Sensitivity Computation with Monte Carlo Methods
(Action C8, WPEC/Sg.39)

IRSN
INSTITUT DE RADIOPROTECTION ET DE SÛRETÉ NUCLÉAIRE
Faire avancer la sûreté nucléaire

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General Remarks

- **Objective** of the exercise is to test continuous energy (CE) cross-section sensitivities and continuous angular distribution sensitivity capabilities implemented in Monte Carlo codes

- Monte Carlo (MC) tools compute CE sensitivity coefficients in terms of Fréshet derivatives, i.e., physical meaning of the coefficient is linear response of k_{eff} on multiplication of cross sections profile on a scalar value

- In contrary with deterministic approaches, Monte Carlo perturbation theory does not use the following bi-orthogonal ration below, where i, j are orders of modes

$$\left\langle \lambda_i \cdot \hat{\mathbf{F}} \cdot \vec{\mathbf{\Phi}}_i , \vec{\mathbf{\Psi}}_j \right\rangle = \left\langle \lambda_j \cdot \hat{\mathbf{F}}^{+} \cdot \vec{\mathbf{\Psi}}_j , \vec{\mathbf{\Phi}}_i \right\rangle = a_{i,j} \cdot \delta_{ij}$$

Selected ICSBEP Benchmarks

- **Popsy** (Flattop-Pu) is a plutonium (94 wt% ^{239}Pu) sphere surrounded by a thick reflector of natural uranium.
  - PU-MET-FAST-006. **Spherical model.**
- **Topsy** (Flattop 25) is a highly enriched (93 wt%) uranium sphere surrounded by a thick reflector of natural uranium.
  - HEU-MET-FAST-028. **Spherical model**.
- **ZPR 9/34** loading 303 is a highly enriched uranium/ iron benchmark, reflected by steel.
  - HEU-MET-INTER-001. **RZ model.**
- **ZPR 6/10** loading 24 is the core with heterogeneous plutonium metal fuel with carbon/stainless steel dilutions, and a steel reflector.
  - PU-MET-INTER-002. **RZ model.**

Codes, Methods, Participants

MONK:	MC Fine-group Derivative operator sampling	AWE
SERPENT v2:	MC CE Iterated Fission Probability (IFP)	PSI
ANISN/PARTISN:	Deterministic MG	IJS
SCALE 6.1/TSUNANI-1D:	Deterministic SN MG	IRSN
SCALE 6.1/TSUNAMI-3D:	MC MG	IRSN
SCALE 6.2β:	MC CE IFP	ORNL, PSI, IRSN
SCALE 6.2β:	MC CE CLUTCH	ORNL, PSI, IRSN
MCNP6:	MC CE IFP	LANL, NEA, IRSN

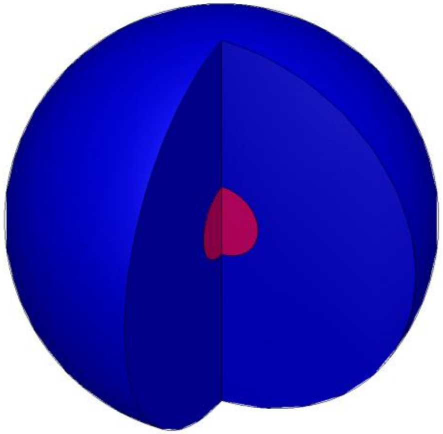
Profiles Computations

Participant	Tool	Model	Cross sections	Method	Output, groups
AWE	MONK	3D	CE ENDF/B-VII.0 JEFF3.1	MC	33
PSI	SERPENT v2	3D	CE ENDF/B-VII	MC	33
NEA, LANL, IRSN	MCNP6	3D	CE, ENDF/B-VII.1	MC	238, 33
IRSN	SCALE 6.1	1D	MG, ENDF/B-VII.0	SN	238
PSI, ORNL, IRSN	SCALE 6.2β	3D	CE, ENDF/B-VII.1, 0	MC	238
JSI	ANISN/PARTISN	1D	See presentation by I. Kodeli	SN	33

- 238-gr. sensitivities converted into 33 gr. by IRSN BERING code (E. Ivanov)
- 33-gr. sensitivities converted to SCALE/sdf format by IRSN scripts (E. Ivanov)
- MCNP6 output converted into SCALE/sdf format by NEA script (I. Hill)
- Sensitivity profiles are presented using SCALE/Javapeno that reads *.sdf

PMF-006 (Flattop-Pu or Popsy)

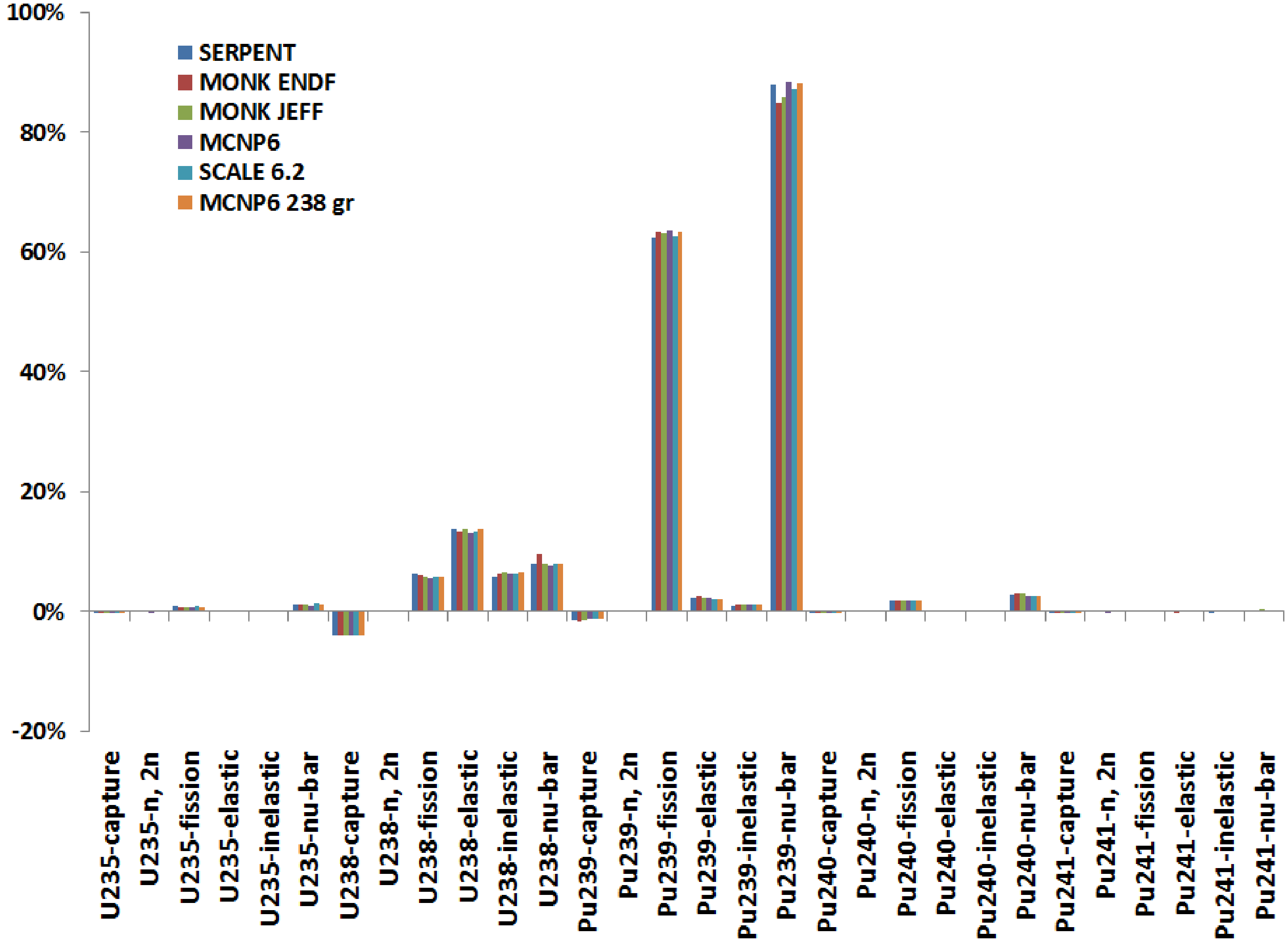
- Plutonium (94 wt ^{239}Pu) sphere surrounded by a thick reflector of natural uranium. Sensitive to scattering on heavy metals, and threshold reactions.
- k_{bench}=1.0000±0.0030



Popsy: Integrated Sensitivities (1/3)

