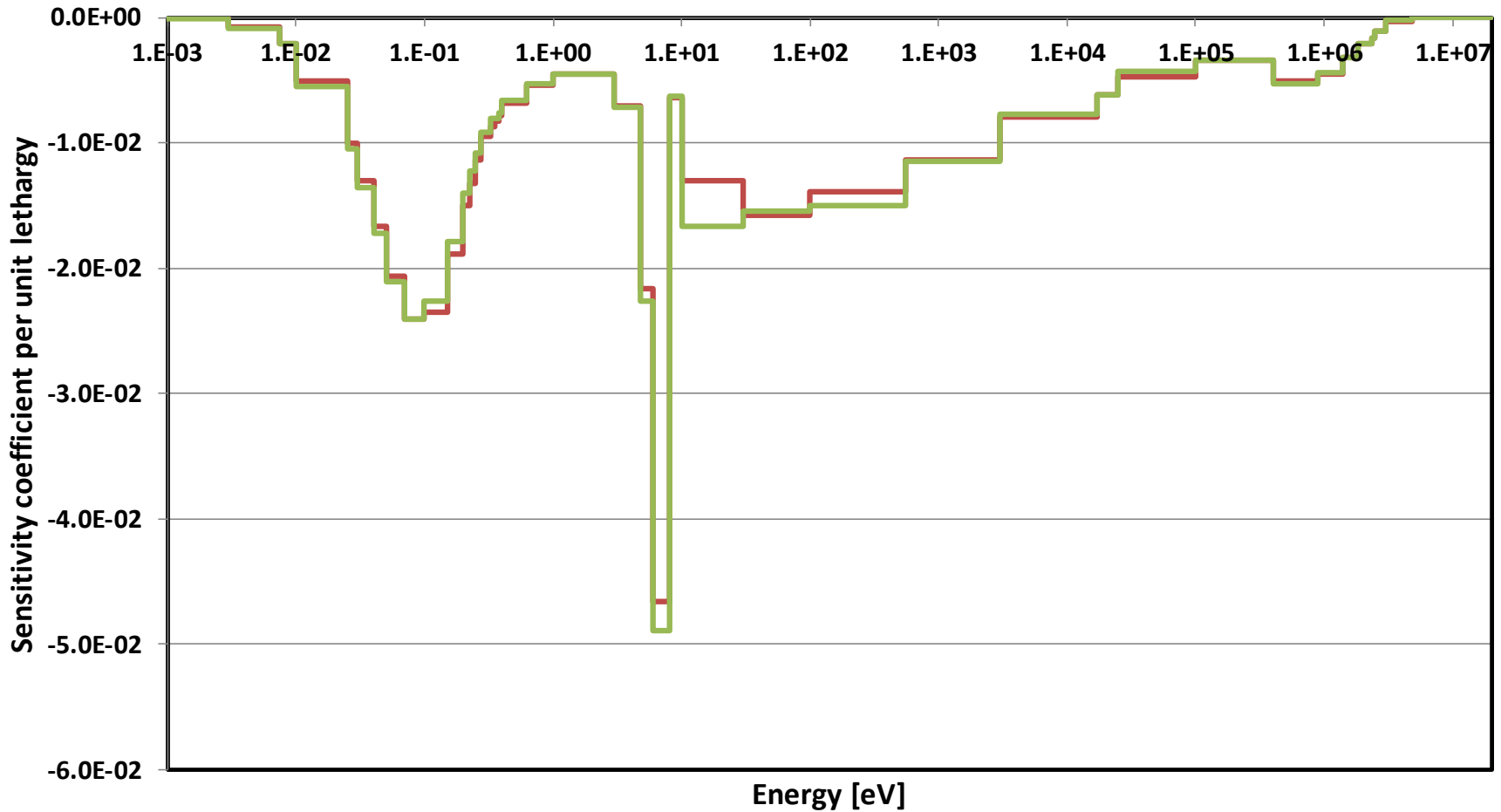
— SERPENT 44 groups    — SCALE 6.1 - 44 groups

## TMI Pin - $k_{\text{eff}}$ - $^{238}\text{U}$ (n,fission)



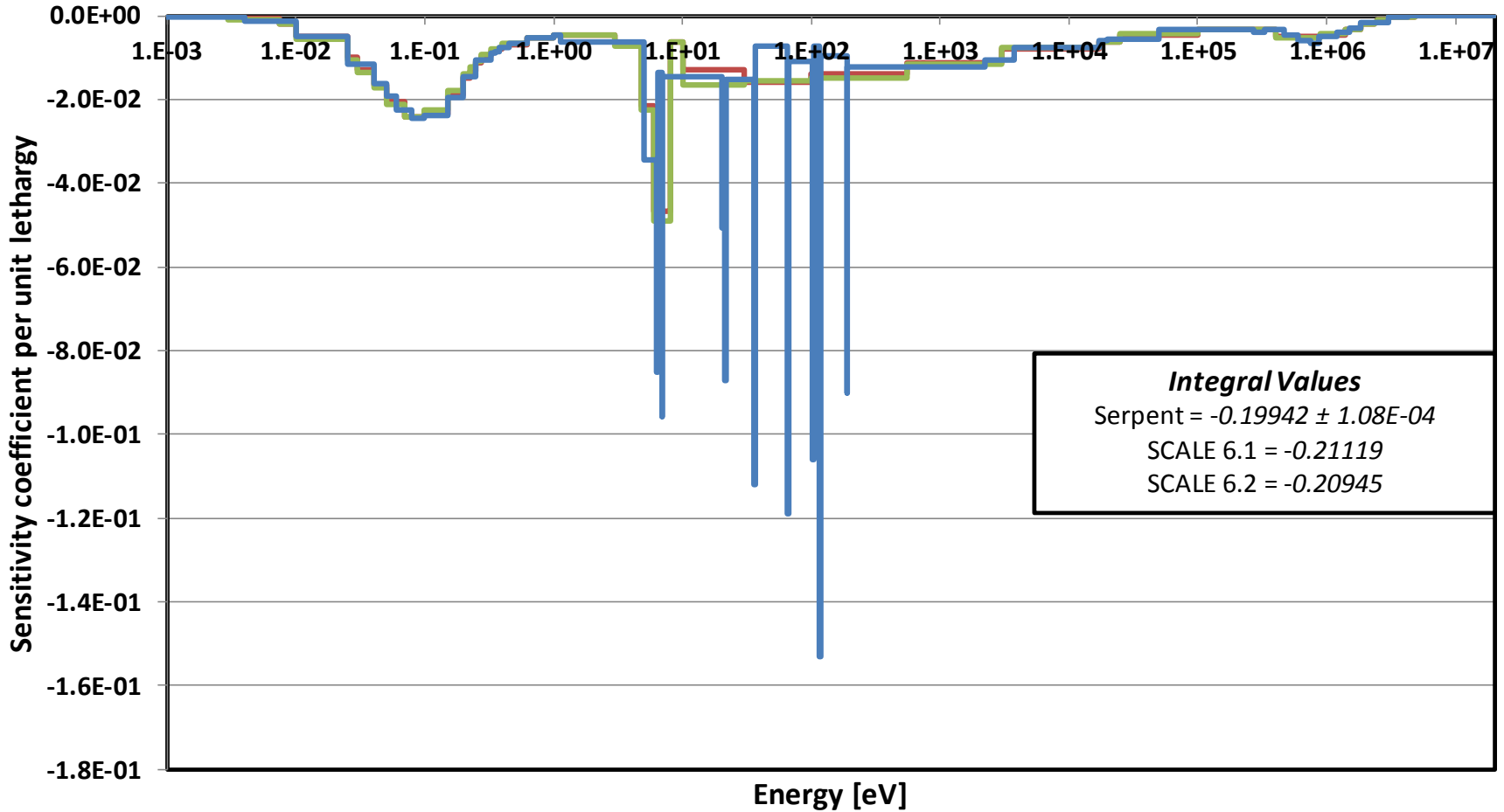
— SERPENT 44 groups    — SCALE 6.1 - 44 groups    — SCALE 6.2 - 56 groups

