



**Nuclear
and
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EEngineering**

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

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- Introduction
- Codes and methods
- Test cases
- Results
 - UAM Exercise I-1
 - ✓ k_{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}U , ^{238}U , ^{16}O and ^1H) 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_{eff}
 - 1 group σ_{capt} , σ_{fiss} , Σ_{capt} and Σ_{fiss}
- Results are compared with SCALE/TSUNAMI-1D

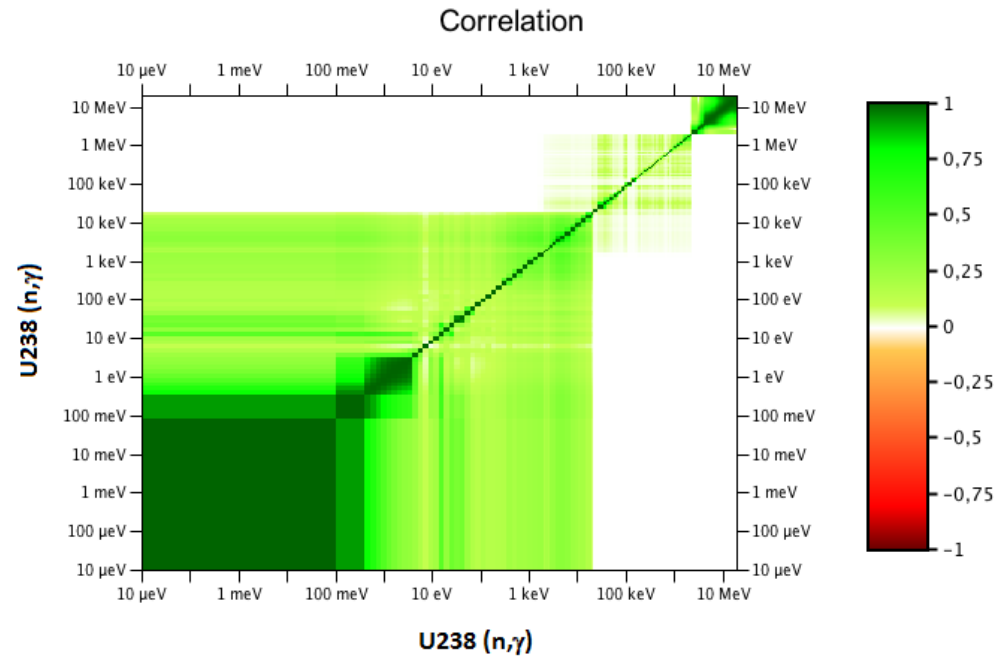
- The effect of a perturbation of a parameter x on the response R is:

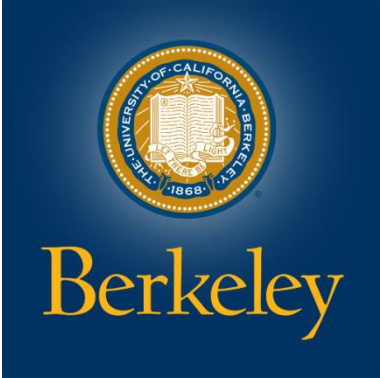
$$S_{R,x} = \frac{dR/R}{dx/x}$$

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

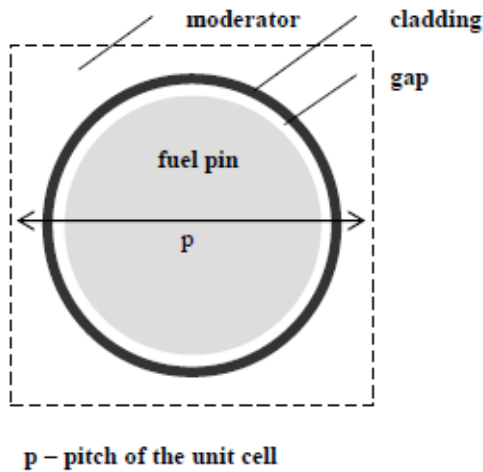
$$Var[R] = S_{R,x} Cov[x] (S_{R,x})^T$$

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



- 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_{eff} , homogenized microscopic and macroscopic cross sections) related to the perturbation of input cross sections.
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- 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

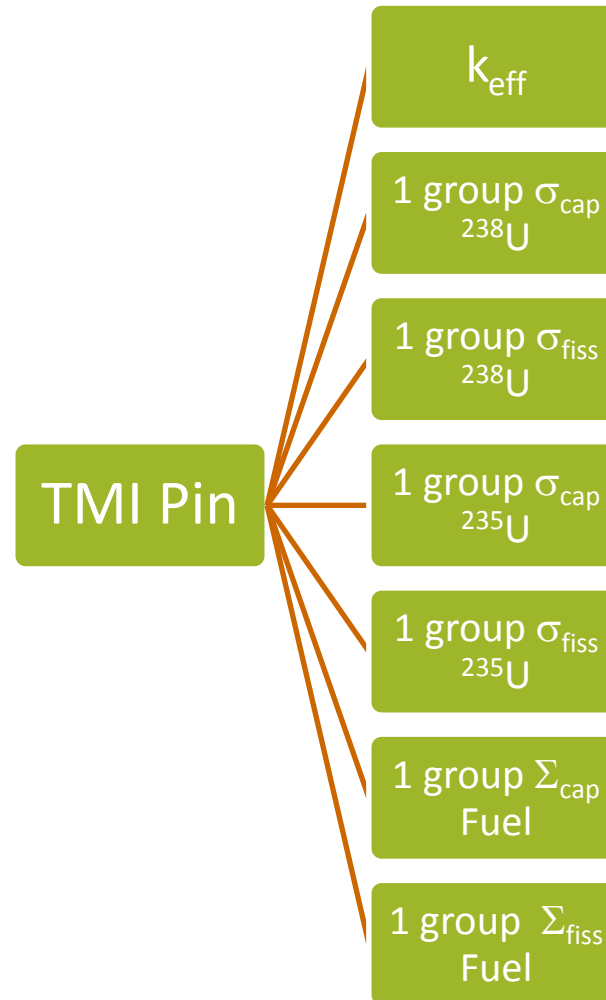


Parameter	Value
Unit cell pitch, [mm]	14.427
Fuel pellet diameter, [mm]	9.391
Fuel pellet material	UO ₂
Fuel density, [g/cm ³]	10.283
Fuel enrichment, w/o	4.85
Cladding outside diameter, [mm]	10.928
Cladding thickness, [mm]	0.673
Cladding material	Zircaloy-4
Cladding density, [g/cm ³]	6.55
Gap material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

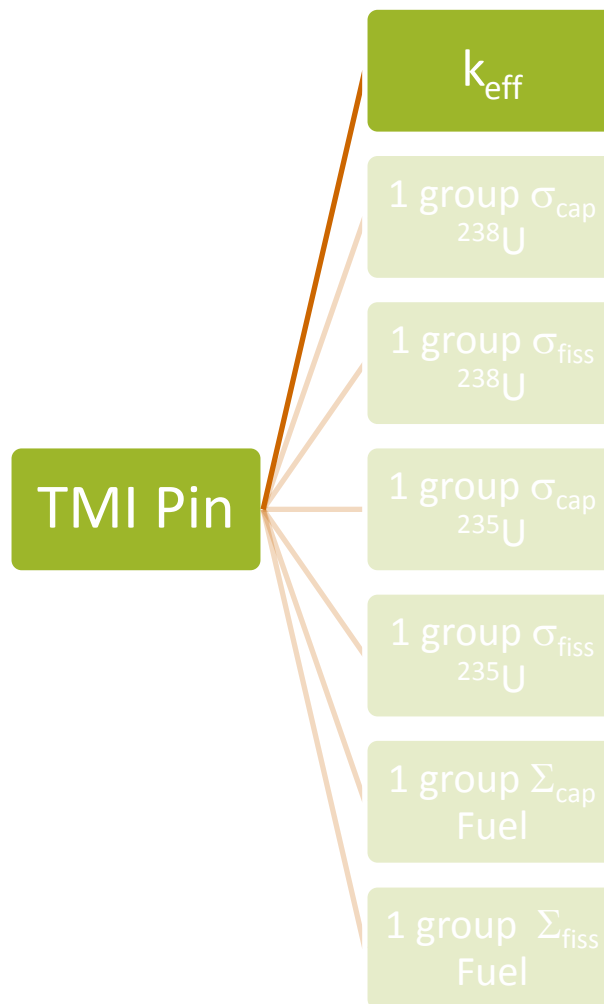
Parameter / Reactor condition	HZP	HFP
Fuel temperature, [K]	551	900
Cladding temperature, [K]	551	600
Moderator (coolant) temperature, [K]	551	562
Moderator (coolant) density, [kg/m ³]	766	748.4
Reactor power, [MWt]	2.772	2.772