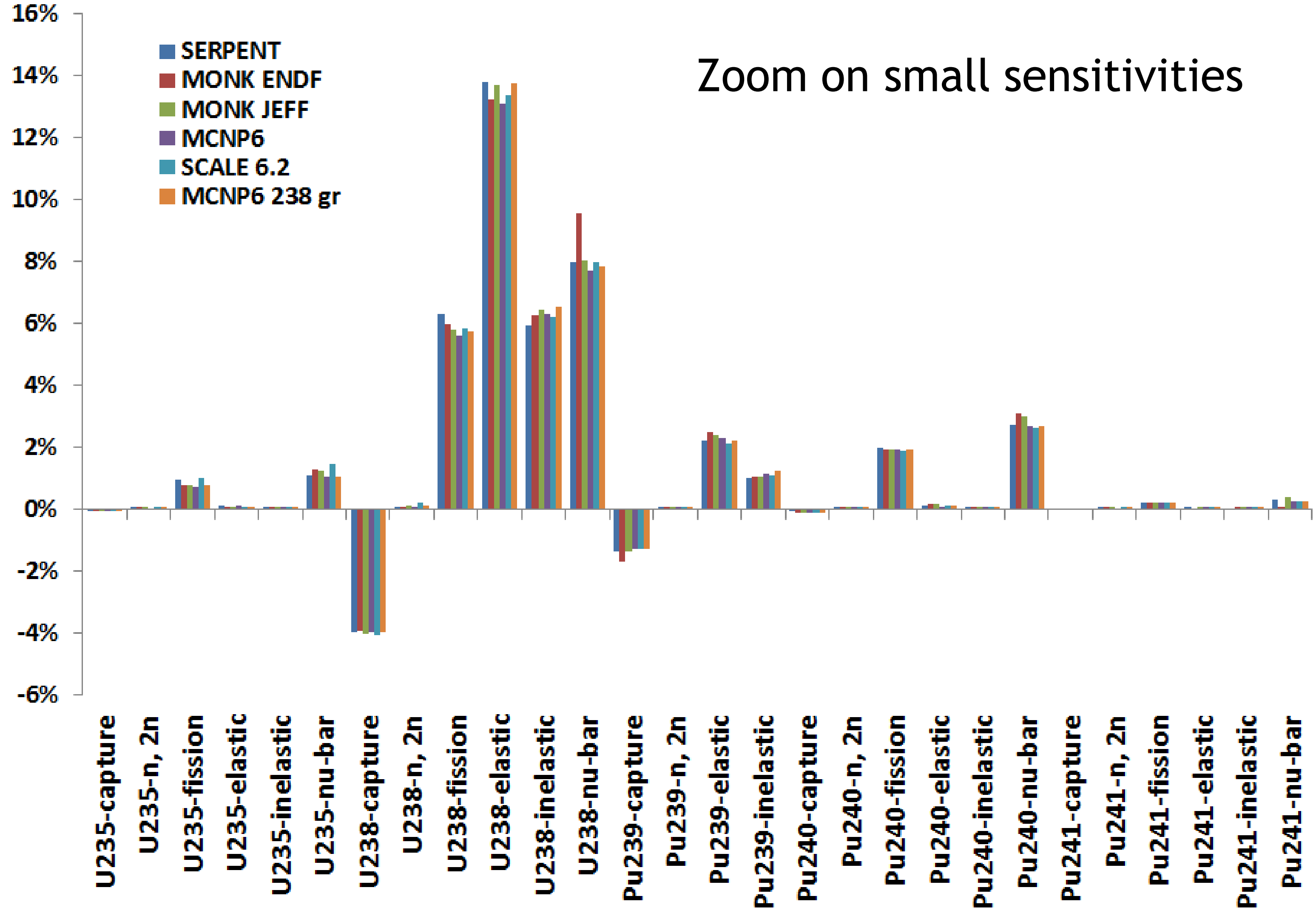
	SERPENT	MONK ENDF	MONK JEFF	MCNP6	SCALE 6.2	MCNP6 238 gr
U235-capture	-0,05	-0,06	-0,05	-0,05	-0,07	-0.05
U235-n, 2n	0,00	0,00	0,00	0,00	0,00	0.00
U235-fission	0,96	0,75	0,75	0,74	1,01	0.75
U235-elastic	0,09	0,07	0,08	0,12	0,08	0.08
U235-inelastic	0,03	0,03	0,03	0,02	0,02	0.03
U235-nu-bar	1,09	1,26	1,22	1,02	1,45	1.04
U238-capture	-4,00	-3,92	-4,04	-3,97	-4,08	-3.97
U238-n, 2n	0,08	0,07	0,10	0,06	0,19	0.10
U238-fission	6,30	5,99	5,81	5,62	5,82	5.73
U238-elastic	13,77	13,25	13,70	13,08	13,39	13.75
U238-inelastic	5,92	6,26	6,41	6,32	6,22	6.51
U238-nu-bar	7,95	9,58	8,03	7,71	7,98	7.83
Pu239-capture	-1,39	-1,71	-1,40	-1,28	-1,28	-1.29
Pu239-n, 2n	0,03	0,02	0,04	0,03	0,02	0.03
Pu239-fission	62,43	63,26	63,21	63,53	62,64	63.32
Pu239-elastic	2,22	2,49	2,37	2,32	2,13	2.19
Pu239-inelastic	1,01	1,06	1,04	1,13	1,10	1.24
Pu239-nu-bar	87,94	84,83	85,79	88,33	87,30	88.20
Pu240-capture	-0,09	-0,12	-0,10	-0,10	-0,10	-0.10
Pu240-n, 2n	0,00	0,00	0,00	0,00	0,00	0.00
Pu240-fission	1,95	1,94	1,91	1,91	1,88	1.91
Pu240-elastic	0,11	0,14	0,15	0,07	0,12	0.12
Pu240-inelastic	0,07	0,07	0,08	0,08	0,05	0.06
Pu240-nu-bar	2,73	3,10	3,00	2,66	2,62	2.65
Pu241-capture	-0,01	-0,01	-0,01	-0,01	-0,01	-0.01
Pu241-n, 2n	0,00	0,00	0,00	0,00	0,00	0.00
Pu241-fission	0,20	0,22	0,19	0,19	0,19	0.19
Pu241-elastic	0,01	0,00	0,01	0,01	0,01	0.01
Pu241-inelastic	0,00	0,00	0,00	0,01	0,00	0.01
Pu241-nu-bar	0,28	0,02	0,40	0,27	0,27	0.27

Popsy: Integrated Sensitivities (2/3)

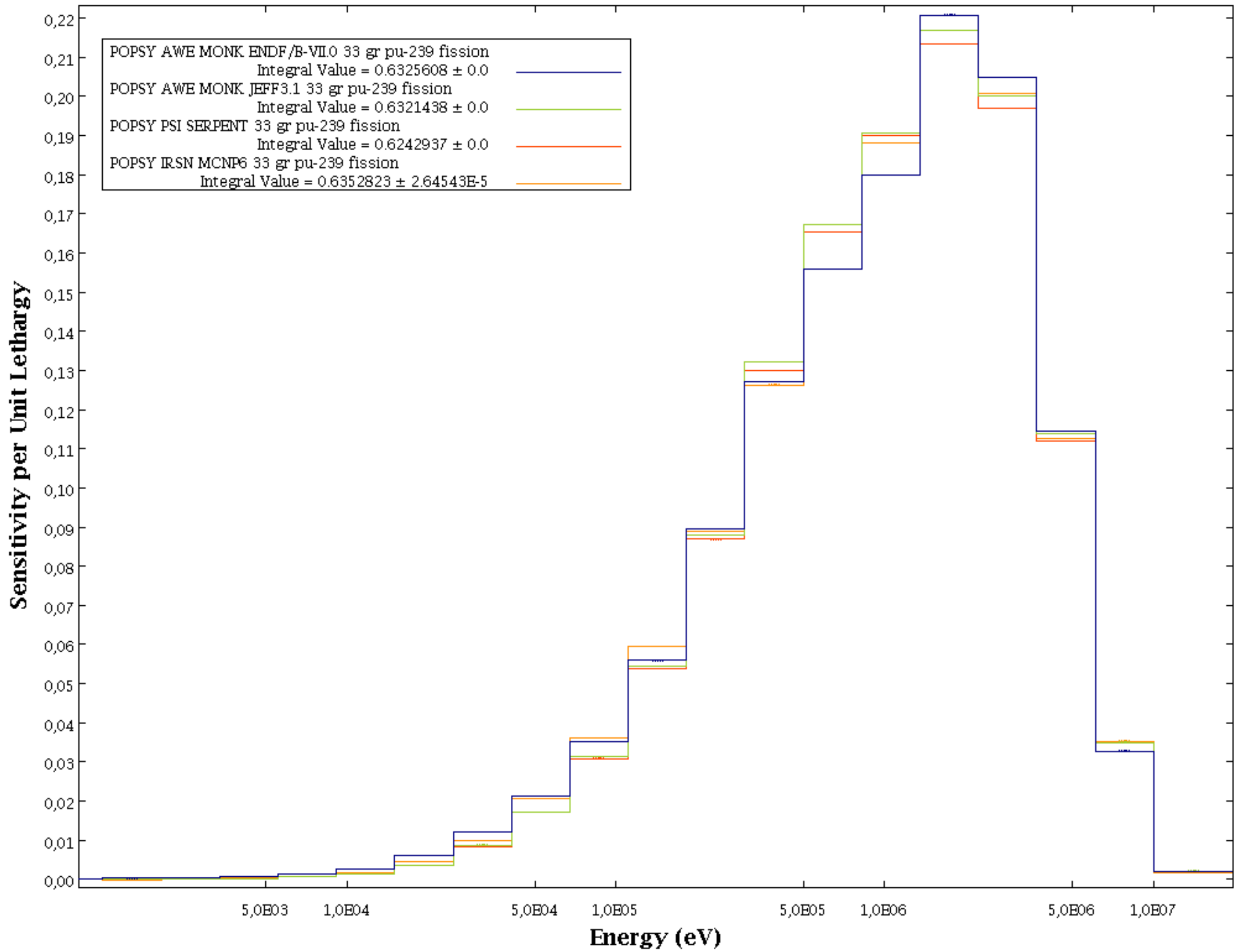


Popsy: Integrated Sensitivities (3/3)