## TMI Pin - $k_{\text{eff}}$ - $^{238}\text{U}$ (n, $\gamma$ )



— SERPENT 44 groups    — SCALE 6.1 - 44 groups

## TMI Pin - $k_{\text{eff}}$ - $^{238}\text{U}$ (n, $\gamma$ )



— SERPENT 44 groups

— SCALE 6.1 - 44 groups

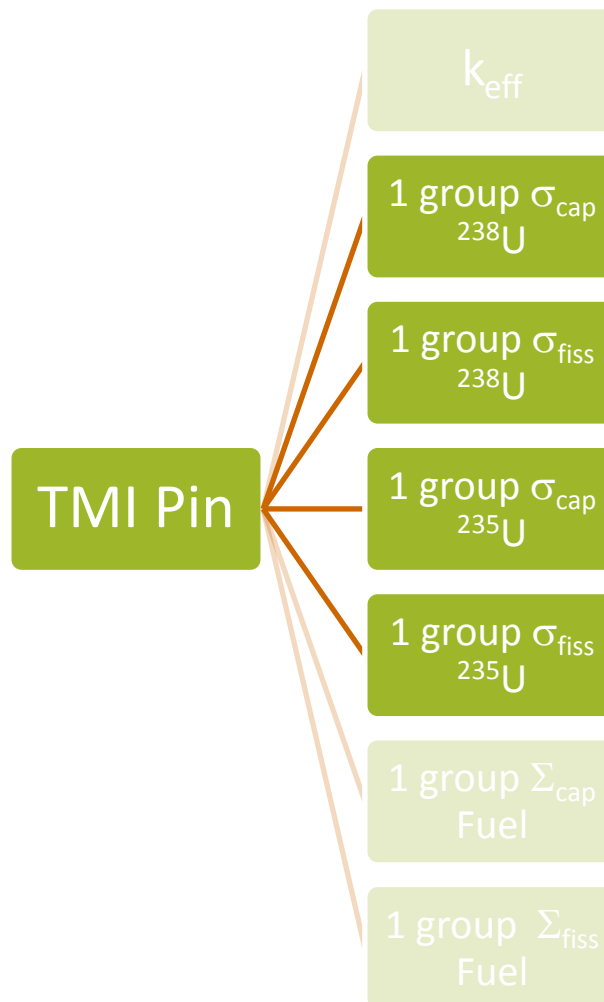
— SCALE 6.2 - 56 groups

## Uncertainty quantification – TMI Pin - $k_{\text{eff}}$

|                                 |                                 | SERPENT 44 groups   | SCALE 6.1 44 groups   | SCALE 6.2 56 groups   |
|---------------------------------|---------------------------------|---|---|---|
| <i>Covariance Matrix</i>        |                                 | <i>Relative standard deviation in <math>k_{\text{eff}}</math> (pcm)</i> | <i>Relative standard deviation in <math>k_{\text{eff}}</math> (pcm)</i> | <i>Relative standard deviation in <math>k_{\text{eff}}</math> (pcm)</i> |
| $^{235}\text{U}$ nubar          | $^{235}\text{U}$ nubar          | 264.63  | 264.78  | 341.22  |
| $^{238}\text{U}$ (n, $\gamma$ ) | $^{238}\text{U}$ (n, $\gamma$ ) | 253.32  | 269.32  | 275.11  |
| $^{235}\text{U}$ (n, $\gamma$ ) | $^{235}\text{U}$ (n, $\gamma$ ) | 208.99  | 210.53  | 196.52  |
| $^{238}\text{U}$ (n,n')         | $^{238}\text{U}$ (n,n')         | 114.25  | 113.08  | 113.60  |
| $^{235}\text{U}$ $\chi$         | $^{235}\text{U}$ $\chi$         | 93.73   | 92.72   | 152.32  |
| $^{235}\text{U}$ (n,fiss)       | $^{235}\text{U}$ (n,fiss)       | 76.86   | 76.26   | 76.65   |
| $^{238}\text{U}$ nubar          | $^{238}\text{U}$ nubar          | 70.47   | 69.66   | 70.41   |
| $^1\text{H}$ (n,el)             | $^1\text{H}$ (n,el)             | 23.97   | 24.90   | 16.15   |

| SERPENT 44 groups          |                | SCALE 6.1 44 groups |                | SCALE 6.2 56 groups |                |
|----------------------------|----------------|---------------------|----------------|---------------------|----------------|
| $k_{\text{eff}}$           | % $\Delta k/k$ | $k_{\text{eff}}$    | % $\Delta k/k$ | $k_{\text{eff}}$    | % $\Delta k/k$ |
| $1.43018 \pm 4\text{E-}05$ | 0.467%         | 1.42394             | 0.483%         | 1.42441             | 0.542%         |