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

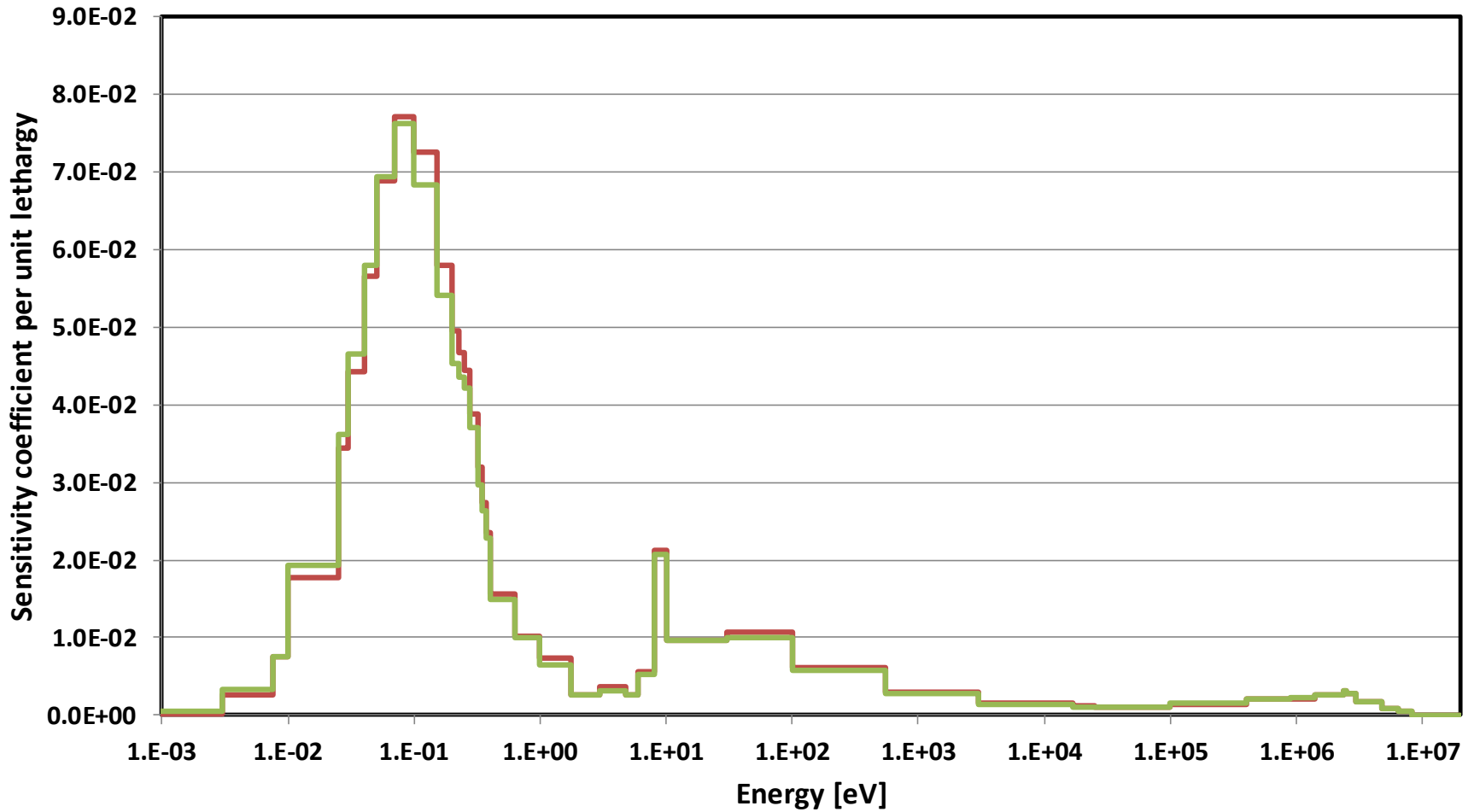
Uncertainty quantification



Uncertainty quantification

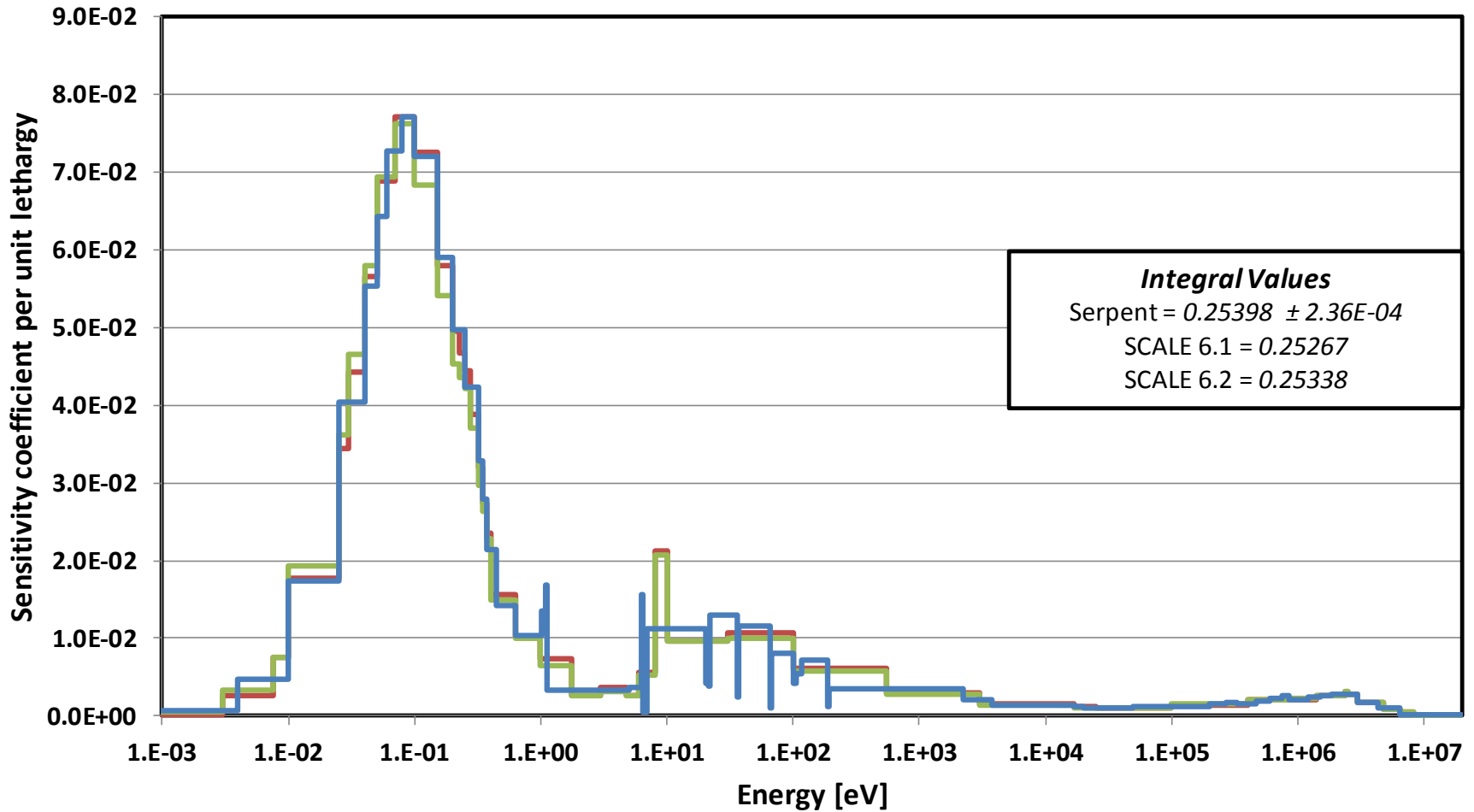


TMI Pin - k_{eff} - ^{235}U (n,fission)



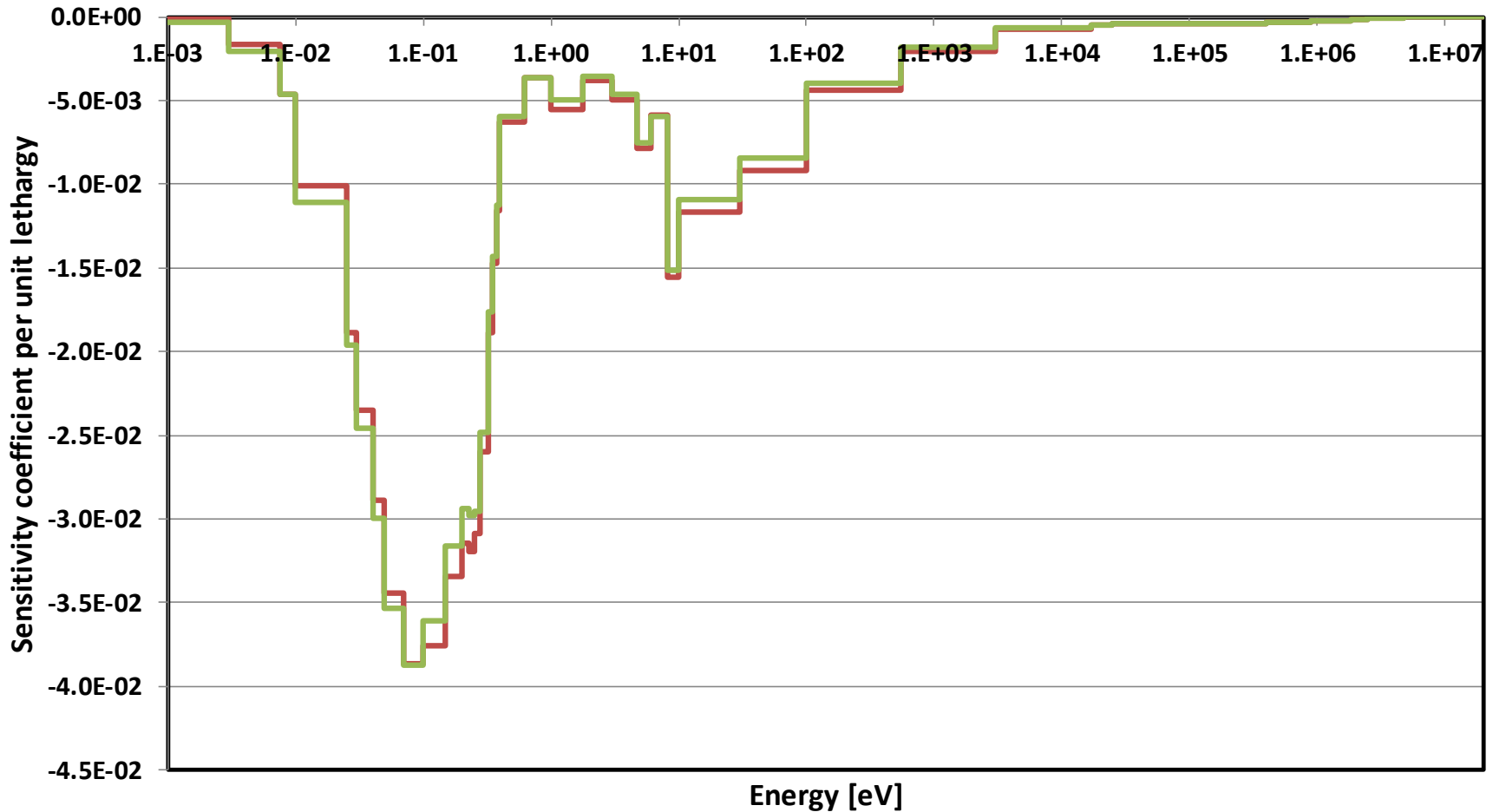
— SERPENT 44 groups — SCALE 6.1 - 44 groups

TMI Pin - k_{eff} - ^{235}U (n,fission)