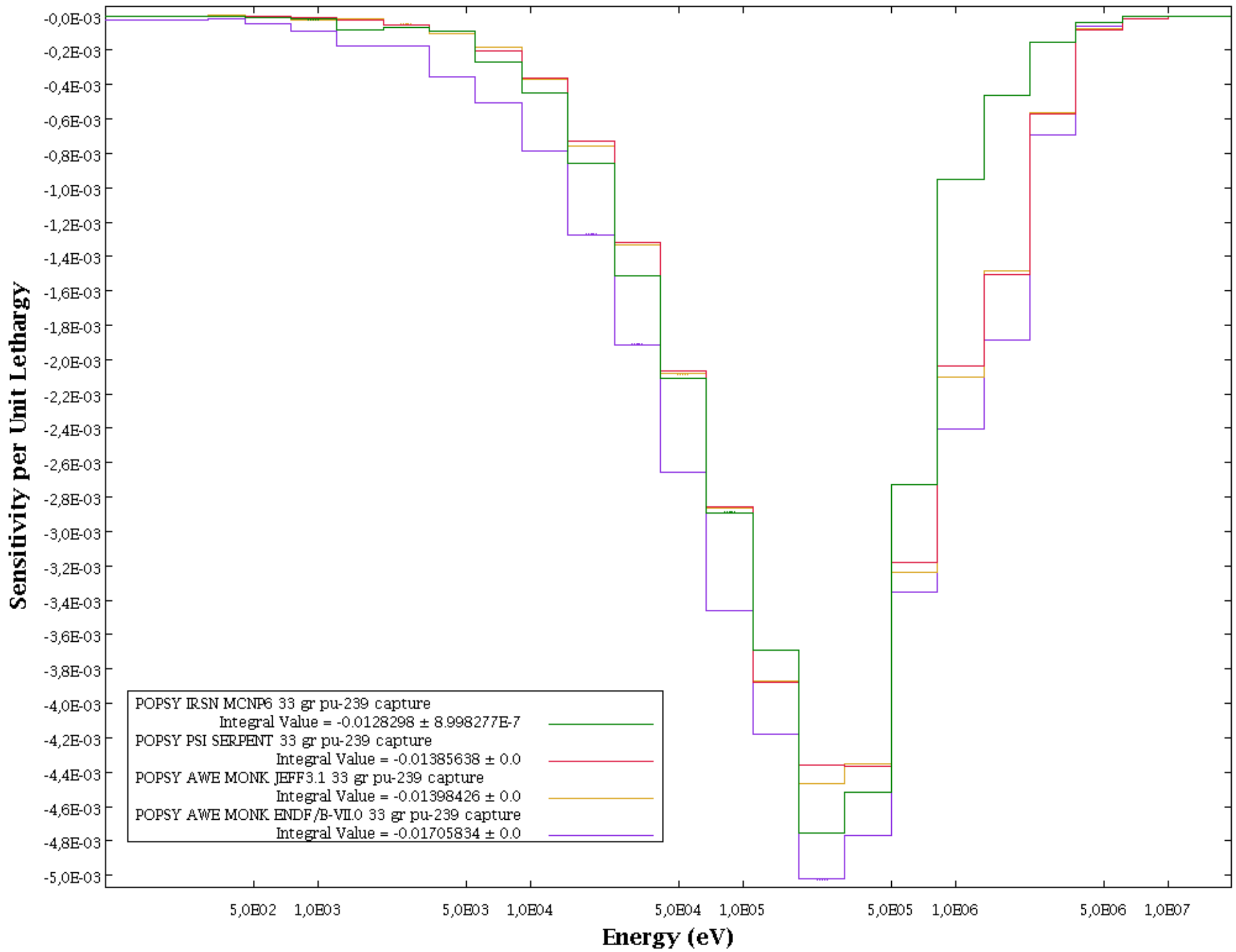
Zoom on small sensitivities



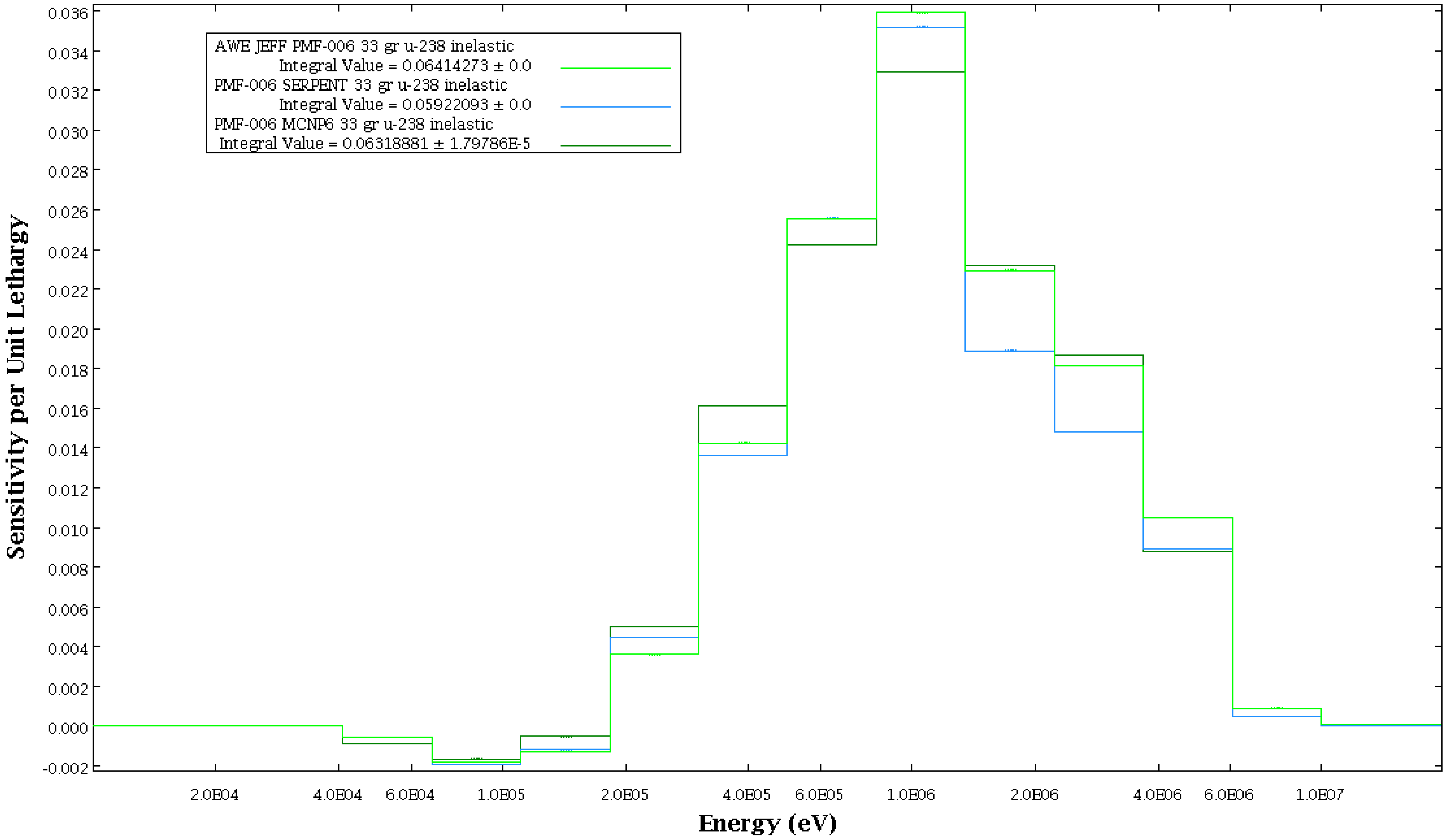
Popsy: Pu-239 Fission Profiles



Popsy: Pu-239 Capture Profiles



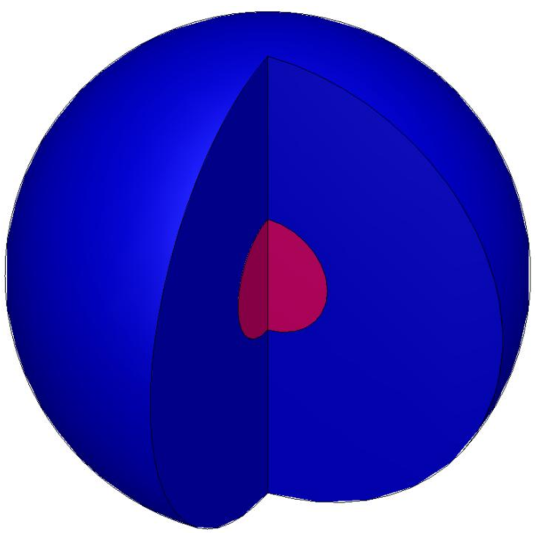
Popsy: U-238 Inelastic Profiles



HMF-028 (Flattop-25 or Topsy)

- **H**ighly enriched (93 wt%) uranium sphere surrounded by a thick reflector of natural uranium.

- k_{bench}=1.0000±0.0030



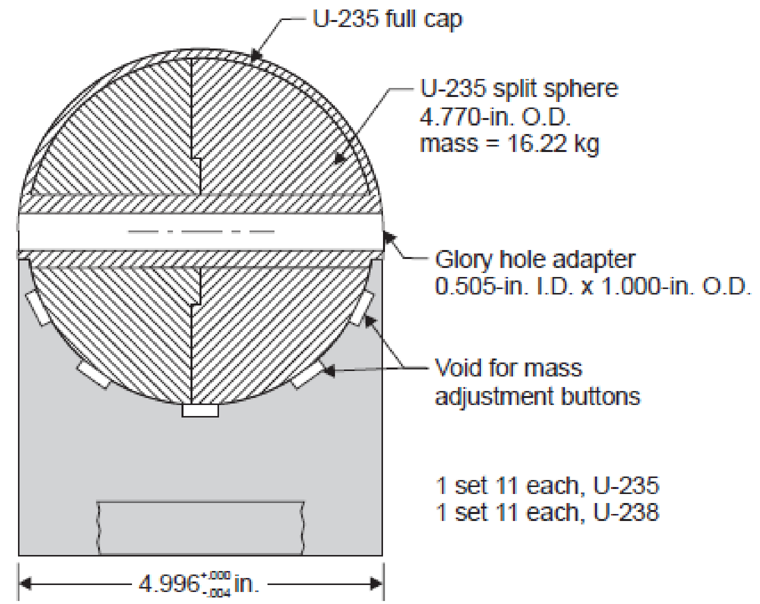
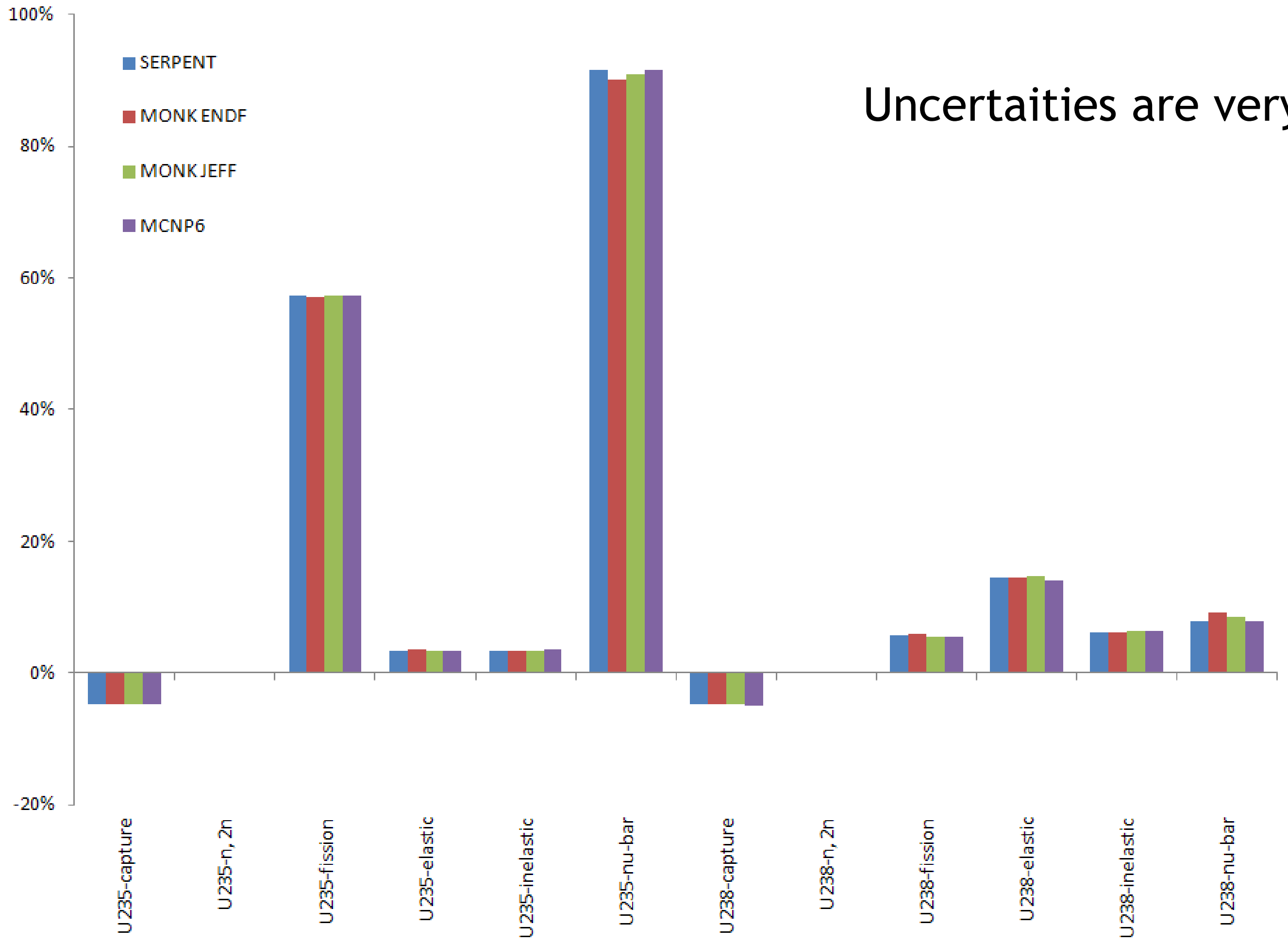