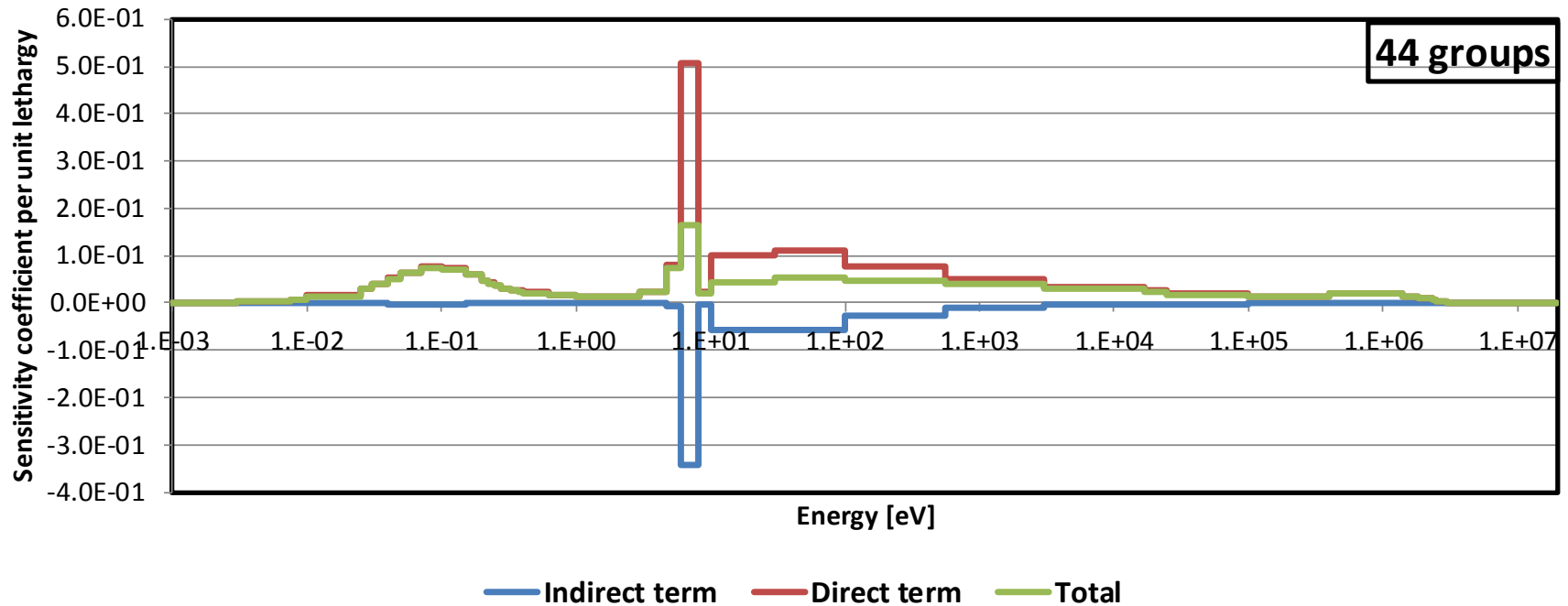
## Uncertainty quantification



## Direct and indirect effects

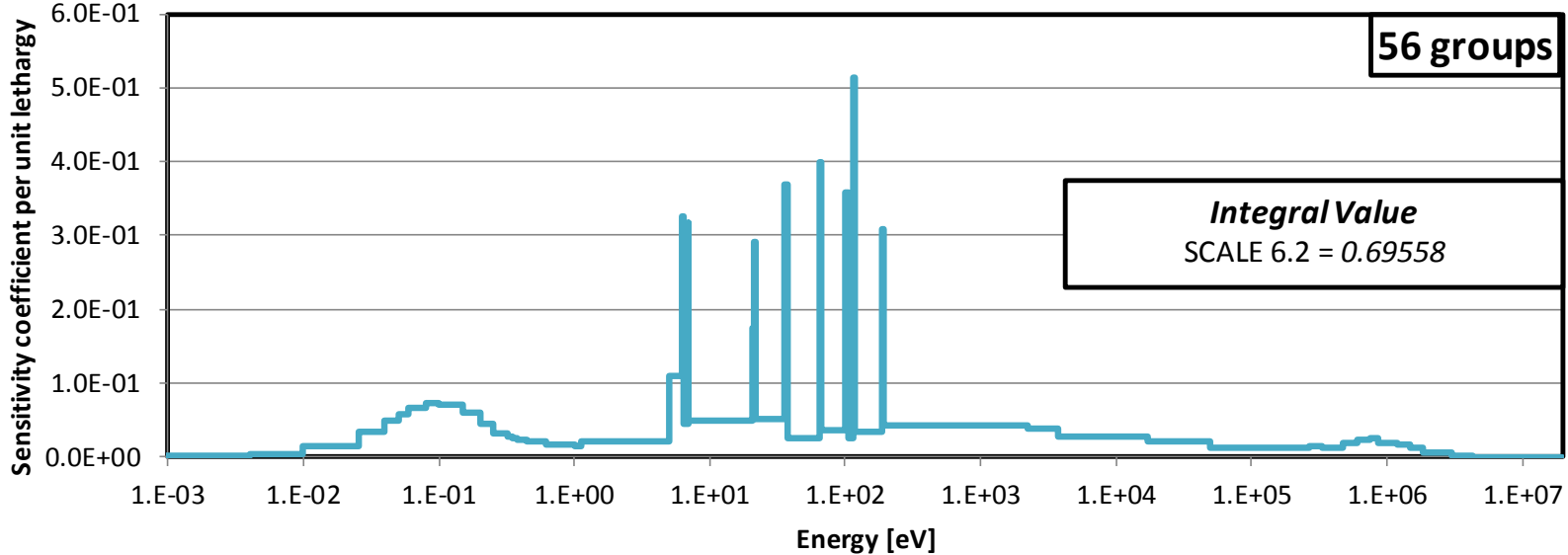
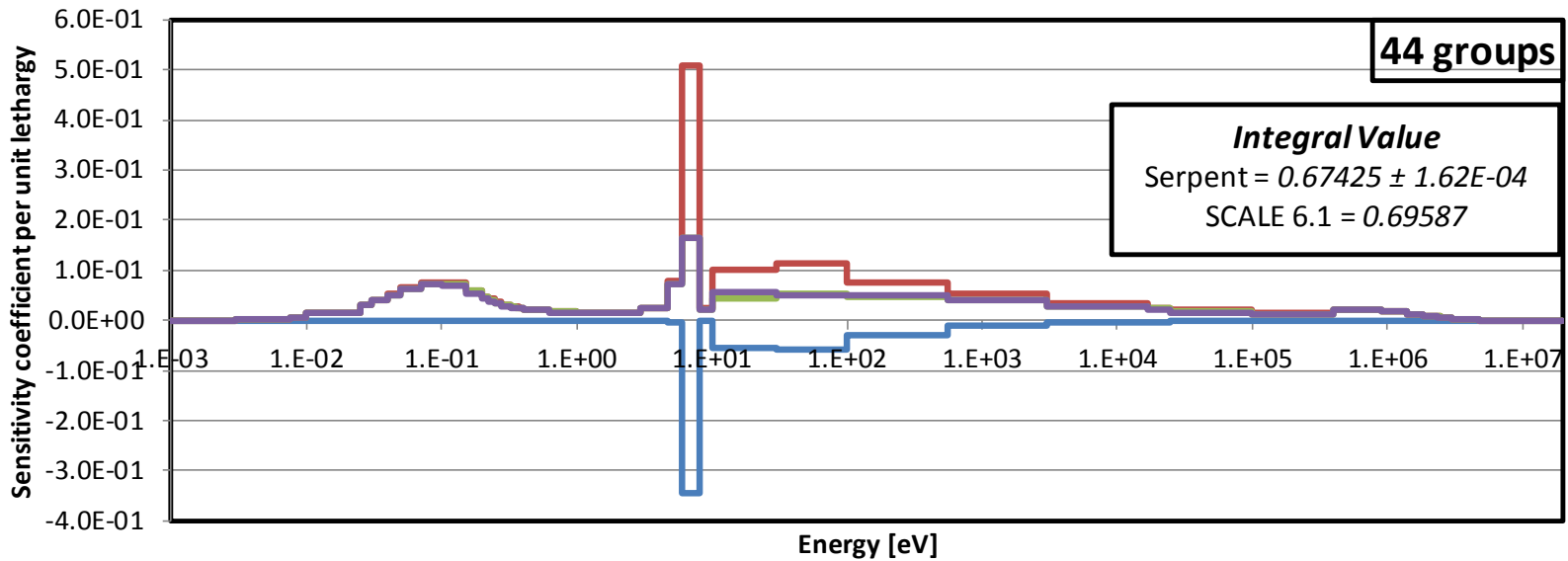
- Sensitivity coefficients based on the Generalized Perturbation Theory expressions consist of 2 different effects:
  - **Direct effects:** due to the perturbation of cross sections appearing directly in the response function
  - **Indirect effects:** due to the perturbation of neutron flux (caused by the cross sections perturbation)
- These effects have been calculated separately with Serpent for the evaluation of the cross sections sensitivity coefficient