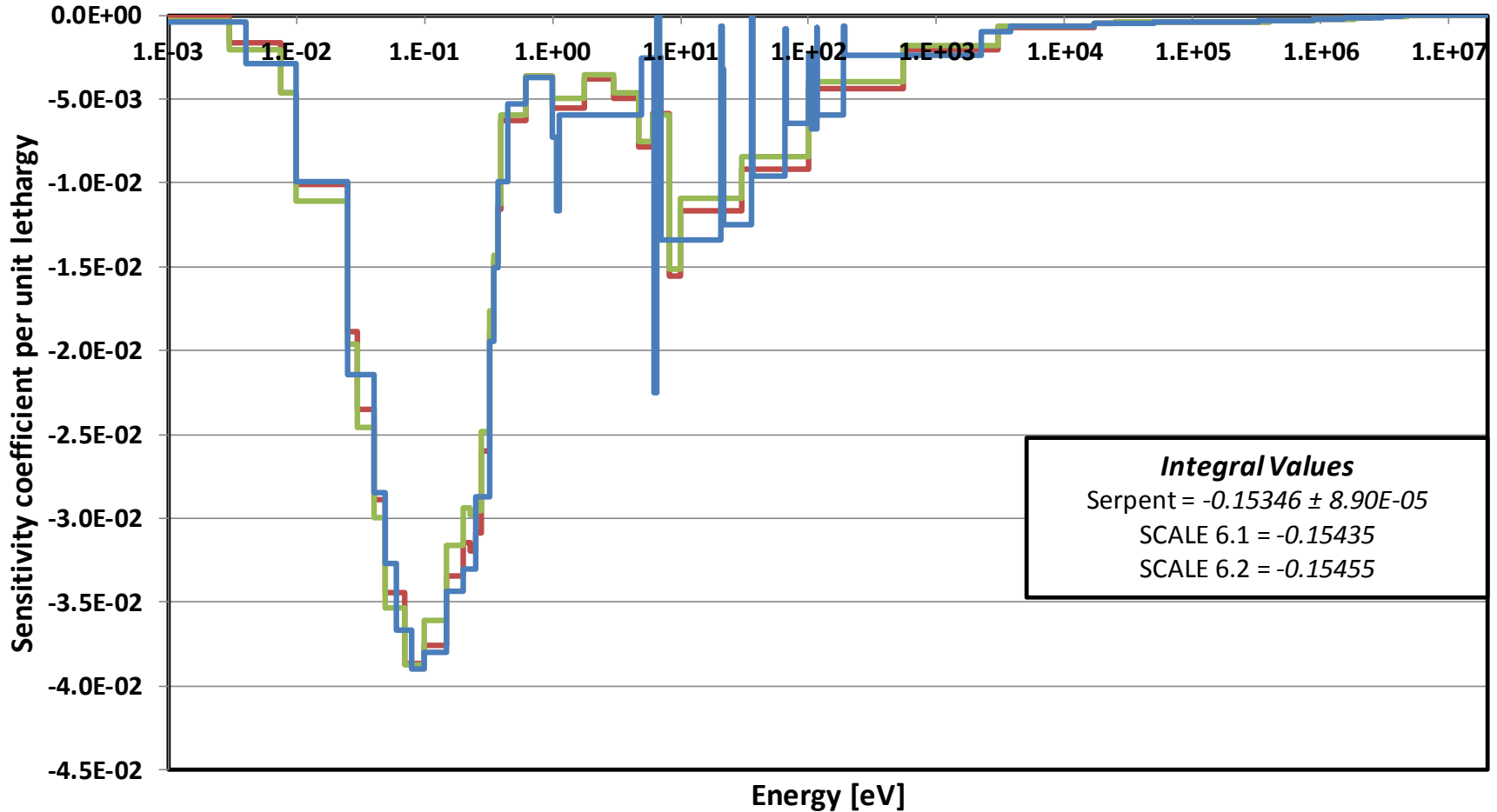
— SERPENT 44 groups
 — SCALE 6.1 - 44 groups
 — SCALE 6.2 - 56 groups

TMI Pin - k_{eff} - ^{235}U (n, γ)



— SERPENT 44 groups — SCALE 6.1 - 44 groups

TMI Pin - k_{eff} - ^{235}U (n, γ)