Figure 3. The HEU Sphere.

Topsy: Integrated Sensitivities (1/3)

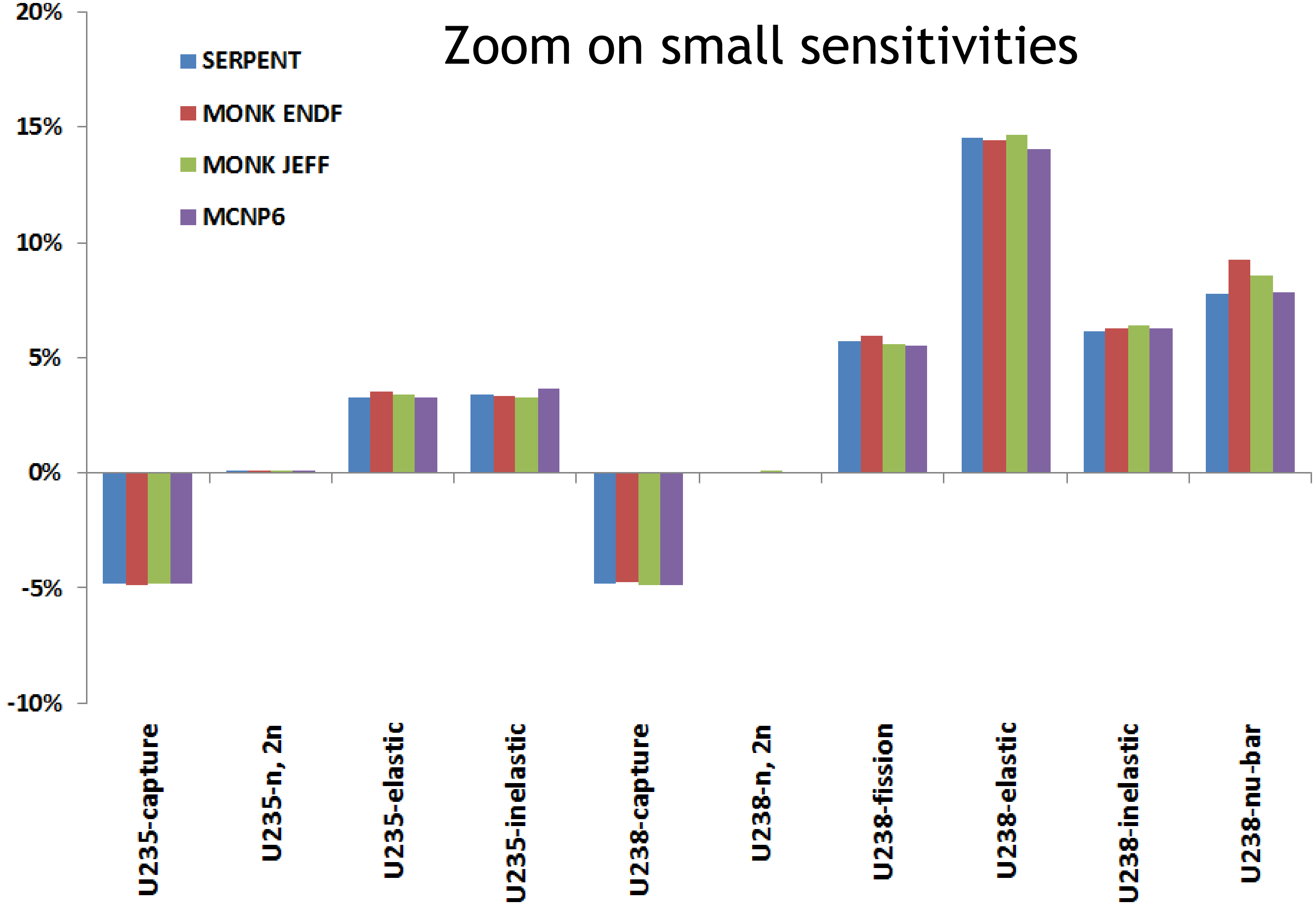
	SERPENT	MONK ENDF	MONK JEFF	MCNP6
U235-capture	-4,79	-4,87	-4,82	-4,84
U235-n, 2n	0,11	0,12	0,12	0,12
U235-fission	57,37	57,17	57,32	57,41
U235-elastic	3,30	3,54	3,43	3,30
U235-inelastic	3,39	3,34	3,28	3,63
U235-nu-bar	91,56	90,10	90,88	91,53
U238-capture	-4,83	-4,74	-4,88	-4,90
U238-n, 2n	0,07	0,05	0,08	0,04
U238-fission	5,72	5,95	5,61	5,54
U238-elastic	14,54	14,43	14,65	14,07
U238-inelastic	6,12	6,24	6,36	6,28
U238-nu-bar	7,78	9,23	8,57	7,81

Topsy: Integrated Sensitivities (2/3)