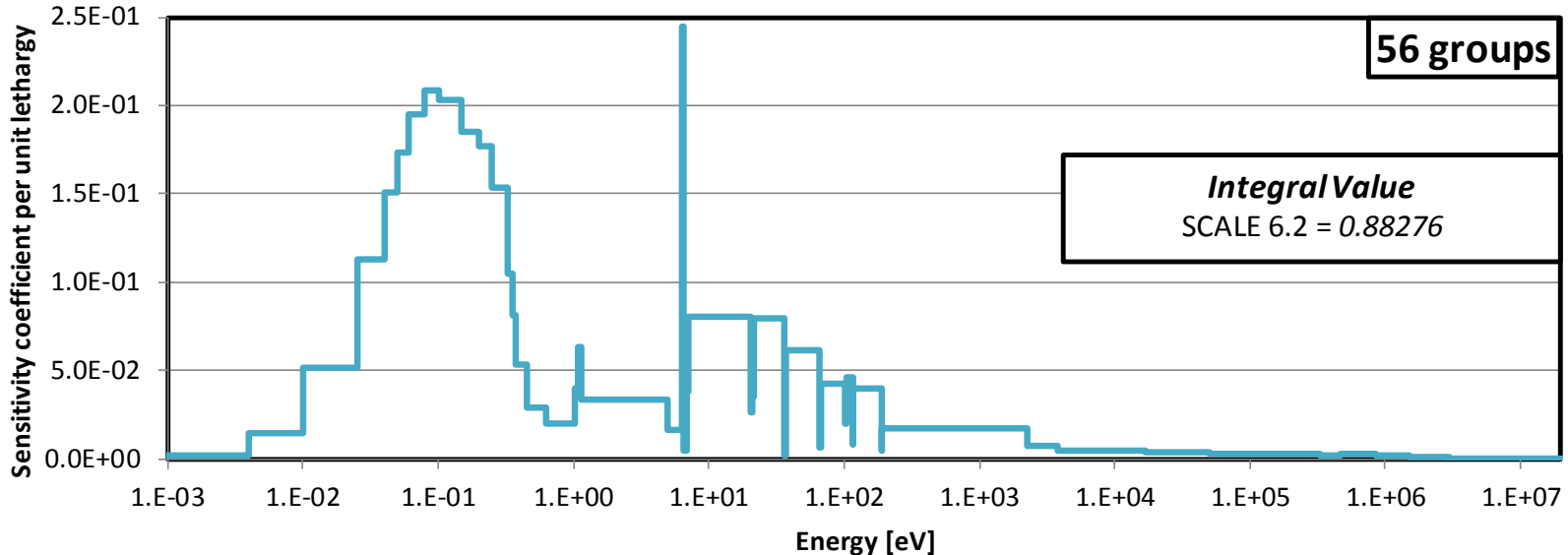
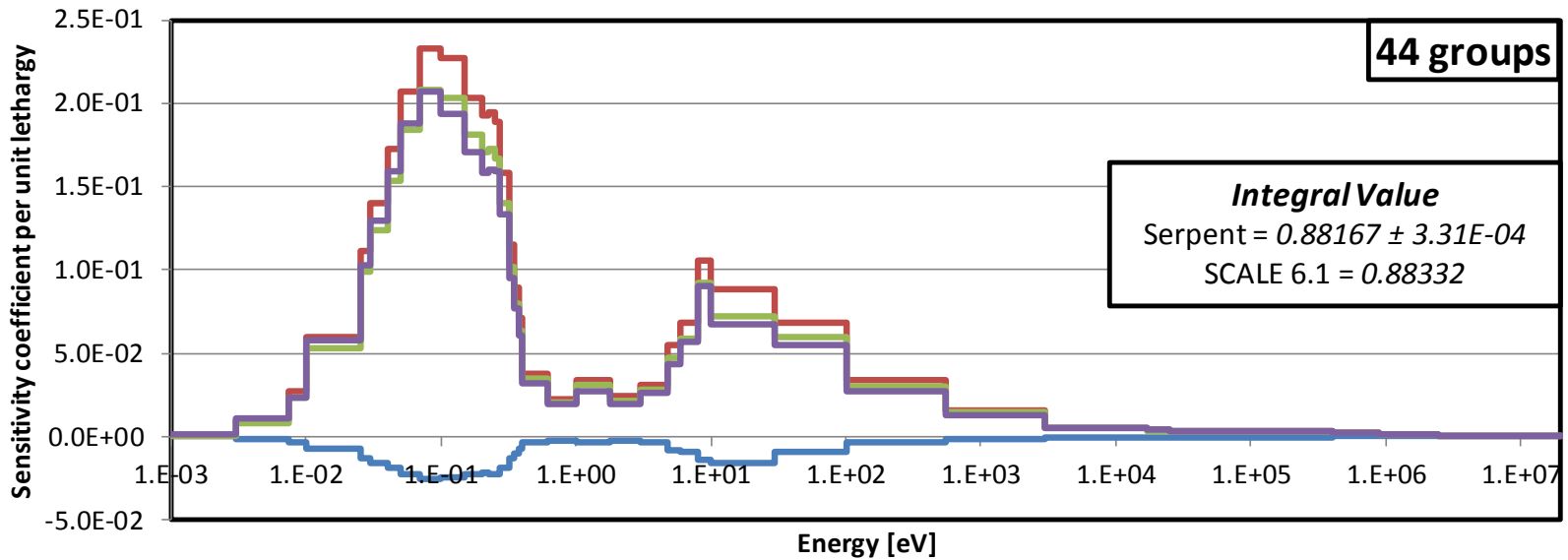
The **indirect term** is negative because an increase in the cross-section data enhances the local depression of the neutron flux, causing a decrease of the 1 group  $\sigma$