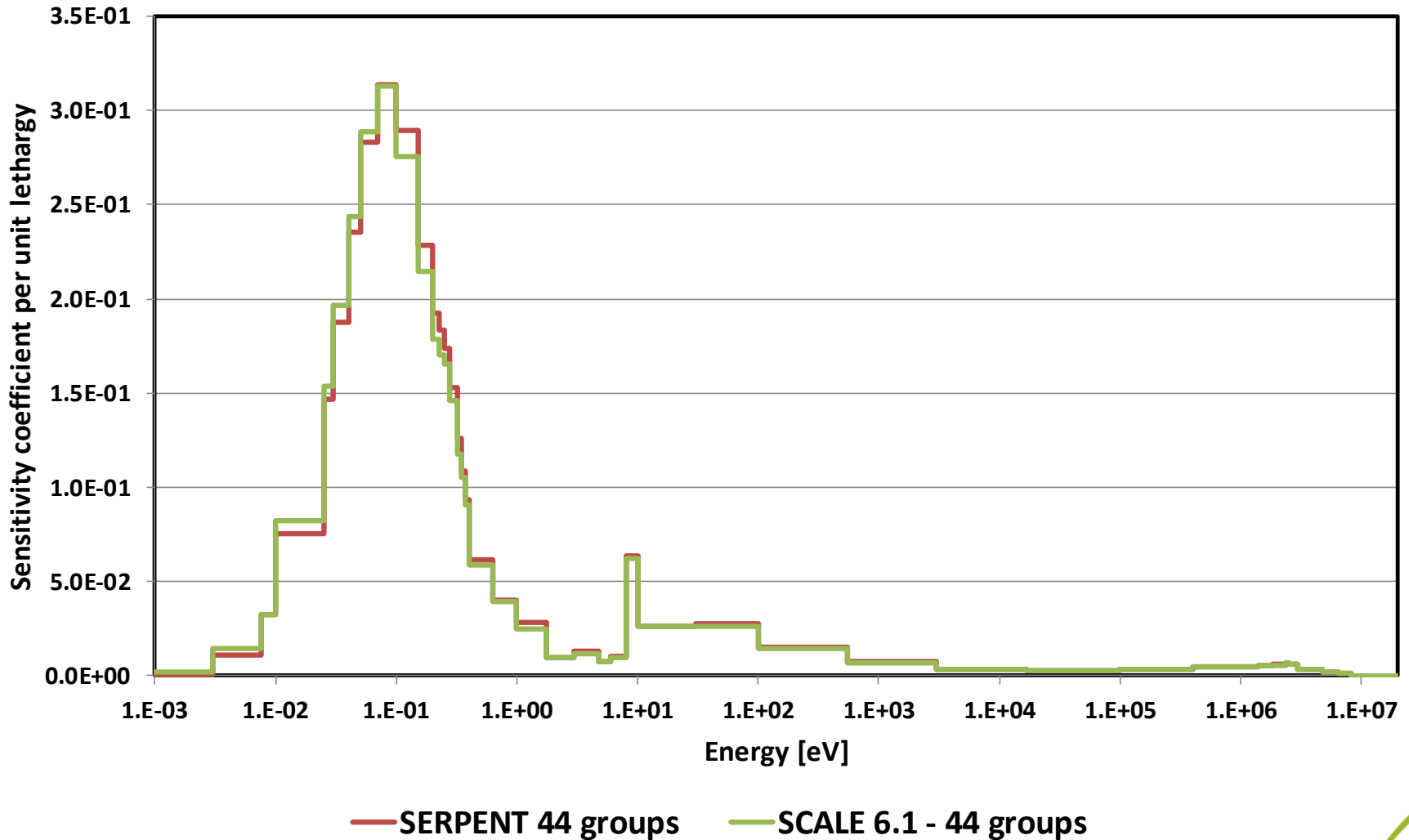


— SERPENT 44 groups

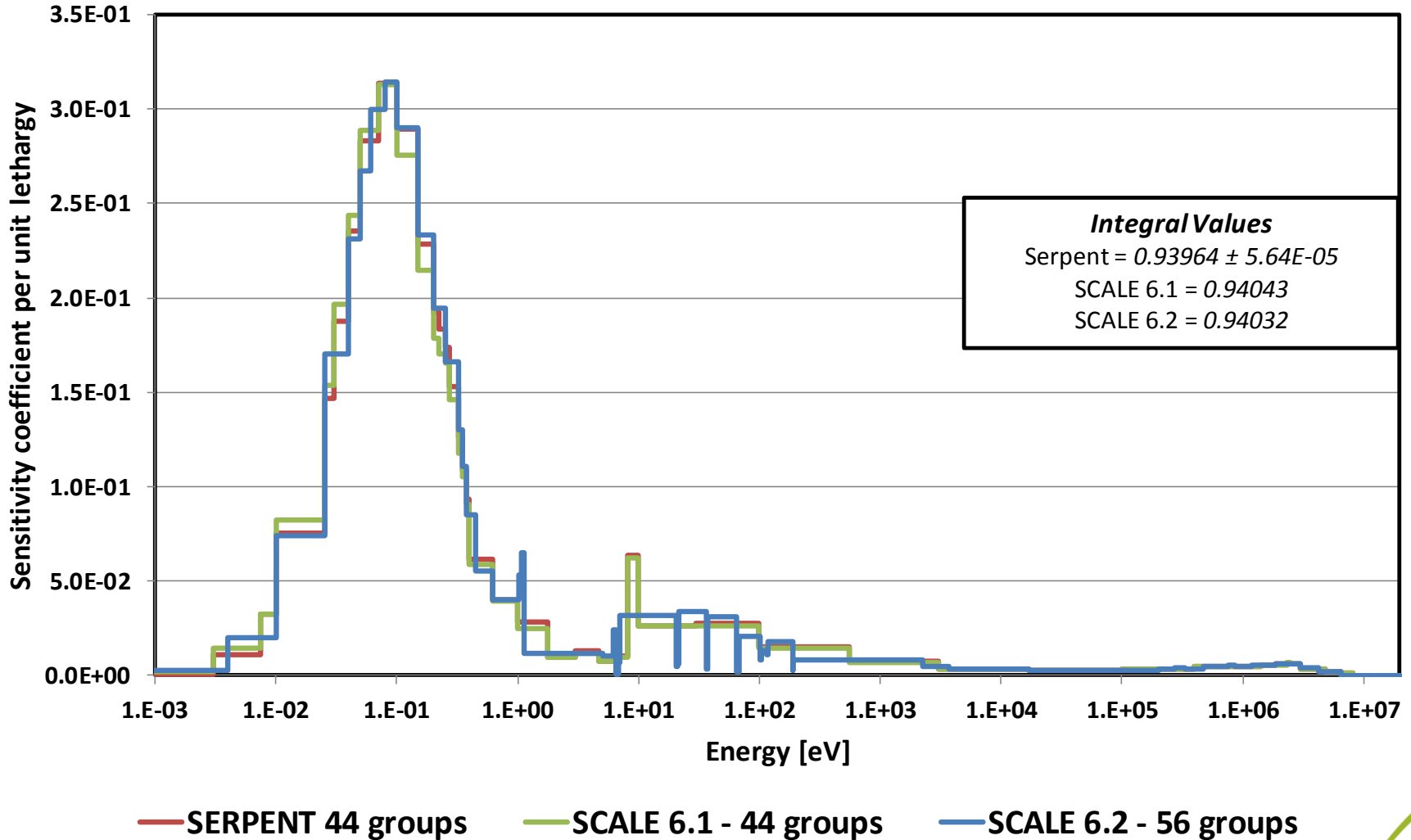
— SCALE 6.1 - 44 groups

— SCALE 6.2 - 56 groups

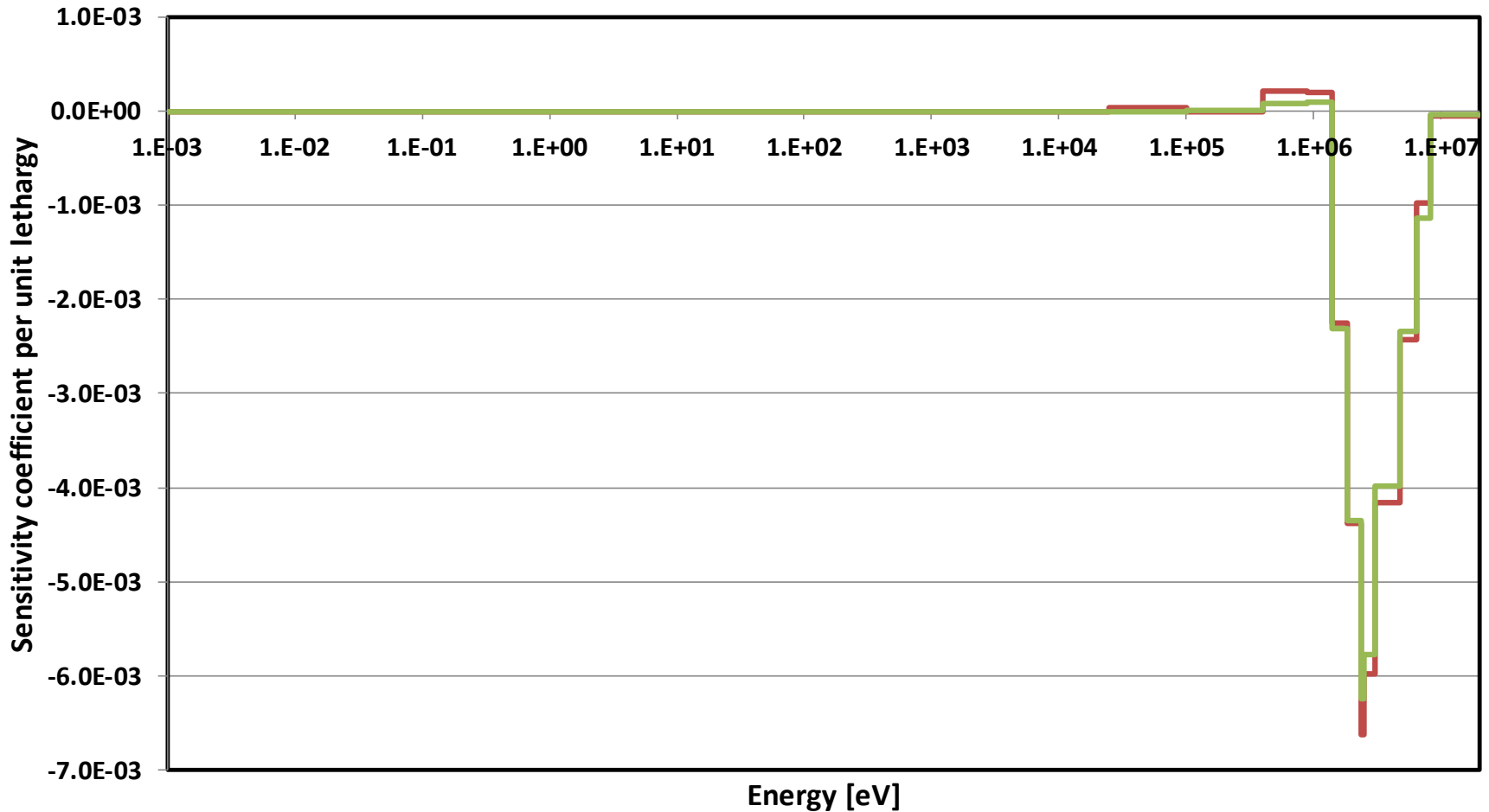
TMI Pin - k_{eff} - ^{235}U nubar



TMI Pin - k_{eff} - ^{235}U nubar

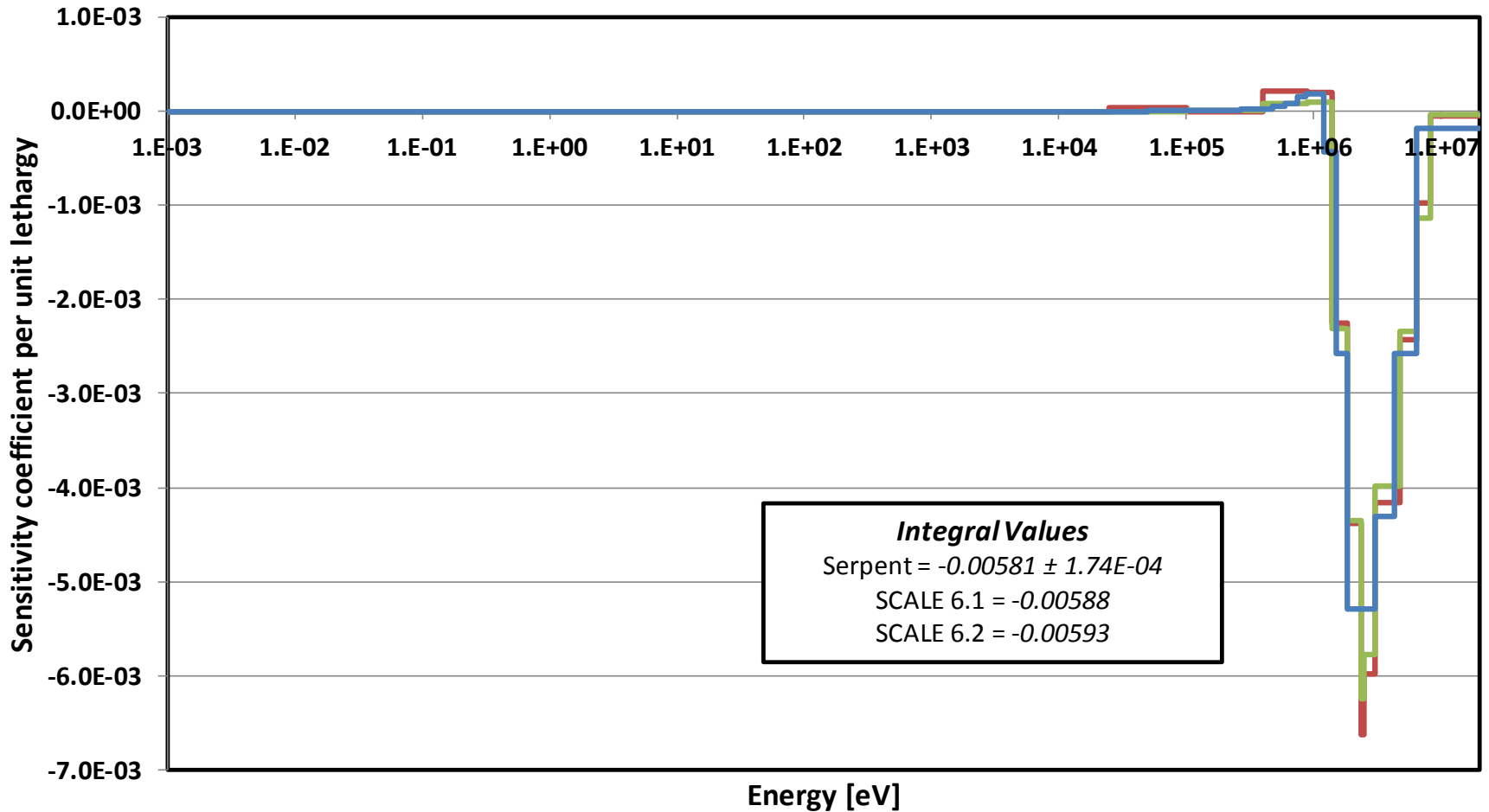


TMI Pin - k_{eff} - ^{238}U (n,n')



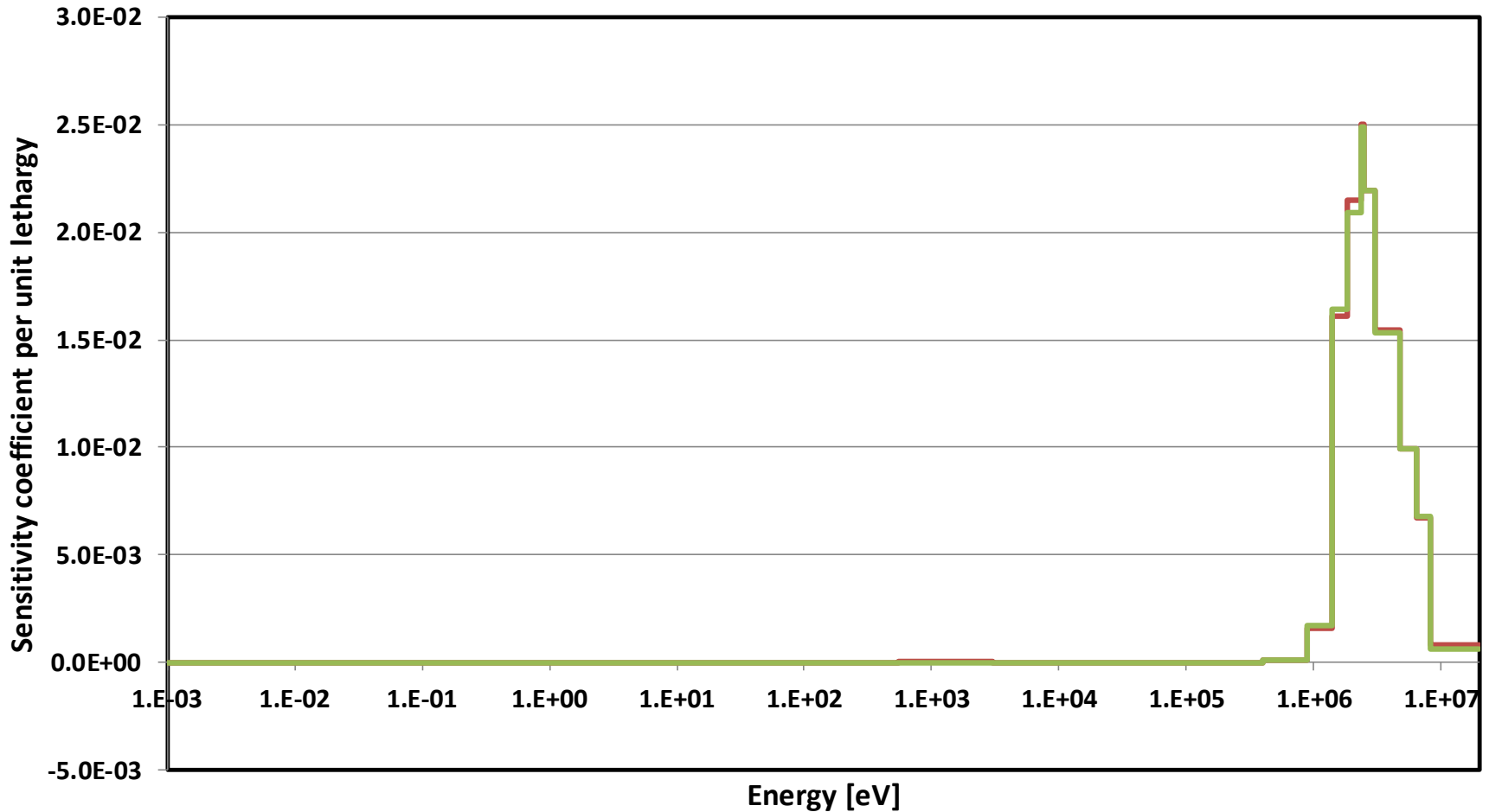
— SERPENT 44 groups — SCALE 6.1 - 44 groups

TMI Pin - k_{eff} - ^{238}U (n,n')