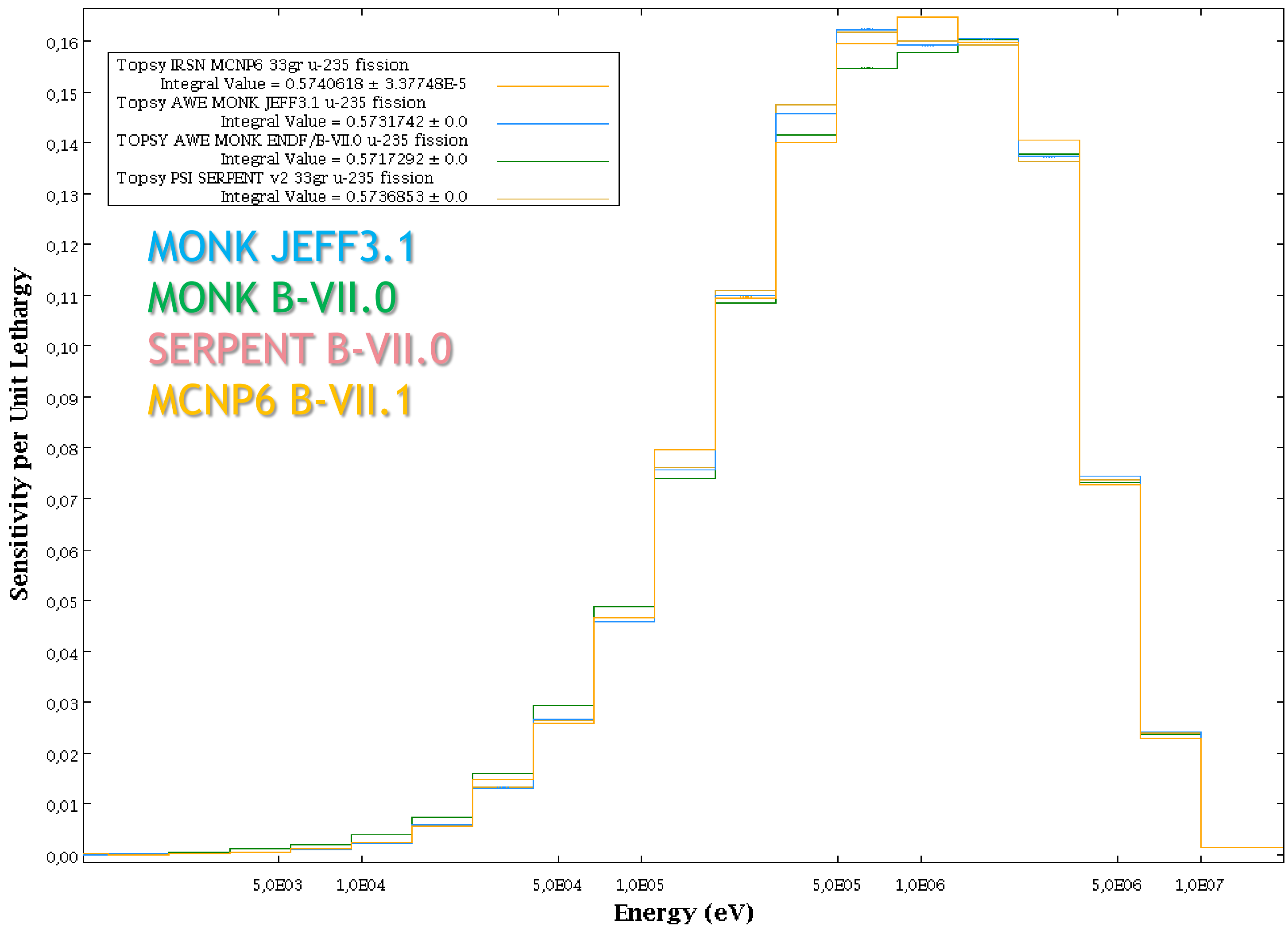


Uncertaities are very small

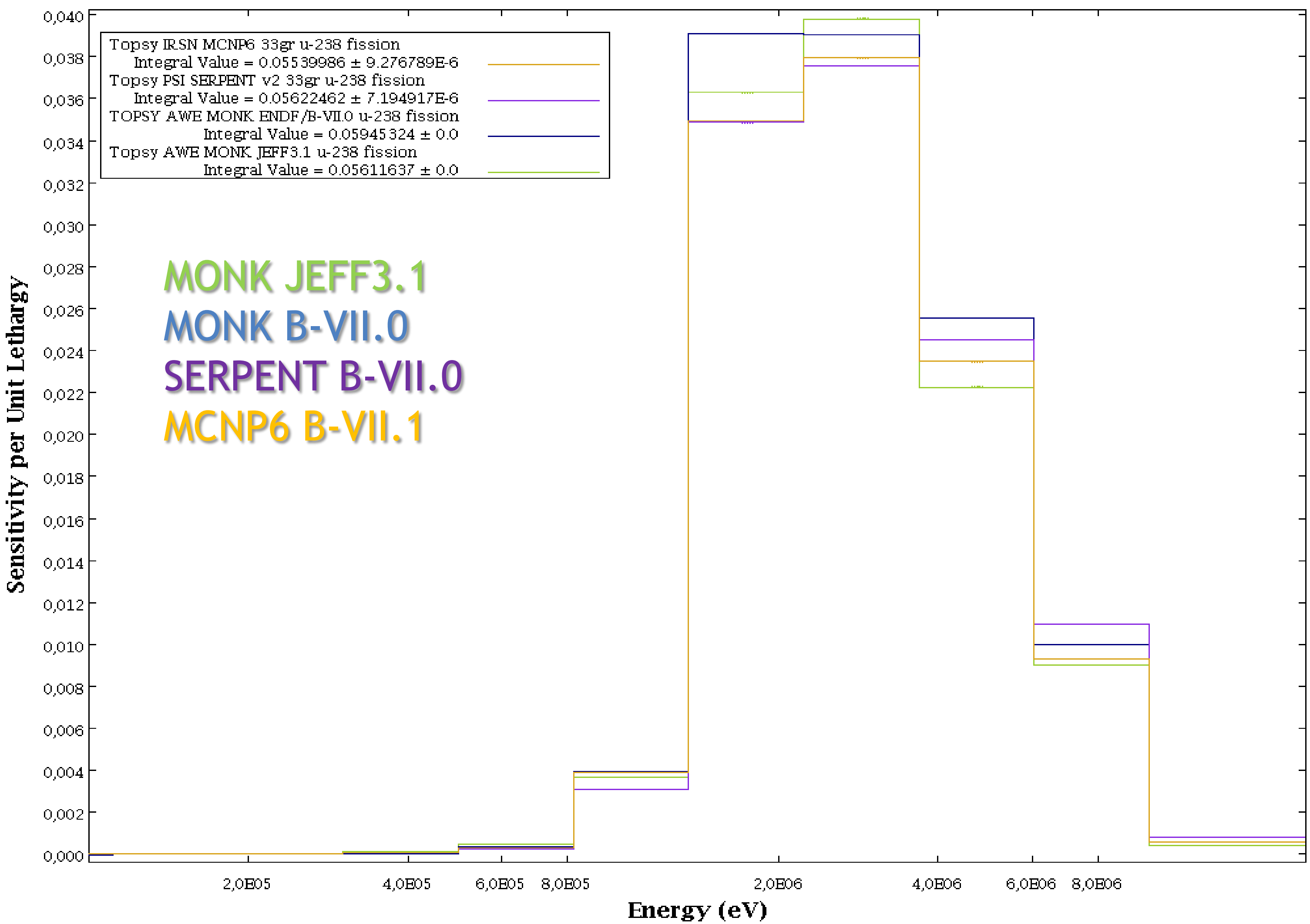
Topsy: Integrated Sensitivities (3/3)