The **direct term** is positive because an increase in the cross-section data directly increase the 1 group  $\sigma$



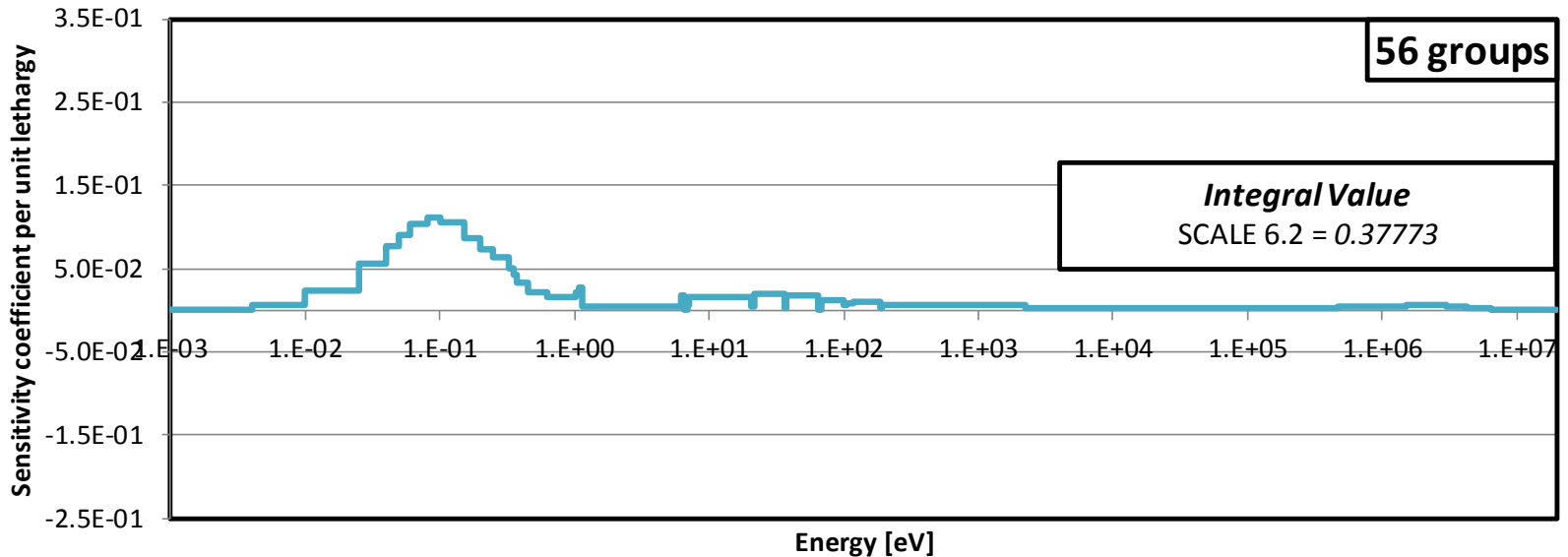
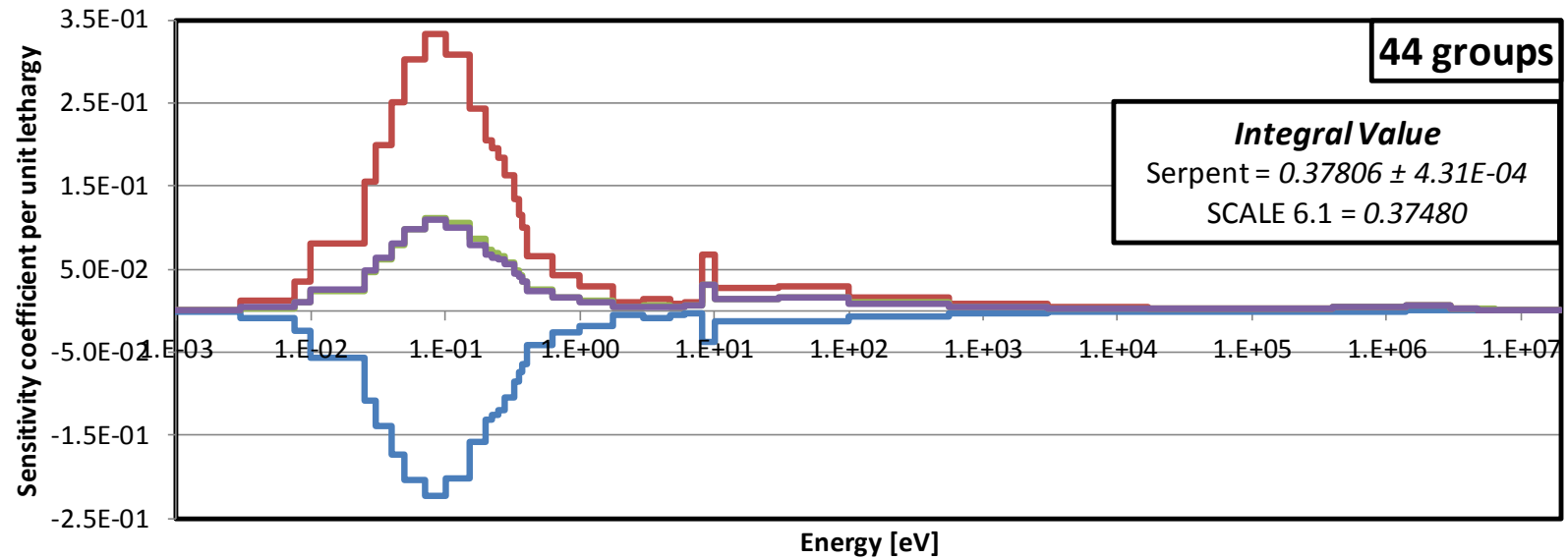
— Serpent - Indirect term   
 — Serpent - Direct term   
 — Serpent - Total   
 — SCALE 6.1   
 — SCALE 6.2