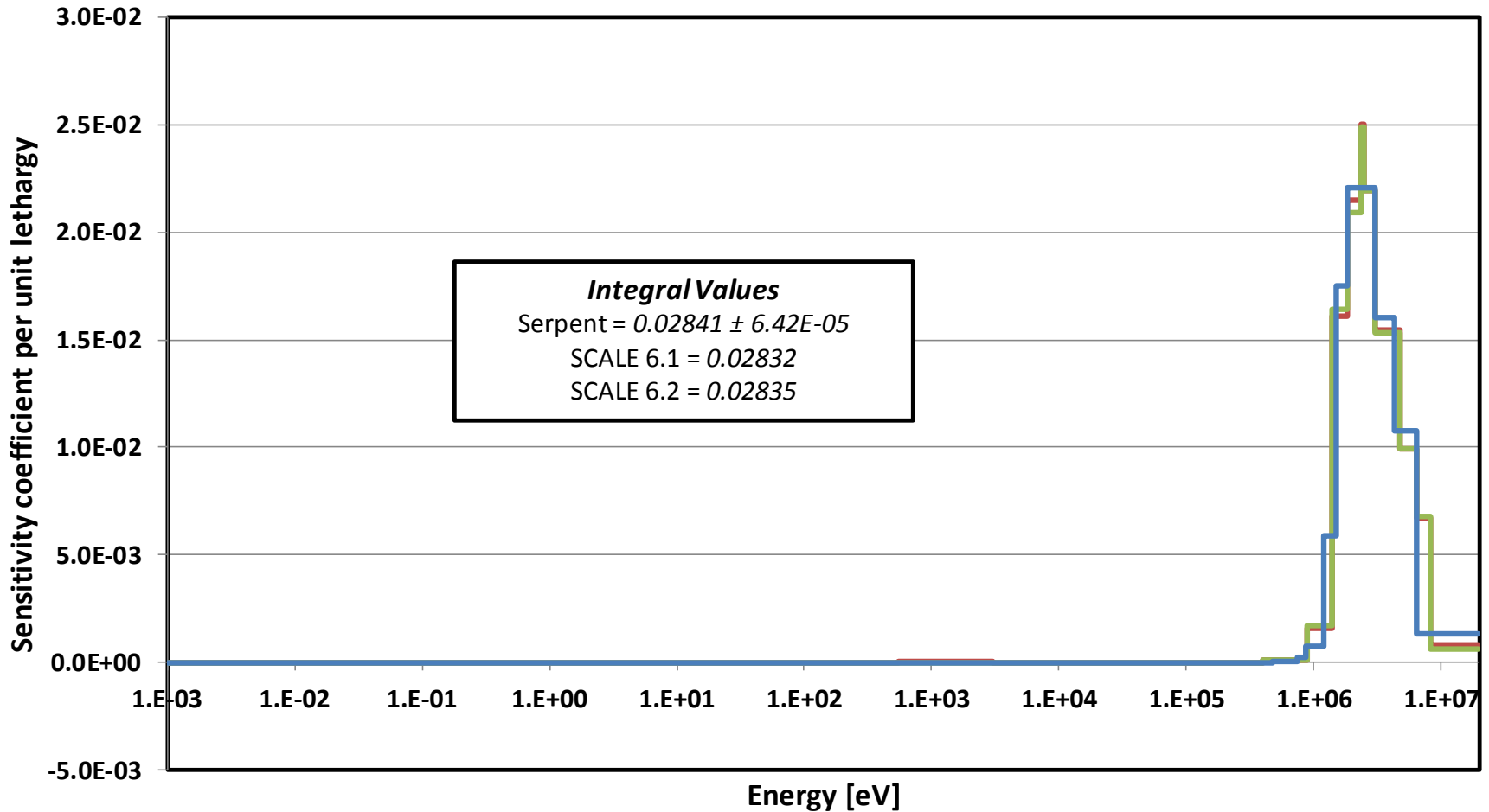
— SERPENT 44 groups — SCALE 6.1 - 44 groups — SCALE 6.2 - 56 groups

TMI Pin - k_{eff} - ^{238}U (n,fission)



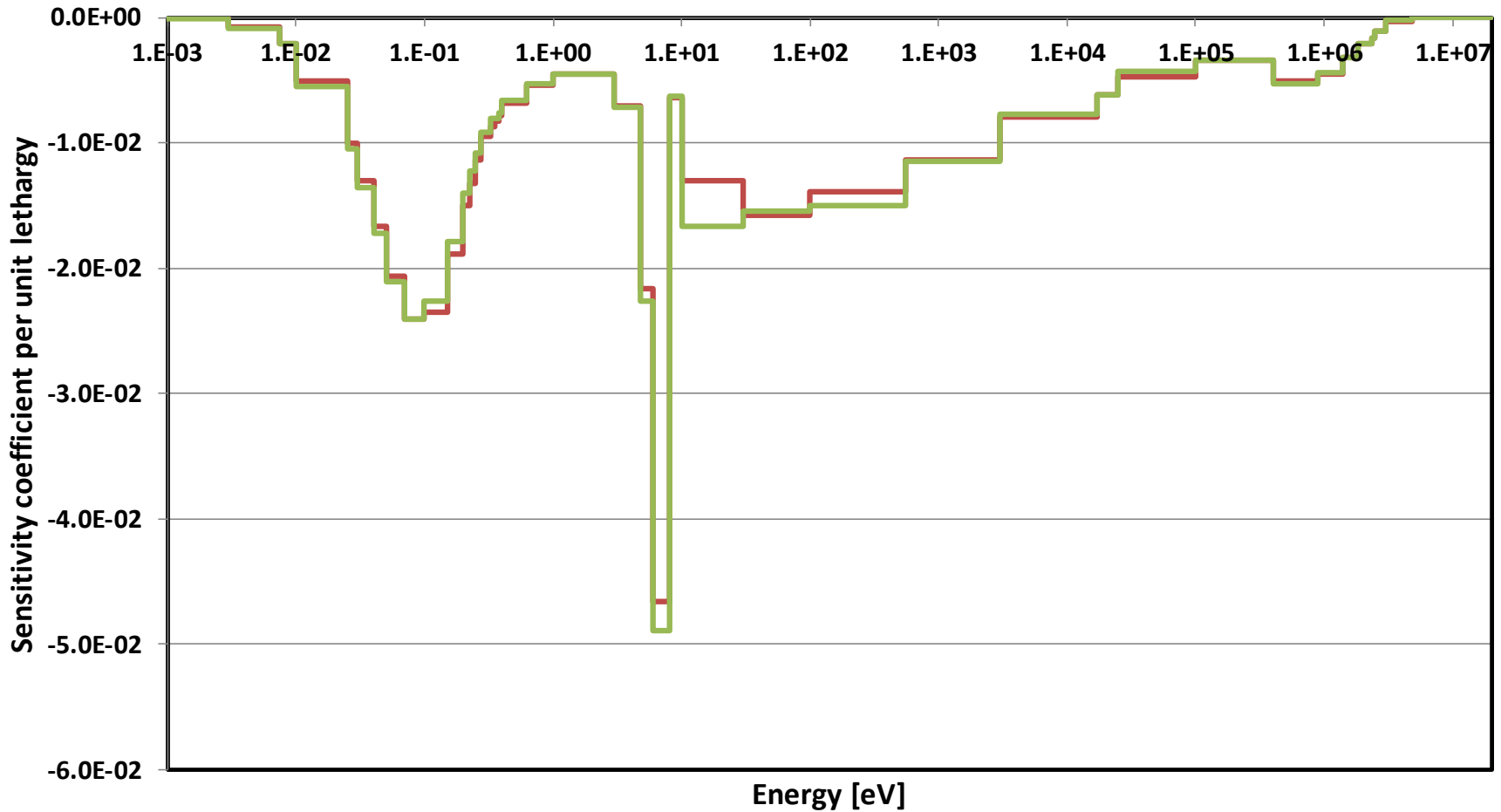
— SERPENT 44 groups — SCALE 6.1 - 44 groups

TMI Pin - k_{eff} - ^{238}U (n,fission)



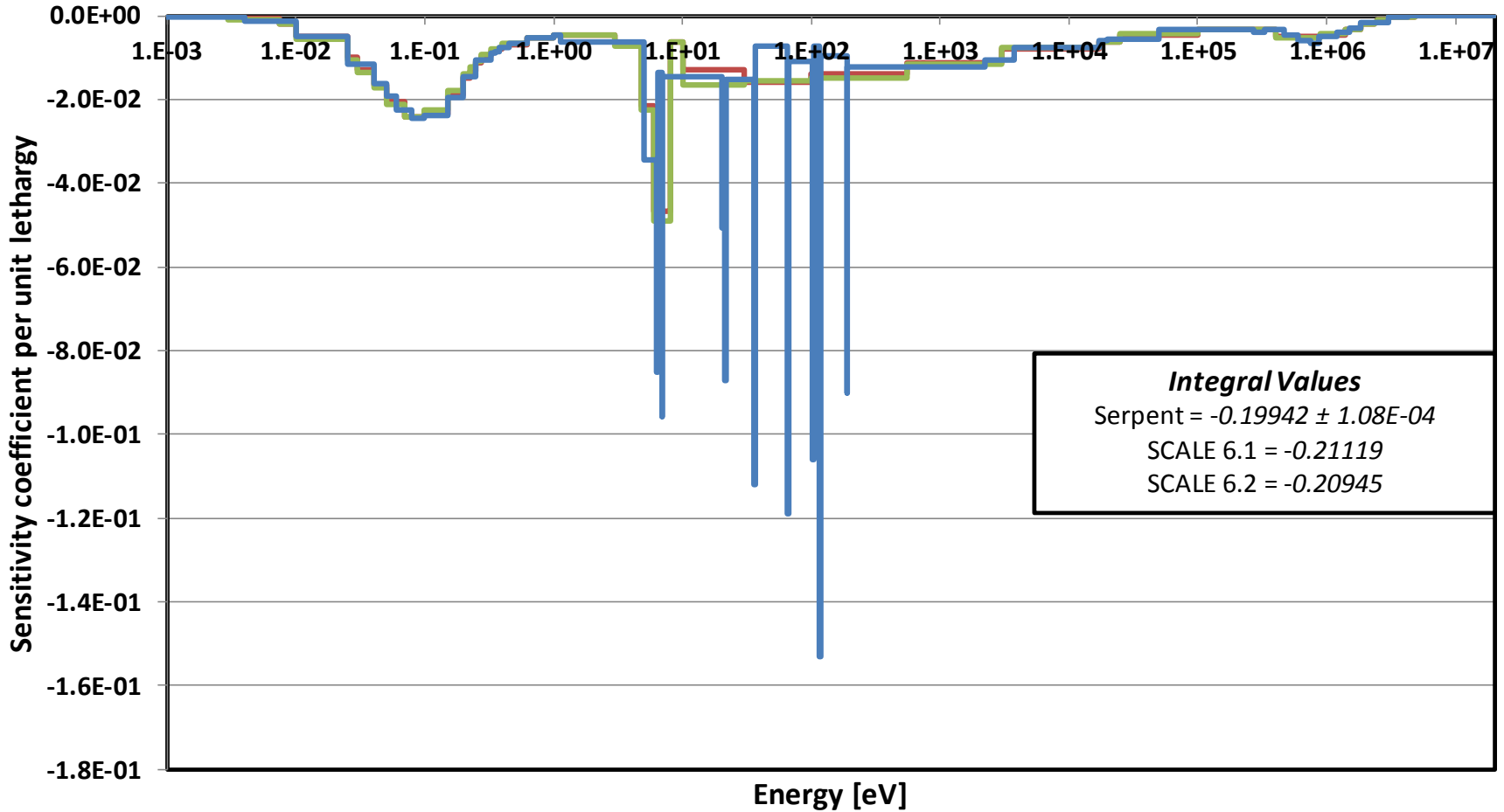
— SERPENT 44 groups — SCALE 6.1 - 44 groups — SCALE 6.2 - 56 groups