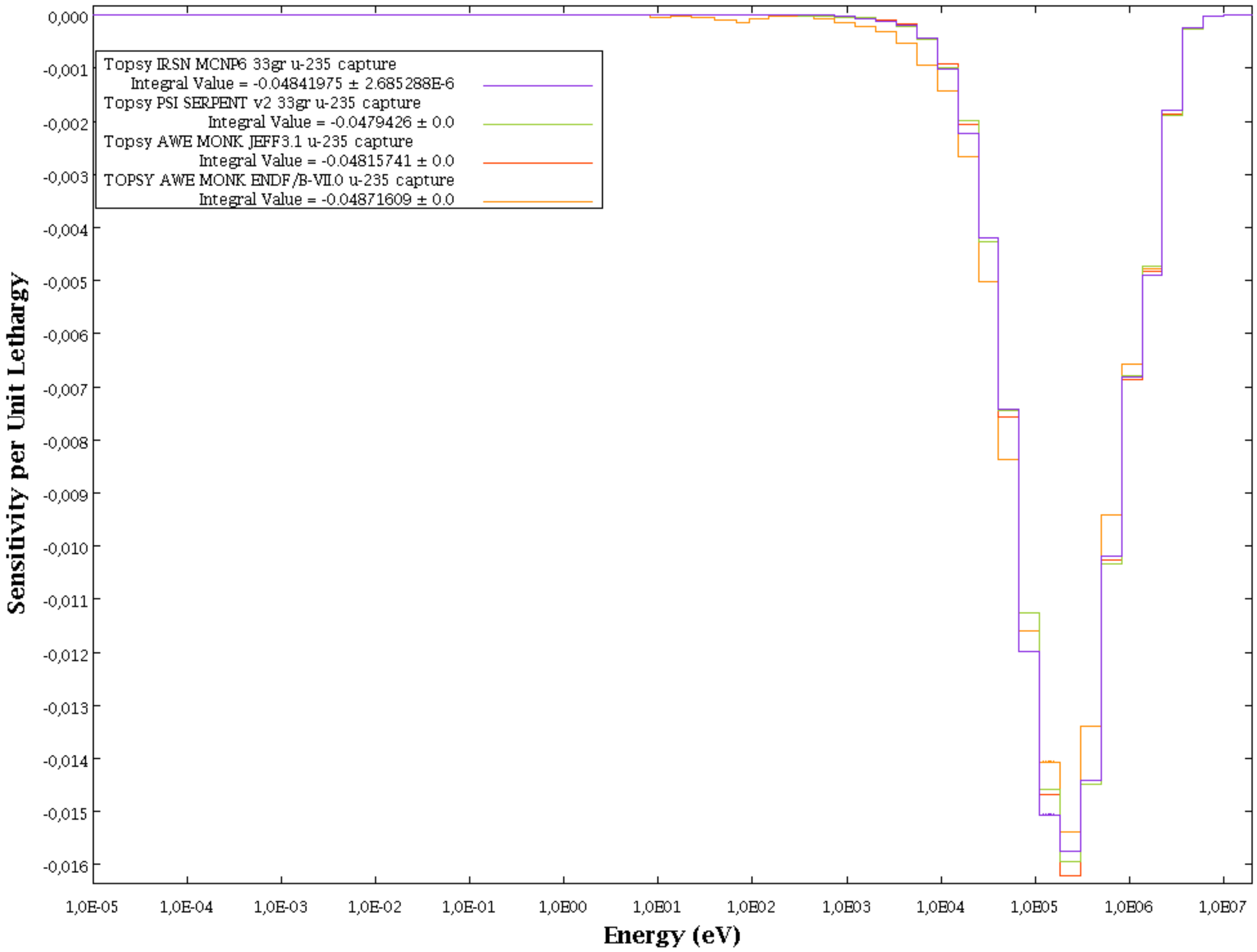
Topsy: U-235 Fission Profile



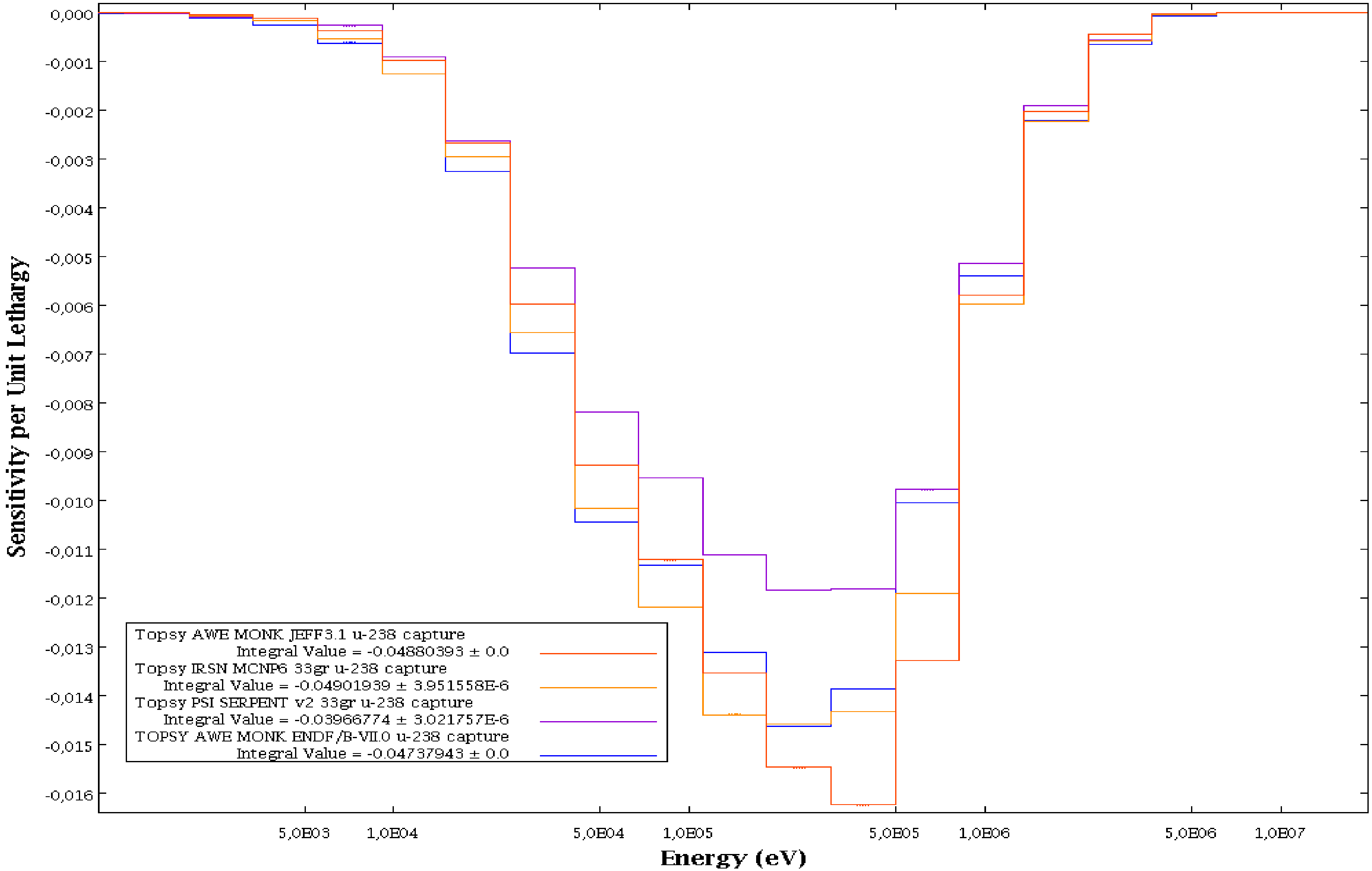
Topsy: U-238 Fission Profile



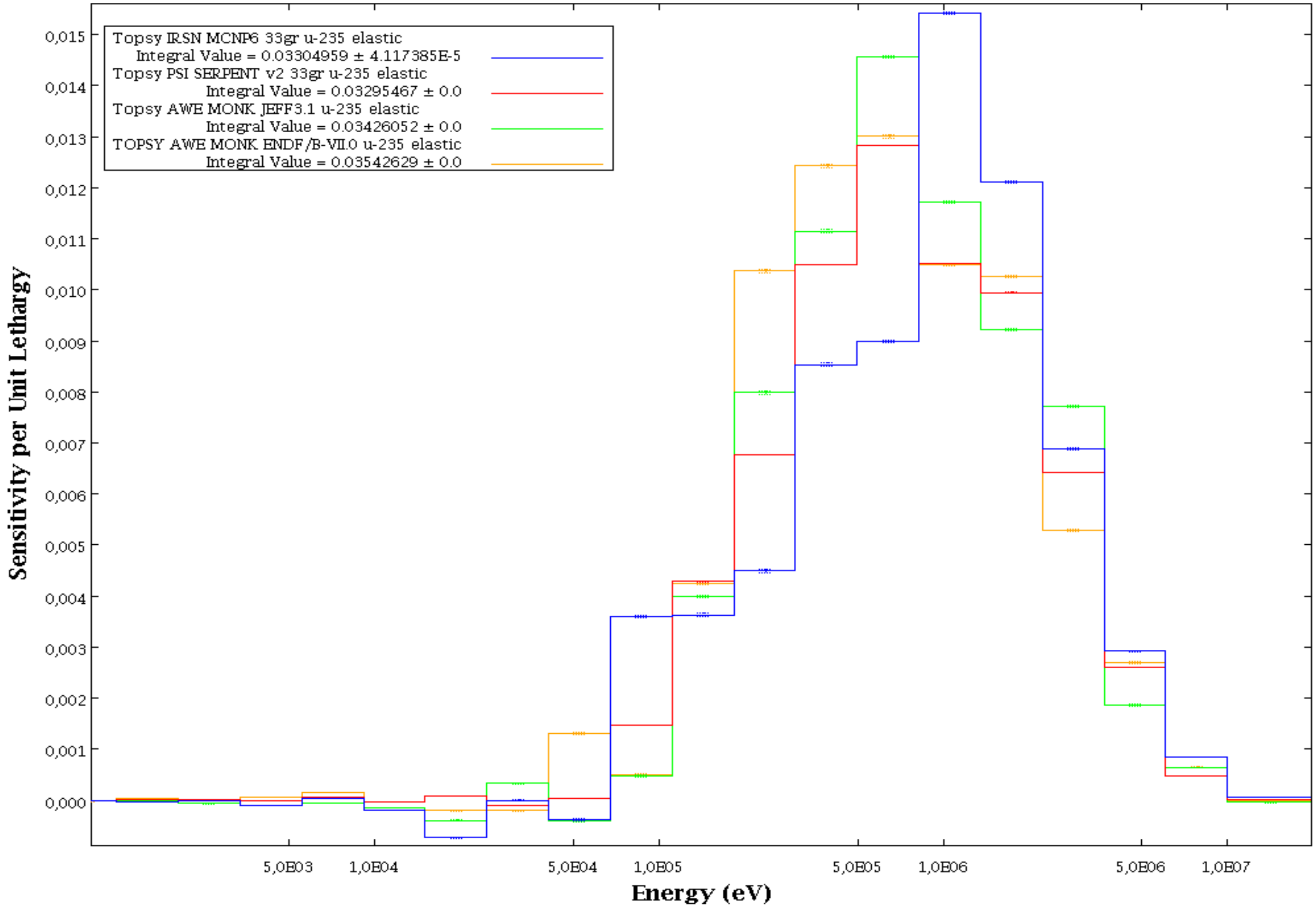
Topsy: U-235 Capture Profile



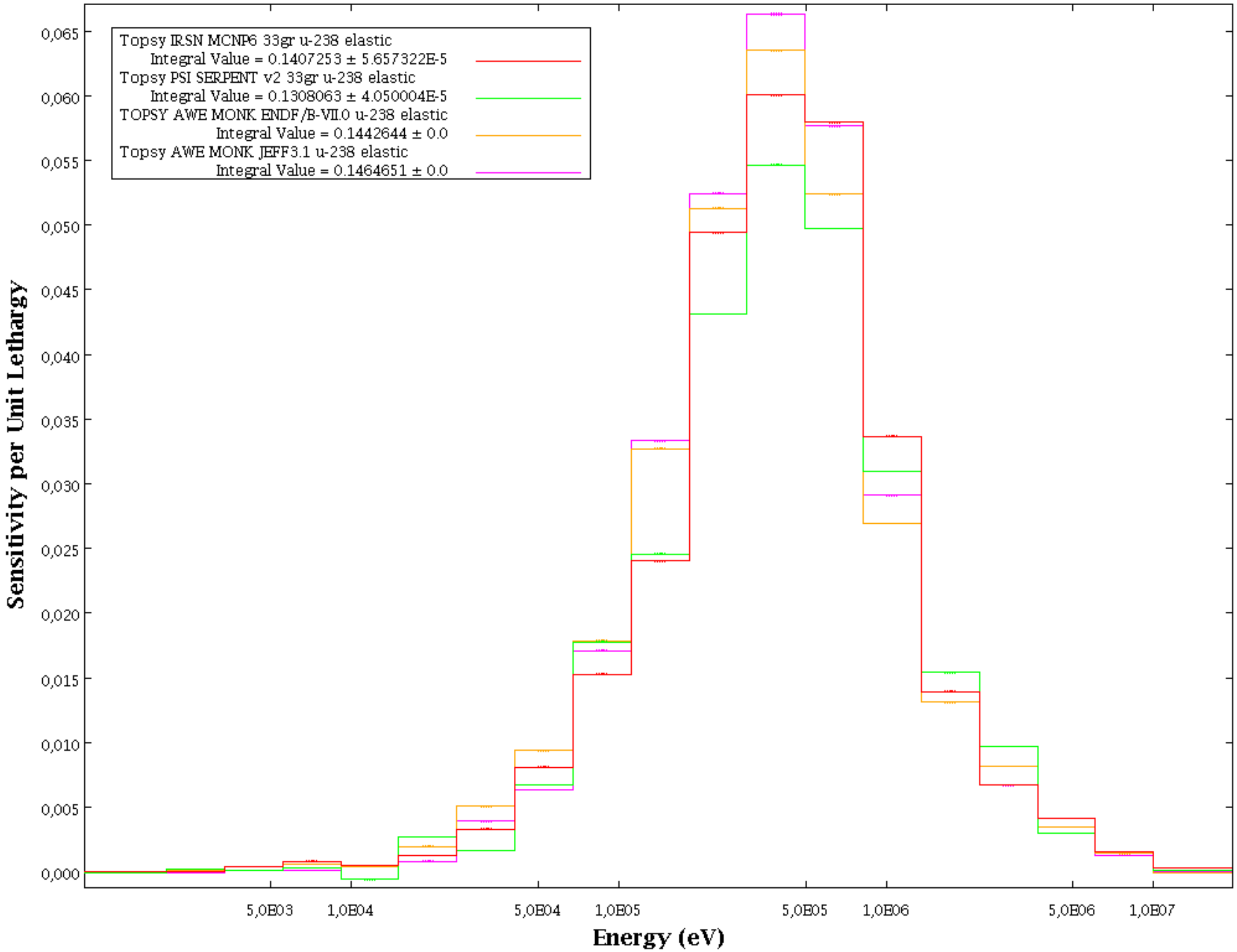
Topsy: U-238 Capture Profile



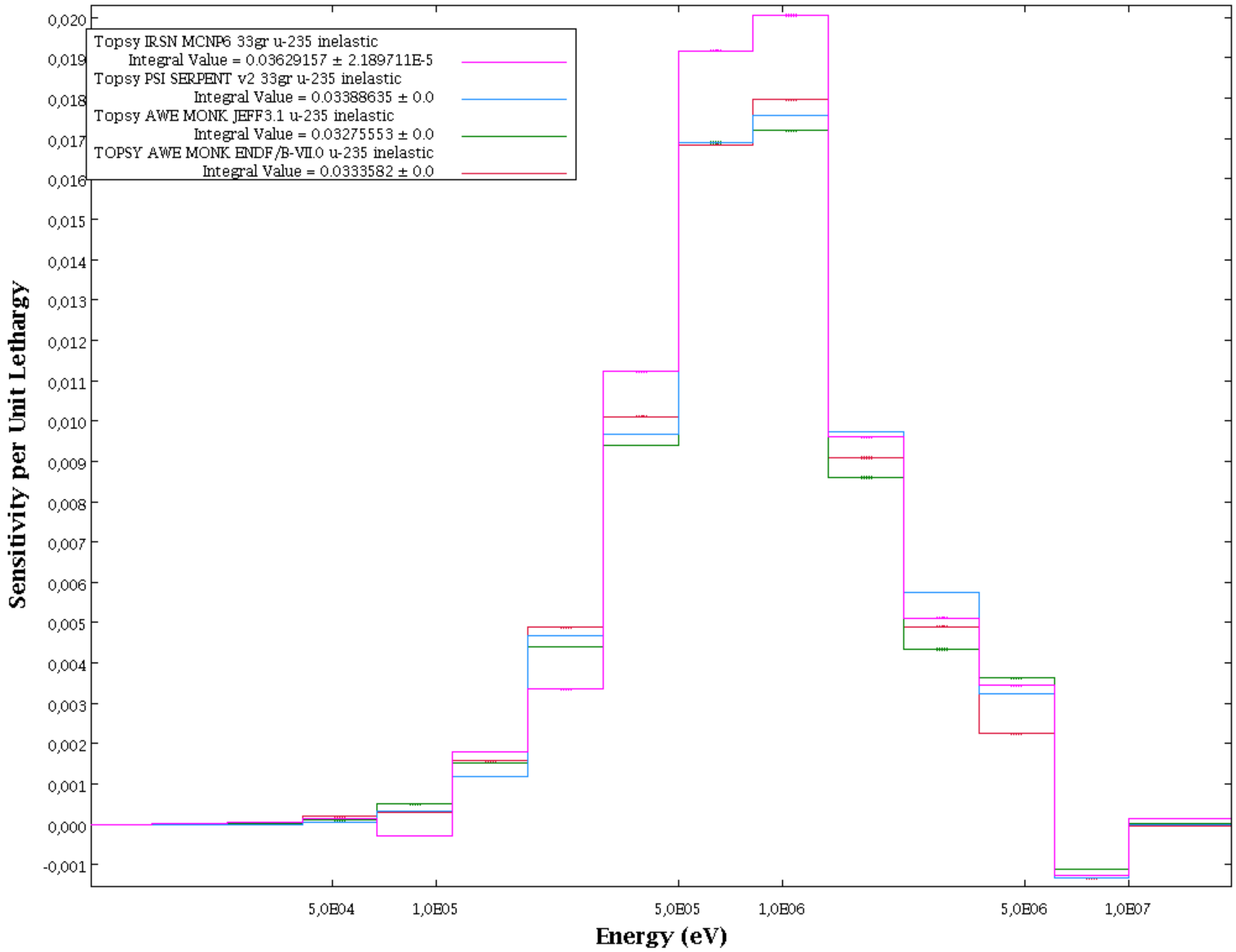
Topsy: U-235 Elastic Profiles



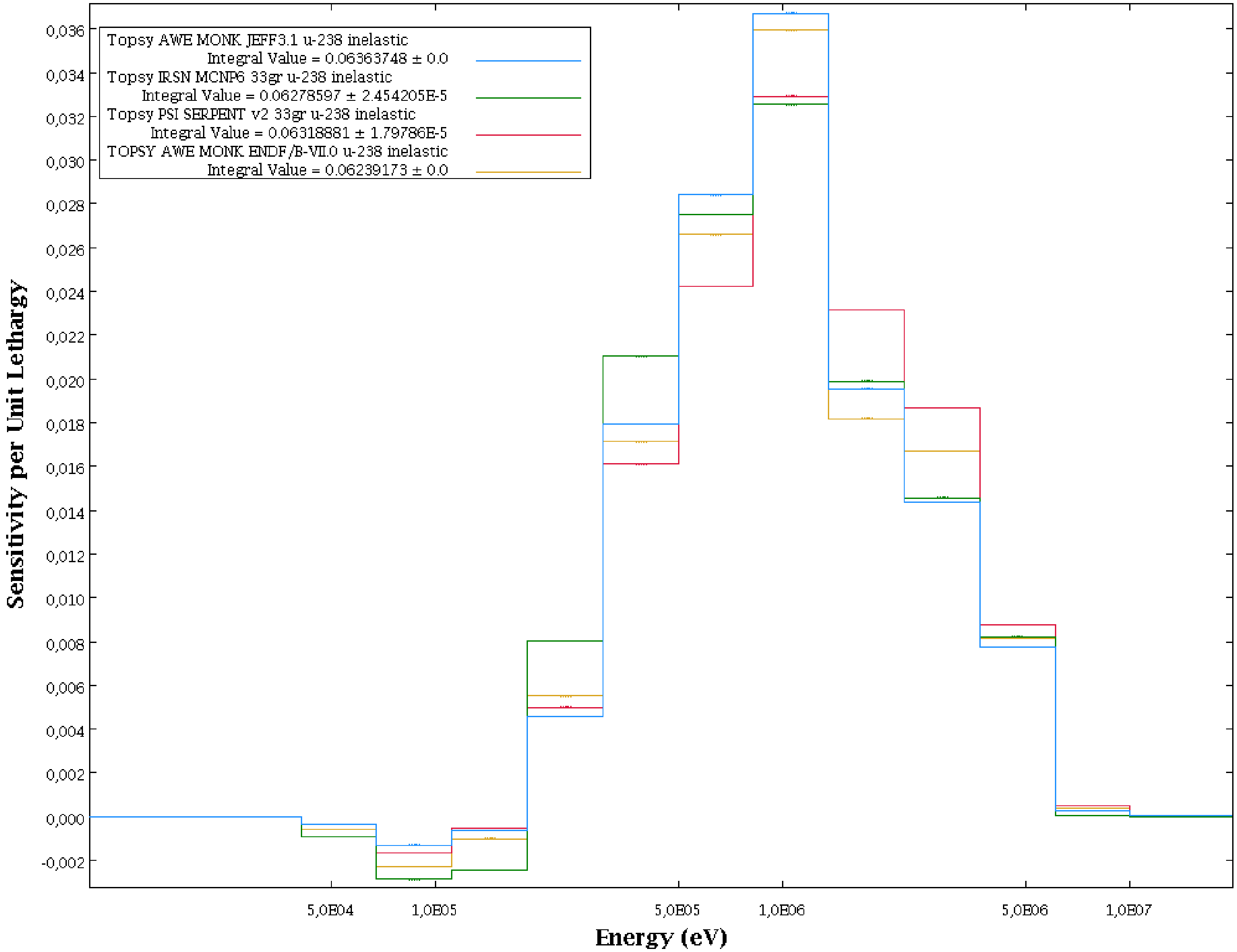