# Results – TMI Pin – $\sigma_{\text{capt, U235}}$ sensitivity to $^{235}\text{U}$ (n, $\gamma$ )

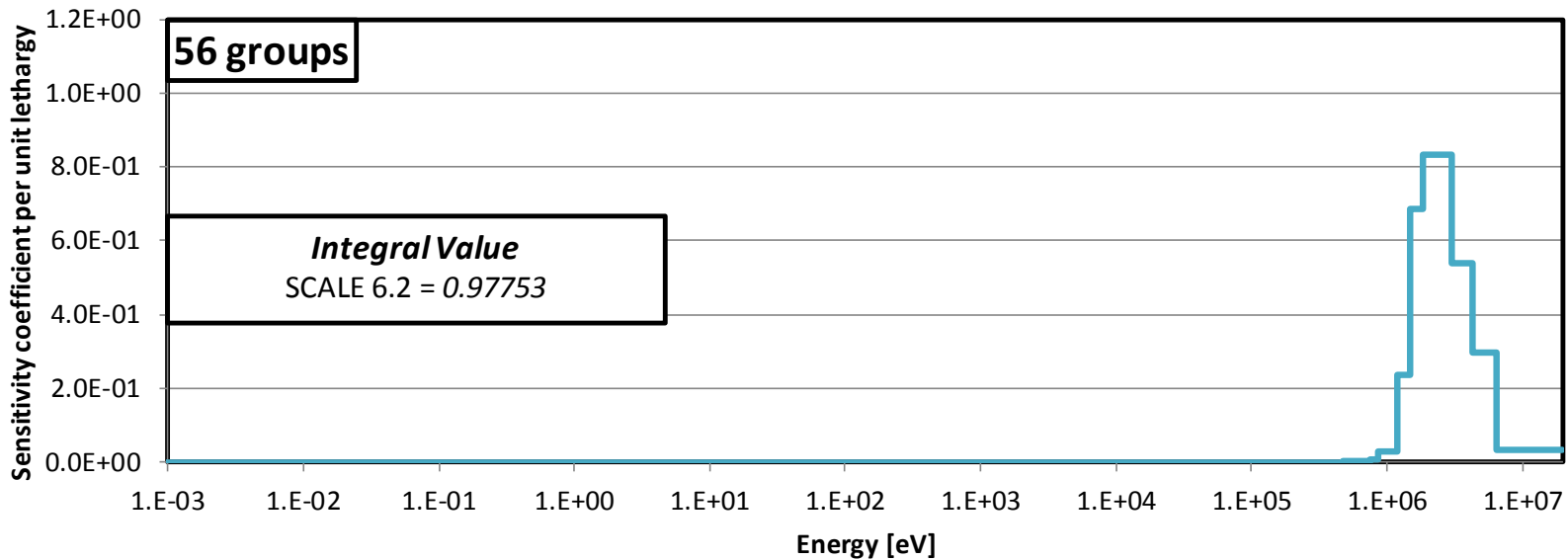
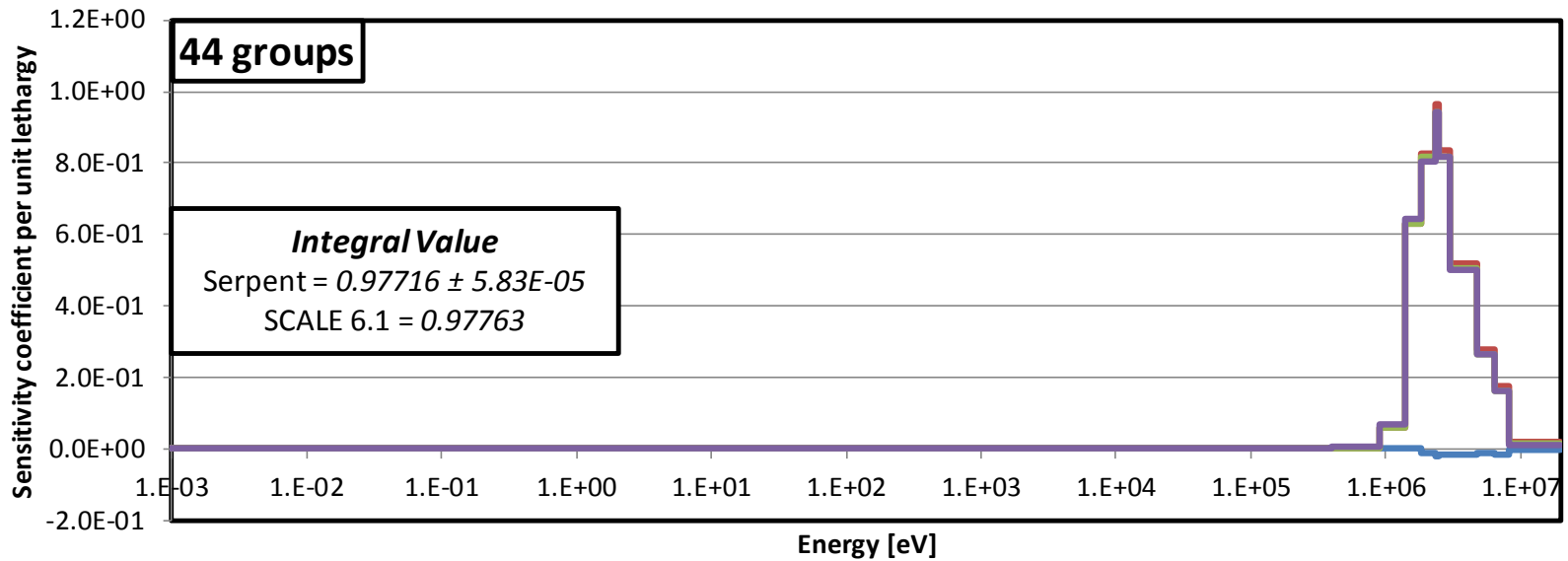


— Serpent - Indirect term    — Serpent - Direct term    — Serpent - Total    — SCALE 6.1    — SCALE 6.2

# Results – TMI Pin – $\sigma_{fiss, U235}$ sensitivity to $^{235}\text{U}$ (n,fiss)



— Serpent - Indirect term   
 — Serpent - Direct term   
 — Serpent - Total   
 — SCALE 6.1   
 — SCALE 6.2



— Serpent - Indirect term   
 — Serpent - Direct term   
 — Serpent - Total   
 — SCALE 6.1   
 — SCALE 6.2

## Uncertainty quantification – TMI Pin – 1 group $\sigma$

| $\sigma_{\text{capt, U235}}$     |                             | SERPENT<br>44 groups | SCALE 6.1<br>44 groups | SCALE 6.2<br>56 groups |
|----------------------------------|-----------------------------|----------------------|------------------------|------------------------|
| <i>Covariance Matrix</i>         |                             | <i>RSD (%)</i>       | <i>RSD (%)</i>         | <i>RSD (%)</i>         |
| $^{235}\text{U} (n,\gamma)$      | $^{235}\text{U} (n,\gamma)$ | 1.284%               | 1.294%                 | 1.171%                 |
| $^{238}\text{U} (n,n')$          | $^{238}\text{U} (n,n')$     | 0.962%               | 0.946%                 | 0.960%                 |
| $^{235}\text{U} \chi$            | $^{235}\text{U} \chi$       | 0.447%               | 0.444%                 | 0.750%                 |
| $^1\text{H} (n,\text{el})$       | $^1\text{H} (n,\text{el})$  | 0.413%               | 0.411%                 | 0.215%                 |
| $^{235}\text{U} (n,\text{fiss})$ | $^{235}\text{U} (n,\gamma)$ | 0.340%               | 0.340%                 | 0.340%                 |