TMI Pin - k_{eff} - ^{238}U (n, γ)



— SERPENT 44 groups — SCALE 6.1 - 44 groups

TMI Pin - k_{eff} - ^{238}U (n, γ)



— SERPENT 44 groups

— SCALE 6.1 - 44 groups

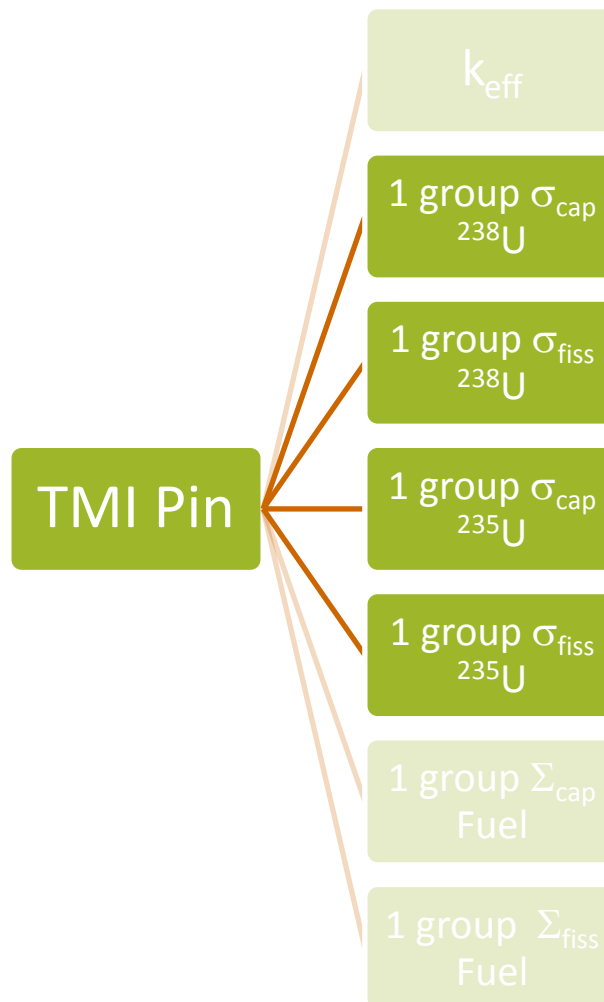
— SCALE 6.2 - 56 groups

Uncertainty quantification – TMI Pin - k_{eff}

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

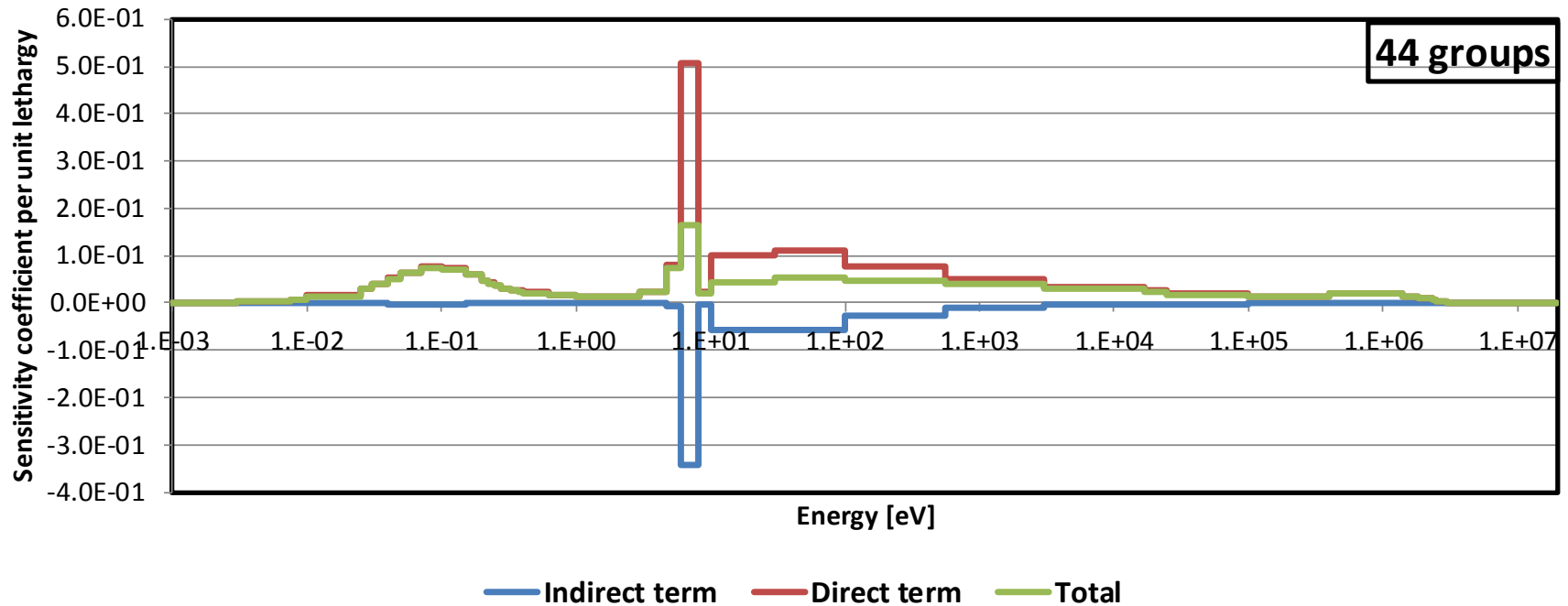
SERPENT 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
k_{eff}	% $\Delta k/k$	k_{eff}	% $\Delta k/k$	k_{eff}	% $\Delta k/k$
$1.43018 \pm 4\text{E-}05$	0.467%	1.42394	0.483%	1.42441	0.542%

Uncertainty quantification



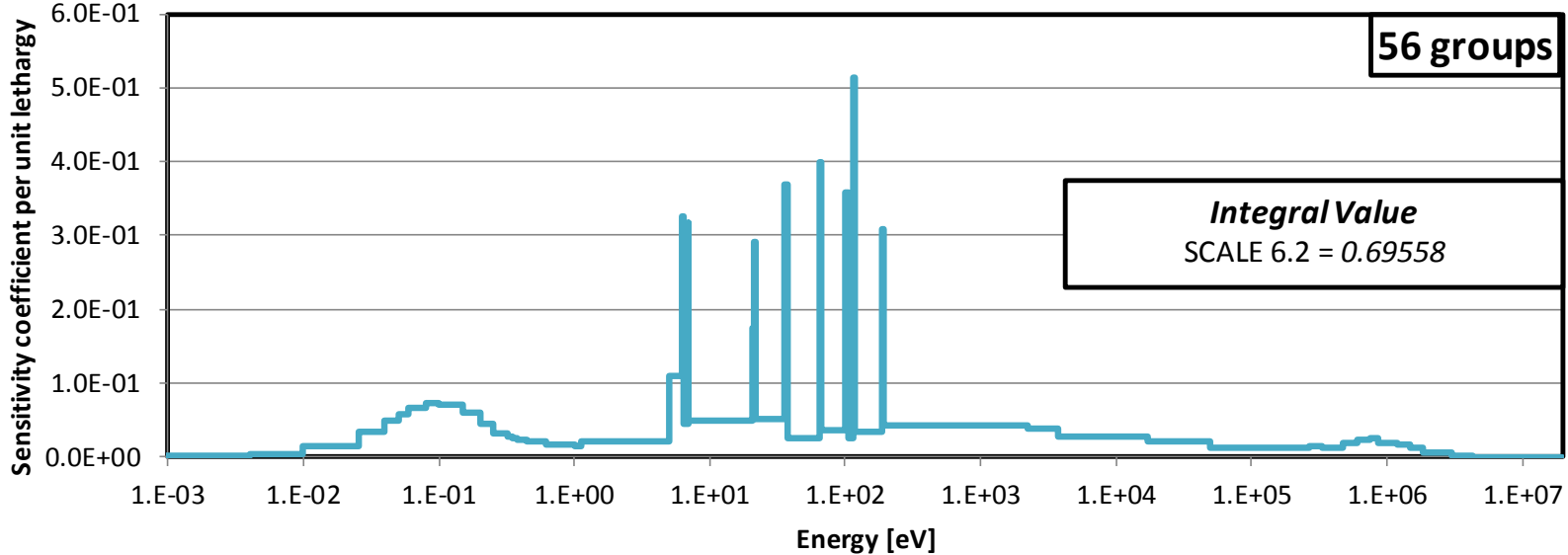
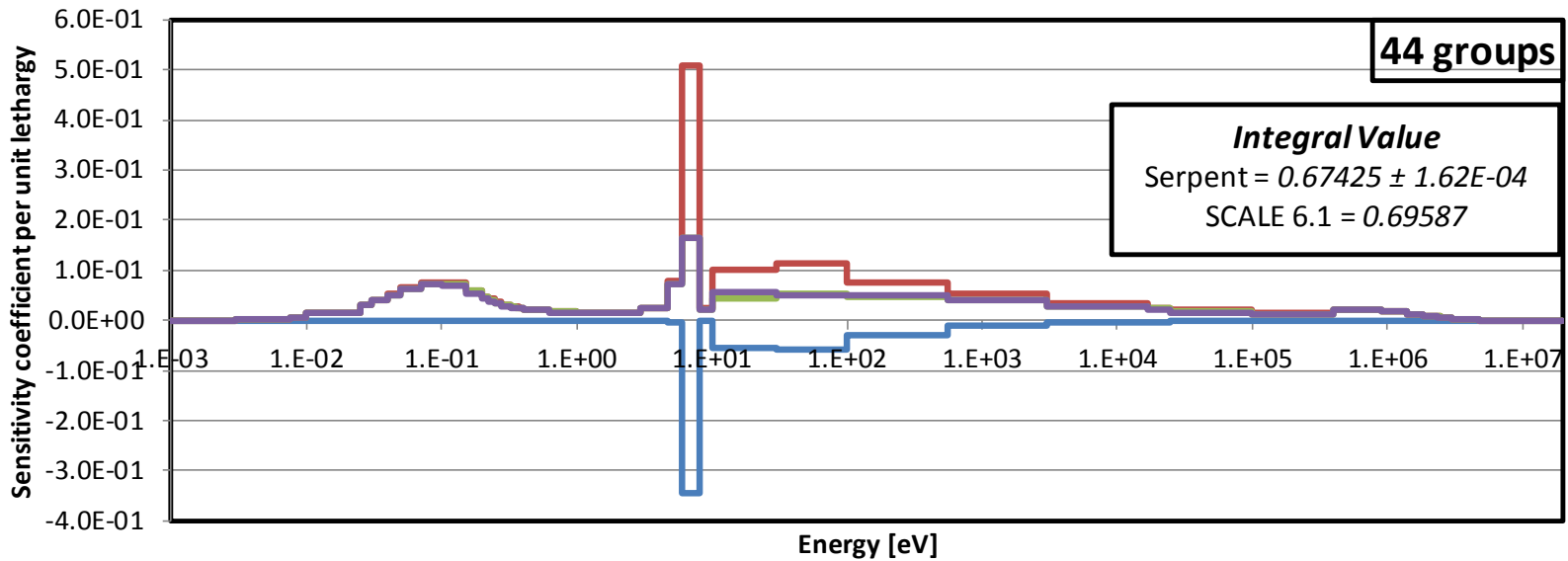
Direct and indirect effects