Topsy: U-238 Elastic Profile



Topsy: U-235 Inelastic Profile



Topsy: U-238 Inelastic Profile



HMI-001 (ZPR 9/34 loading 303)

- Highly enriched uranium/ iron benchmark, moderated, reflected by steel. **RZ model**

- k_{bench}=0.9966±0.0026

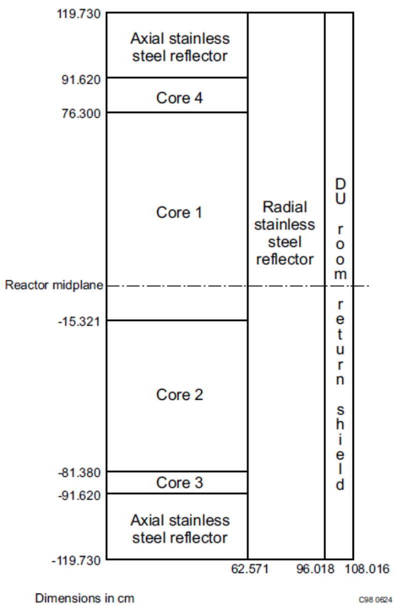
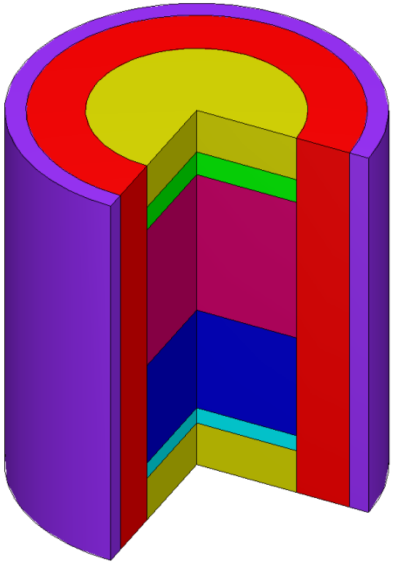
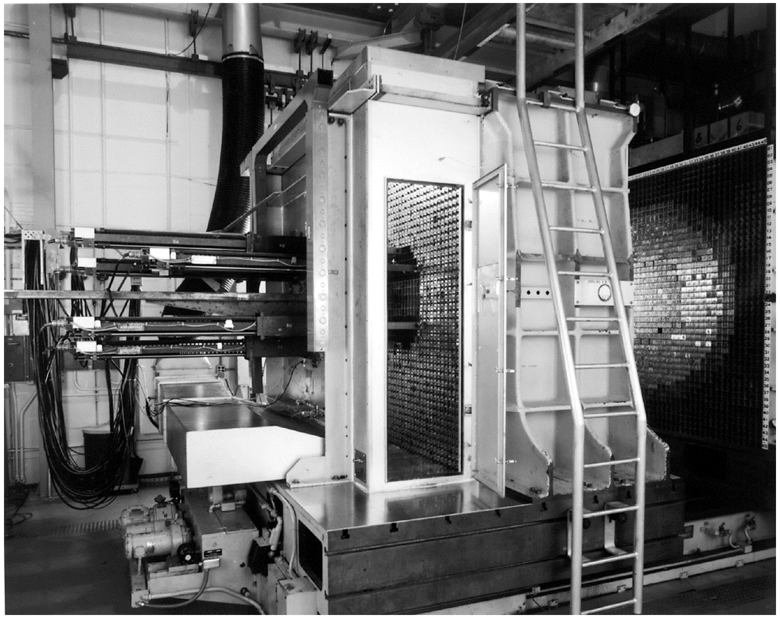


Figure 12. Benchmark Model Geometry.