| $\sigma_{\text{fiss, U235}}$ |                             | SERPENT<br>44 groups | SCALE 6.1<br>44 groups | SCALE 6.2<br>56 groups |
|------------------------------|-----------------------------|----------------------|------------------------|------------------------|
| <i>Covariance Matrix</i>     |                             | <i>RSD (%)</i>       | <i>RSD (%)</i>         | <i>RSD (%)</i>         |
| $^{238}\text{U} (n,n')$      | $^{238}\text{U} (n,n')$     | 0.930%               | 0.918%                 | 0.931%                 |
| $^{235}\text{U} \chi$        | $^{235}\text{U} \chi$       | 0.433%               | 0.430%                 | 0.725%                 |
| $^1\text{H} (n,\text{el})$   | $^1\text{H} (n,\text{el})$  | 0.409%               | 0.407%                 | 0.241%                 |
| $^{238}\text{U} (n,\gamma)$  | $^{238}\text{U} (n,\gamma)$ | 0.200%               | 0.211%                 | 0.216%                 |
| $^{235}\text{U} (n,\gamma)$  | $^{235}\text{U} (n,\gamma)$ | 0.172%               | 0.172%                 | 0.166%                 |

| $\sigma_{\text{capt, U238}}$ |                             | SERPENT<br>44 groups | SCALE 6.1<br>44 groups | SCALE 6.2<br>56 groups |
|------------------------------|-----------------------------|----------------------|------------------------|------------------------|
| <i>Covariance Matrix</i>     |                             | <i>RSD (%)</i>       | <i>RSD (%)</i>         | <i>RSD (%)</i>         |
| $^{238}\text{U} (n,n')$      | $^{238}\text{U} (n,n')$     | 0.919%               | 0.902%                 | 0.914%                 |
| $^{238}\text{U} (n,\gamma)$  | $^{238}\text{U} (n,\gamma)$ | 0.844%               | 0.877%                 | 0.901%                 |
| $^{235}\text{U} \chi$        | $^{235}\text{U} \chi$       | 0.444%               | 0.437%                 | 0.735%                 |
| $^1\text{H} (n,\text{el})$   | $^1\text{H} (n,\text{el})$  | 0.362%               | 0.361%                 | 0.149%                 |
| $^{235}\text{U} (n,\gamma)$  | $^{235}\text{U} (n,\gamma)$ | 0.064%               | 0.065%                 | 0.052%                 |

| $\sigma_{\text{fiss, U238}}$     |                                  | SERPENT<br>44 groups | SCALE 6.1<br>44 groups | SCALE 6.2<br>56 groups |
|----------------------------------|----------------------------------|----------------------|------------------------|------------------------|
| <i>Covariance Matrix</i>         |                                  | <i>RSD (%)</i>       | <i>RSD (%)</i>         | <i>RSD (%)</i>         |
| $^{238}\text{U} (n,n')$          | $^{238}\text{U} (n,n')$          | 3.273 %              | 3.222%                 | 3.231%                 |
| $^{235}\text{U} \chi$            | $^{235}\text{U} \chi$            | 2.200 %              | 2.198%                 | 3.623%                 |
| $^1\text{H} (n,\text{el})$       | $^1\text{H} (n,\text{el})$       | 0.518 %              | 0.513%                 | 0.202%                 |
| $^{238}\text{U} (n,\text{fiss})$ | $^{238}\text{U} (n,\text{fiss})$ | 0.509 %              | 0.510%                 | 0.510%                 |
| $^{238}\text{U} \chi$            | $^{238}\text{U} \chi$            | 0.166 %              | 0.166%                 | 0.569%                 |

## Uncertainty quantification – TMI Pin – 1 group $\sigma$

| SERPENT 44 groups            |               | SCALE 6.1 44 groups          |               | SCALE 6.2 56 groups          |               |
|------------------------------|---------------|------------------------------|---------------|------------------------------|---------------|
| $\sigma_{\text{capt, U235}}$ | Total RSD (%) | $\sigma_{\text{capt, U235}}$ | Total RSD (%) | $\sigma_{\text{capt, U235}}$ | Total RSD (%) |
| $8.263 \pm 4E-05$            | 1.753 %       | 8.297E+00                    | 1.765%        | 8.286E+00                    | 1.758%        |

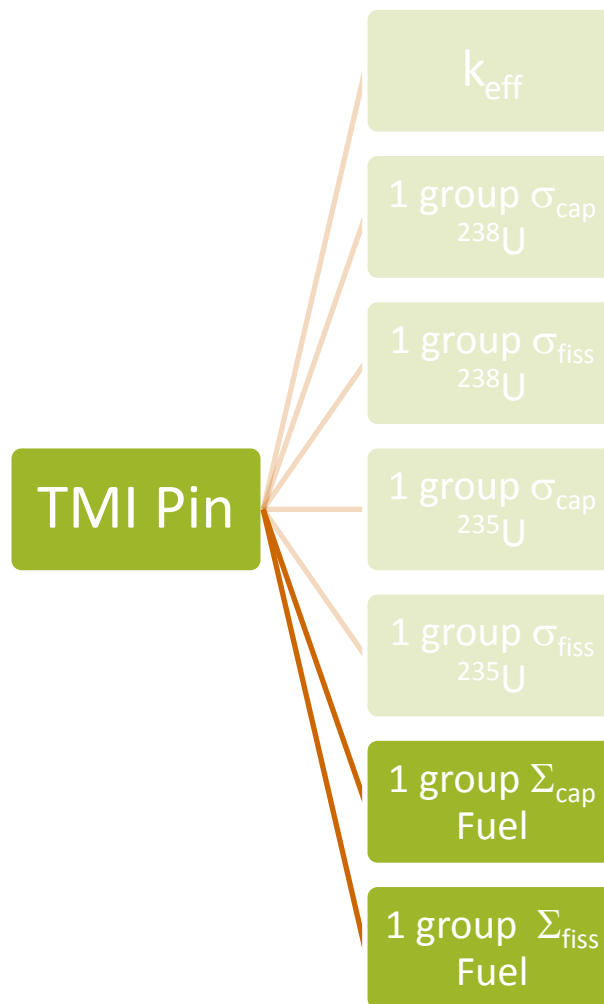
| SERPENT 44 groups            |               | SCALE 6.1 44 groups          |               | SCALE 6.2 56 groups          |               |
|------------------------------|---------------|------------------------------|---------------|------------------------------|---------------|
| $\sigma_{\text{fiss, U235}}$ | Total RSD (%) | $\sigma_{\text{fiss, U235}}$ | Total RSD (%) | $\sigma_{\text{fiss, U235}}$ | Total RSD (%) |
| $3.517E+01 \pm 5E-05$        | 1.145 %       | 3.532E+01                    | 1.140%        | 3.517E+01                    | 1.252%        |