- 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

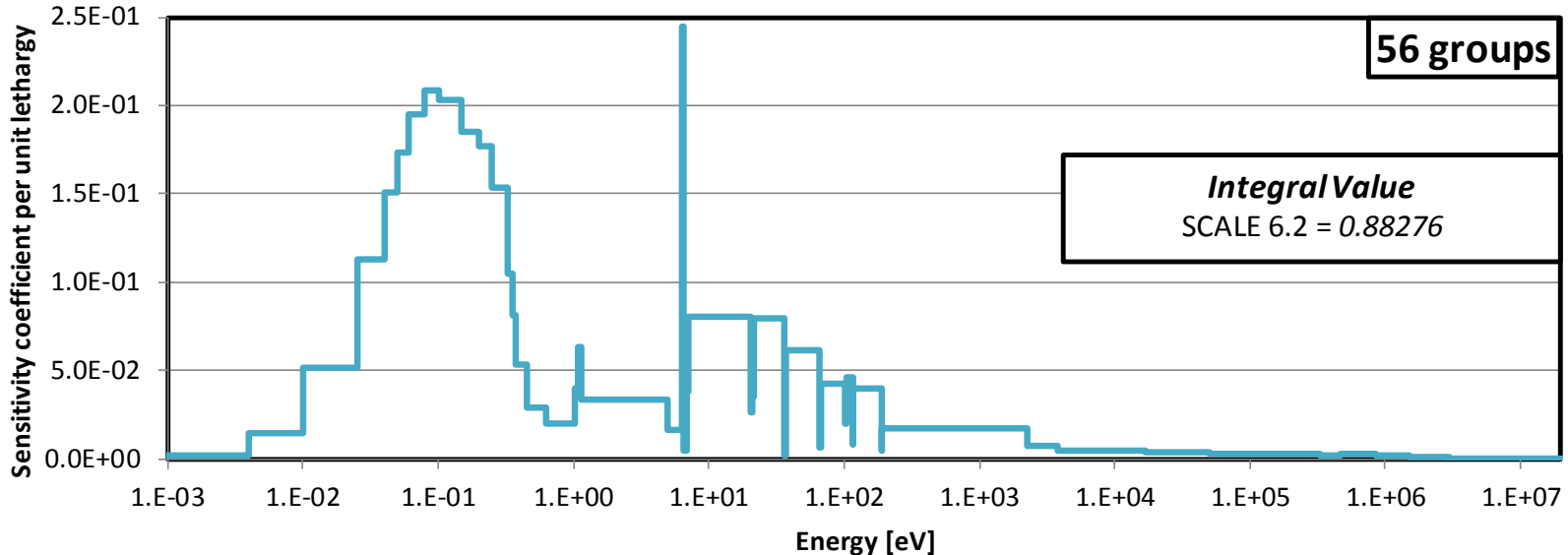
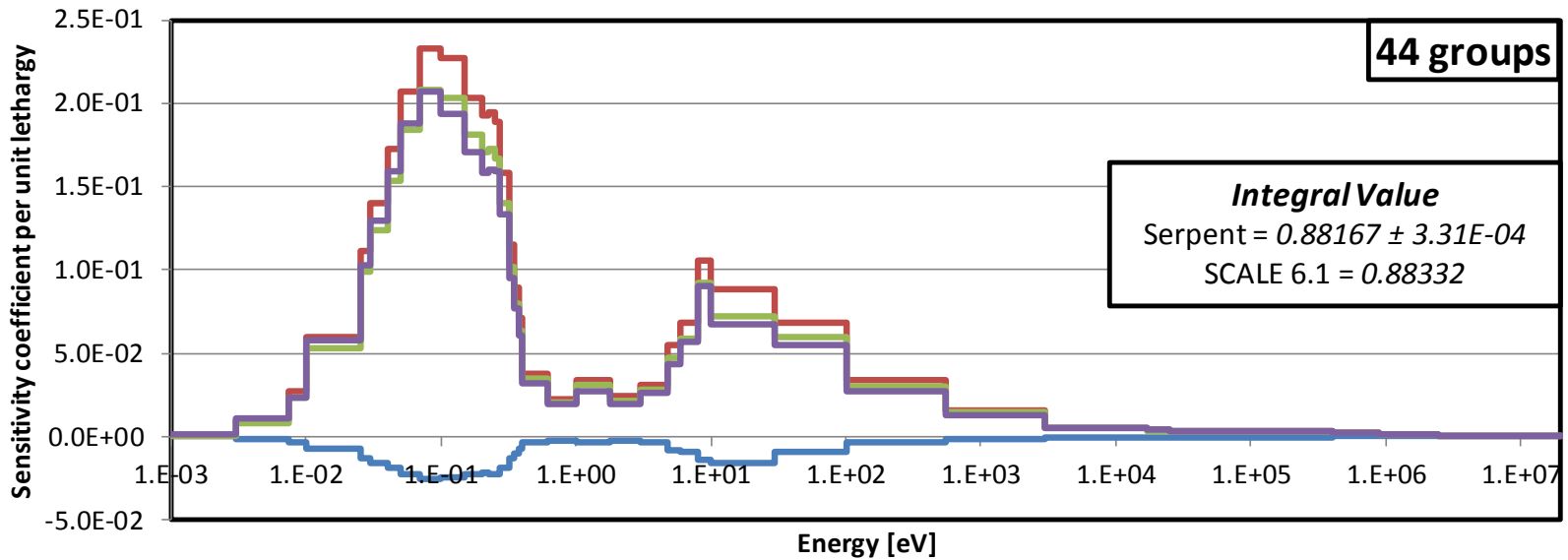


The **indirect term** is negative because an increase in the cross-section data enhances the local depression of the neutron flux, causing a decrease of the 1 group σ

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

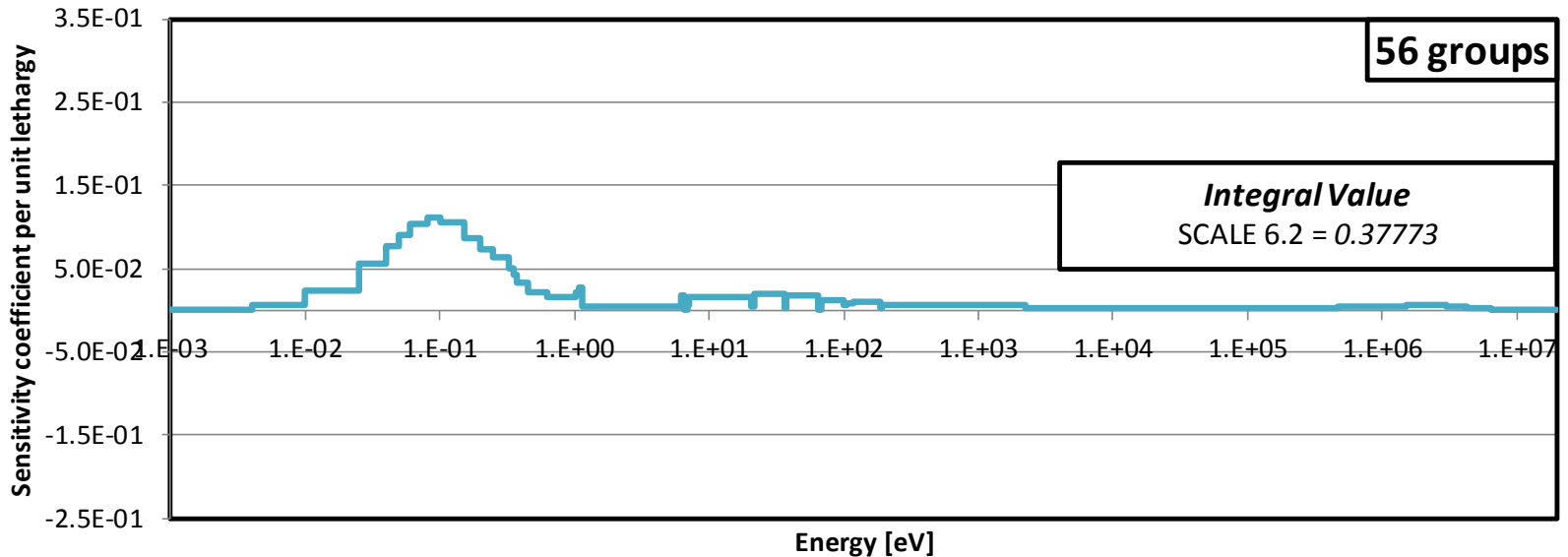
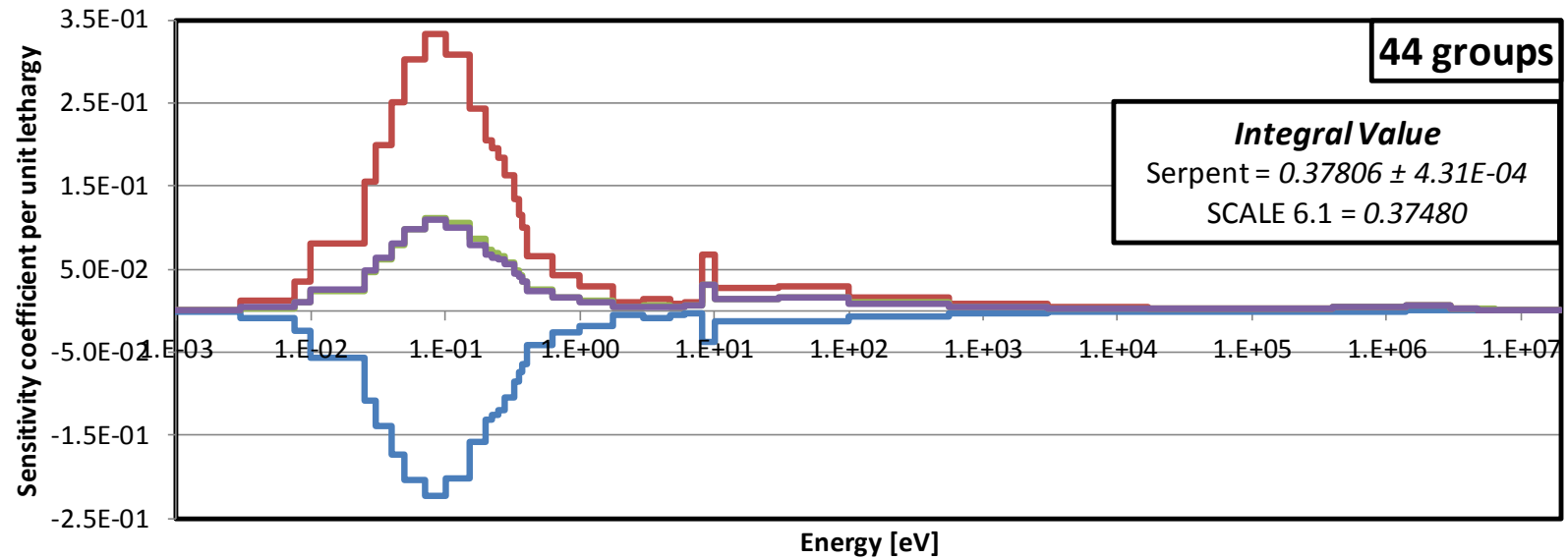