Uncertainty in  $\sigma_{\text{fiss, U238}}$  is big mainly due to the contribution of  $^{238}\text{U} (n,n')$  and  $^{235}\text{U} \chi$

| SERPENT 44 groups            |               | SCALE 6.1 44 groups          |               | SCALE 6.2 56 groups          |               |
|------------------------------|---------------|------------------------------|---------------|------------------------------|---------------|
| $\sigma_{\text{capt, U238}}$ | Total RSD (%) | $\sigma_{\text{capt, U238}}$ | Total RSD (%) | $\sigma_{\text{capt, U238}}$ | Total RSD (%) |
| $8.136E-01 \pm 6E-05$        | 1.378 %       | 8.350E-01                    | 1.385%        | 8.266E-01                    | 1.500%        |

| SERPENT 44 groups            |               | SCALE 6.1 44 groups          |               | SCALE 6.2 56 groups          |               |
|------------------------------|---------------|------------------------------|---------------|------------------------------|---------------|
| $\sigma_{\text{fiss, U238}}$ | Total RSD (%) | $\sigma_{\text{fiss, U238}}$ | Total RSD (%) | $\sigma_{\text{fiss, U238}}$ | Total RSD (%) |
| $1.019E-01 \pm 7E-05$        | 4.013 %       | 1.010E-01                    | 3.963%        | 1.008E-01                    | 4.913%        |

## Uncertainty quantification





## Uncertainty quantification – TMI Pin – 1 group $\Sigma$

| $\Sigma_{\text{capt, Fuel}}$ |                              | SERPENT<br>44 groups | SCALE 6.1<br>44 groups | SCALE 6.2<br>56 groups |
|------------------------------|------------------------------|----------------------|------------------------|------------------------|
| <i>Covariance Matrix</i>     |                              | <i>RSD (%)</i>       | <i>RSD (%)</i>         | <i>RSD (%)</i>         |
| $^{238}\text{U} (n, n')$     | $^{238}\text{U} (n, n')$     | 0.919%               | 0.917%                 | 0.929%                 |
| $^{238}\text{U} (n, \gamma)$ | $^{238}\text{U} (n, \gamma)$ | 0.492%               | 0.516%                 | 0.529%                 |
| $^{235}\text{U} \chi$        | $^{235}\text{U} \chi$        | 0.418%               | 0.440%                 | 0.740%                 |
| $^{235}\text{U} (n, \gamma)$ | $^{235}\text{U} (n, \gamma)$ | 0.403%               | 0.401%                 | 0.370%                 |
| $^1\text{H} (n, el)$         | $^1\text{H} (n, el)$         | 0.375%               | 0.377%                 | 0.171%                 |

| $\Sigma_{\text{fiss, Fuel}}$ |                              | SERPENT<br>44 groups | SCALE 6.1<br>44 groups | SCALE 6.2<br>56 groups |
|------------------------------|------------------------------|----------------------|------------------------|------------------------|
| <i>Covariance Matrix</i>     |                              | <i>RSD (%)</i>       | <i>RSD (%)</i>         | <i>RSD (%)</i>         |
| $^{238}\text{U} (n, n')$     | $^{238}\text{U} (n, n')$     | 0.707%               | 0.702%                 | 0.713%                 |
| $^1\text{H} (n, el)$         | $^1\text{H} (n, el)$         | 0.360%               | 0.359%                 | 0.218%                 |
| $^{235}\text{U} \chi$        | $^{235}\text{U} \chi$        | 0.293%               | 0.292%                 | 0.502%                 |
| $^{238}\text{U} (n, \gamma)$ | $^{238}\text{U} (n, \gamma)$ | 0.185%               | 0.196%                 | 0.200%                 |
| $^{235}\text{U} (n, \gamma)$ | $^{235}\text{U} (n, \gamma)$ | 0.160%               | 0.161%                 | 0.155%                 |

| SERPENT 44<br>groups                |                  | SCALE 6.1 44<br>groups       |                  | SCALE 6.2 56<br>groups       |                  |
|-------------------------------------|------------------|------------------------------|------------------|------------------------------|------------------|
| $\Sigma_{\text{capt, Fuel}}$        | Total<br>RSD (%) | $\Sigma_{\text{capt, Fuel}}$ | Total<br>RSD (%) | $\Sigma_{\text{capt, Fuel}}$ | Total<br>RSD (%) |
| $2.720\text{E-}02 \pm 4\text{E-}05$ | 1.260 %          | $2.759\text{E-}02$           | 1.278%           | $2.740\text{E-}02$           | 1.380%           |

| SERPENT 44<br>groups                |                  | SCALE 6.1 44<br>groups       |                  | SCALE 6.2 56<br>groups       |                  |
|-------------------------------------|------------------|------------------------------|------------------|------------------------------|------------------|
| $\Sigma_{\text{fiss, Fuel}}$        | Total<br>RSD (%) | $\Sigma_{\text{fiss, Fuel}}$ | Total<br>RSD (%) | $\Sigma_{\text{fiss, Fuel}}$ | Total<br>RSD (%) |
| $4.184\text{E-}02 \pm 4\text{E-}05$ | 0.893 %          | $4.199\text{E-}02$           | 0.896%           | $4.182\text{E-}02$           | 0.954%           |

- SERPENT-2 GPT and SCALE 6.1 & 6.2 /TSUNAMI1D sensitivity calculations are in good agreement, regarding the TMI HZP pin analysis.
- In general uncertainty calculations with 44 & 56 groups covariance matrices are in good agreement (single contributions).
- Some discrepancies can be found in the contributions of  $^{235}\text{U}$  nubar,  $^{238}\text{U}$  &  $^{235}\text{U}$   $\chi$  and  $^1\text{H}$  (n,el), between 44 and 56 groups calculation. This is probably due to some update in the new 56 groups libraries of SCALE 6.2 (check  $\Delta\sigma/\sigma$ ).
- $^{235}\text{U}$  nubar and  $^{238}\text{U}$  (n, $\gamma$ ) are the major contributors in  $k_{\text{eff}}$  uncertainty. With the used options in SCALE,  $^{238}\text{U}$  (n, $\gamma$ ) uncertainty may be slightly overestimated.
- $^{238}\text{U}$  (n,n') has a strong influence on the uncertainty of homogenized cross sections (both in pin and assembly). Also  $^1\text{H}$  (n,el) plays an important role.

## Future work

- Include other sets
  - HFP
  - BWR and VVER cases
- Extend the calculation to the fuel assembly and full core (exercises I-2 & I-3)
- Include other isotopes
  - Zr
  - Gd
- Use the new 56 and 252 groups covariance libraries of SCALE 6.2 with Serpent 2

THANK YOU FOR YOUR  
ATTENTION!