— Serpent - Indirect term
 — Serpent - Direct term
 — Serpent - Total
 — SCALE 6.1
 — SCALE 6.2

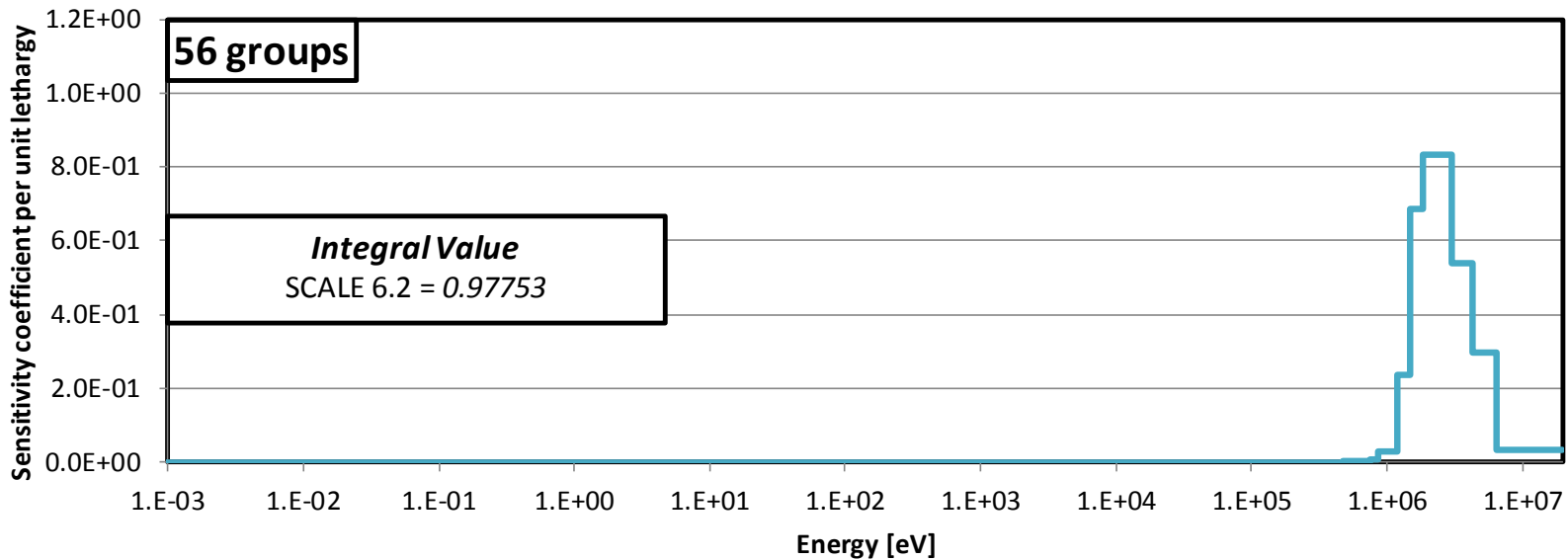
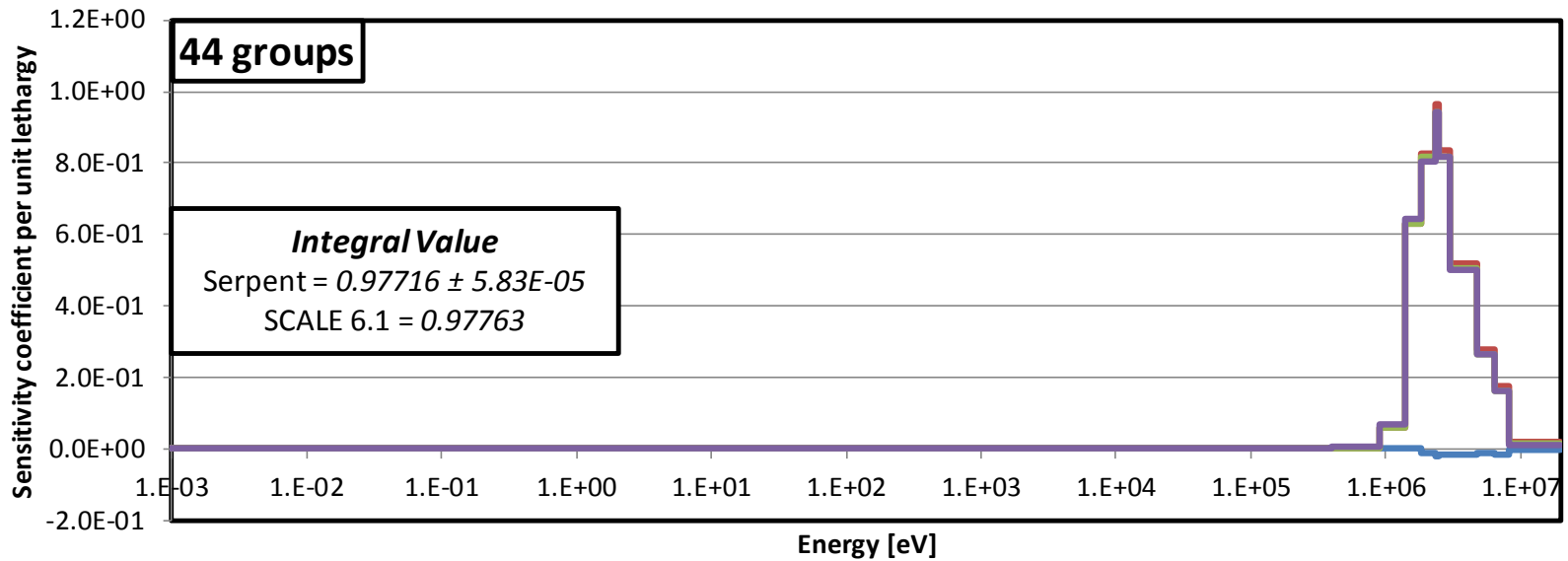


— Serpent - Indirect term
 — Serpent - Direct term
 — Serpent - Total
 — SCALE 6.1
 — SCALE 6.2

Results – TMI Pin – $\sigma_{fiss, U235}$ sensitivity to ^{235}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 σ

$\sigma_{\text{capt, U235}}$		SERPENT 44 groups	SCALE 6.1 44 groups	SCALE 6.2 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 44 groups	SCALE 6.1 44 groups	SCALE 6.2 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 44 groups	SCALE 6.1 44 groups	SCALE 6.2 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 44 groups	SCALE 6.1 44 groups	SCALE 6.2 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 σ

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%

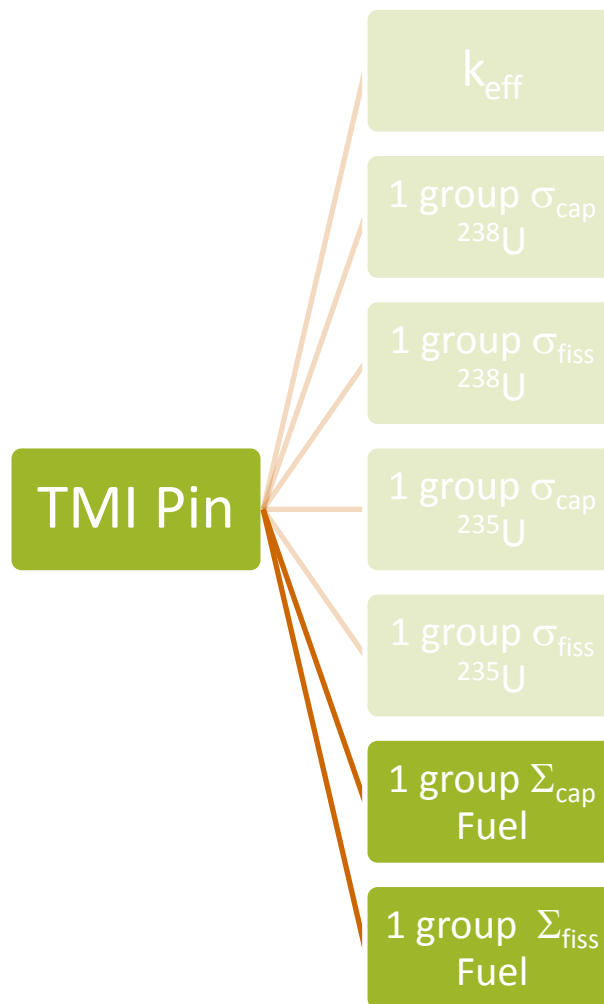
SERPENT 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\sigma_{\text{fiss, U235}}$	Total RSD (%)	$\sigma_{\text{fiss, U235}}$	Total RSD (%)	$\sigma_{\text{fiss, U235}}$	Total RSD (%)
$3.517E+01 \pm 5E-05$	1.145 %	3.532E+01	1.140%	3.517E+01	1.252%

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 Σ

$\Sigma_{\text{capt, Fuel}}$		SERPENT 44 groups	SCALE 6.1 44 groups	SCALE 6.2 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 44 groups	SCALE 6.1 44 groups	SCALE 6.2 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 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\Sigma_{\text{capt, Fuel}}$	Total RSD (%)	$\Sigma_{\text{capt, Fuel}}$	Total RSD (%)	$\Sigma_{\text{capt, Fuel}}$	Total 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 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\Sigma_{\text{fiss, Fuel}}$	Total RSD (%)	$\Sigma_{\text{fiss, Fuel}}$	Total RSD (%)	$\Sigma_{\text{fiss, Fuel}}$	Total 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}U nubar, ^{238}U & ^{235}U χ and ^1H (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}U nubar and ^{238}U (n, γ) are the major contributors in k_{eff} uncertainty. With the used options in SCALE, ^{238}U (n, γ) uncertainty may be slightly overestimated.
- ^{238}U (n,n') has a strong influence on the uncertainty of homogenized cross sections (both in pin and assembly). Also ^1H (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!