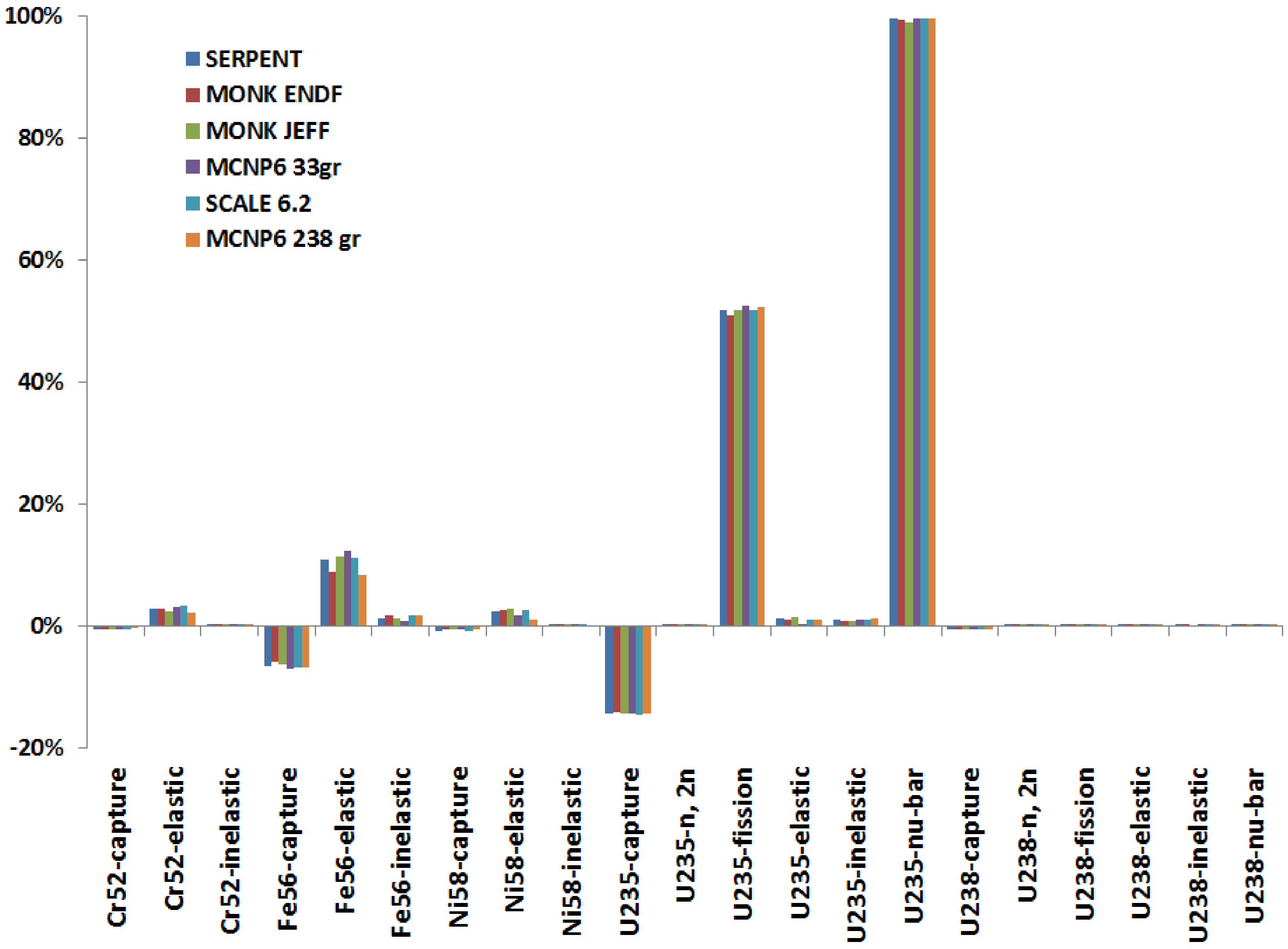




ZPR-9/34: Integrates Sensitivities (1/3)

	SERPENT	MONK ENDF	MONK JEFF	MCNP6	SCALE 6.2	MCNP6 238 gr*
Cr52-capture	-0,53	-0,54	-0,52	-0,53	-0,52	-0,47
Cr52-elastic	2,76	2,91	2,40	3,04	3,26	2,22
Cr52-inelastic	0,05	0,09	0,03	0,04	0,08	0,04
Fe56-capture	-6,53	-5,95	-6,34	-7,11	-6,89	-6,75
Fe56-elastic	10,84	8,79	11,40	12,31	11,14	8,36
Fe56-inelastic	1,31	1,64	1,32	0,71	1,70	1,76
Ni58-capture	-0,78	-0,62	-0,64	-0,66	-0,77	-0,66
Ni58-elastic	2,47	2,51	2,75	1,66	2,55	0,90
Ni58-inelastic	0,02	0,01	0,03	0,07	0,02	-0,03
U235-capture	-14,45	-14,28	-14,42	-14,32	-14,54	-14,38
U235-n, 2n	0,01	0,01	0,01	0,02	0,01	0,00
U235-fission	51,83	50,79	51,82	52,54	51,85	52,29
U235-elastic	1,30	0,99	1,34	0,11	1,07	1,05
U235-inelastic	0,91	0,87	0,87	0,99	0,92	1,22
U235-nu-bar	99,71	99,42	99,04	99,72	99,71	99,71
U238-capture	-0,70	-0,68	-0,68	-0,69	-0,68	-0,67
U238-n, 2n	0,00	0,00	0,00	0,00	0,00	0,00
U238-fission	0,07	0,06	0,07	0,06	0,07	0,07
U238-elastic	0,41	0,36	0,39	0,23	0,39	0,41
U238-inelastic	0,01	0,02	-0,02	0,15	0,01	0,01
U238-nu-bar	0.11	0,08	0,12	0,10	0,11	0,11

ZPR-9/34: Integrates Sensitivities (2/3)



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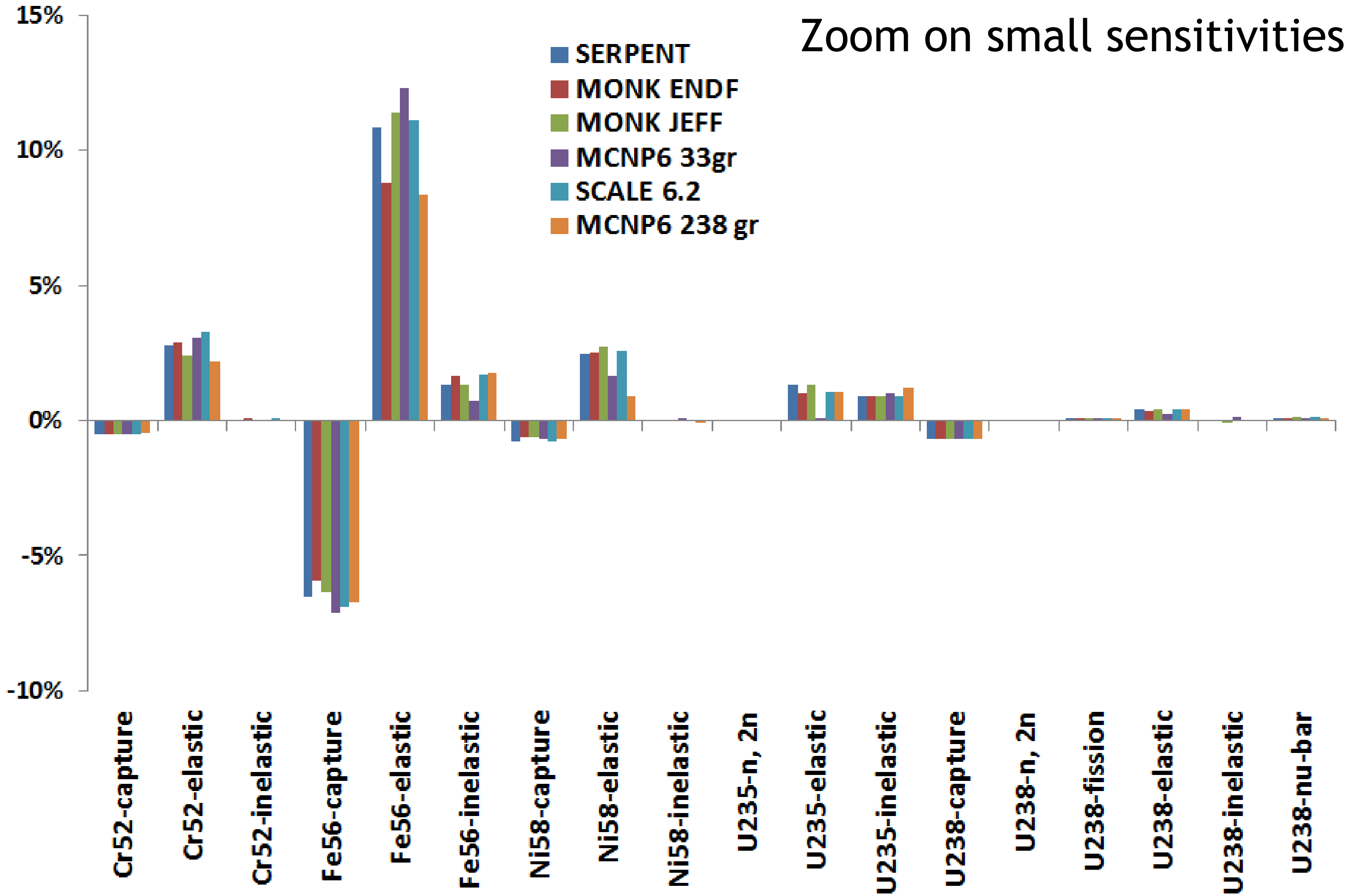
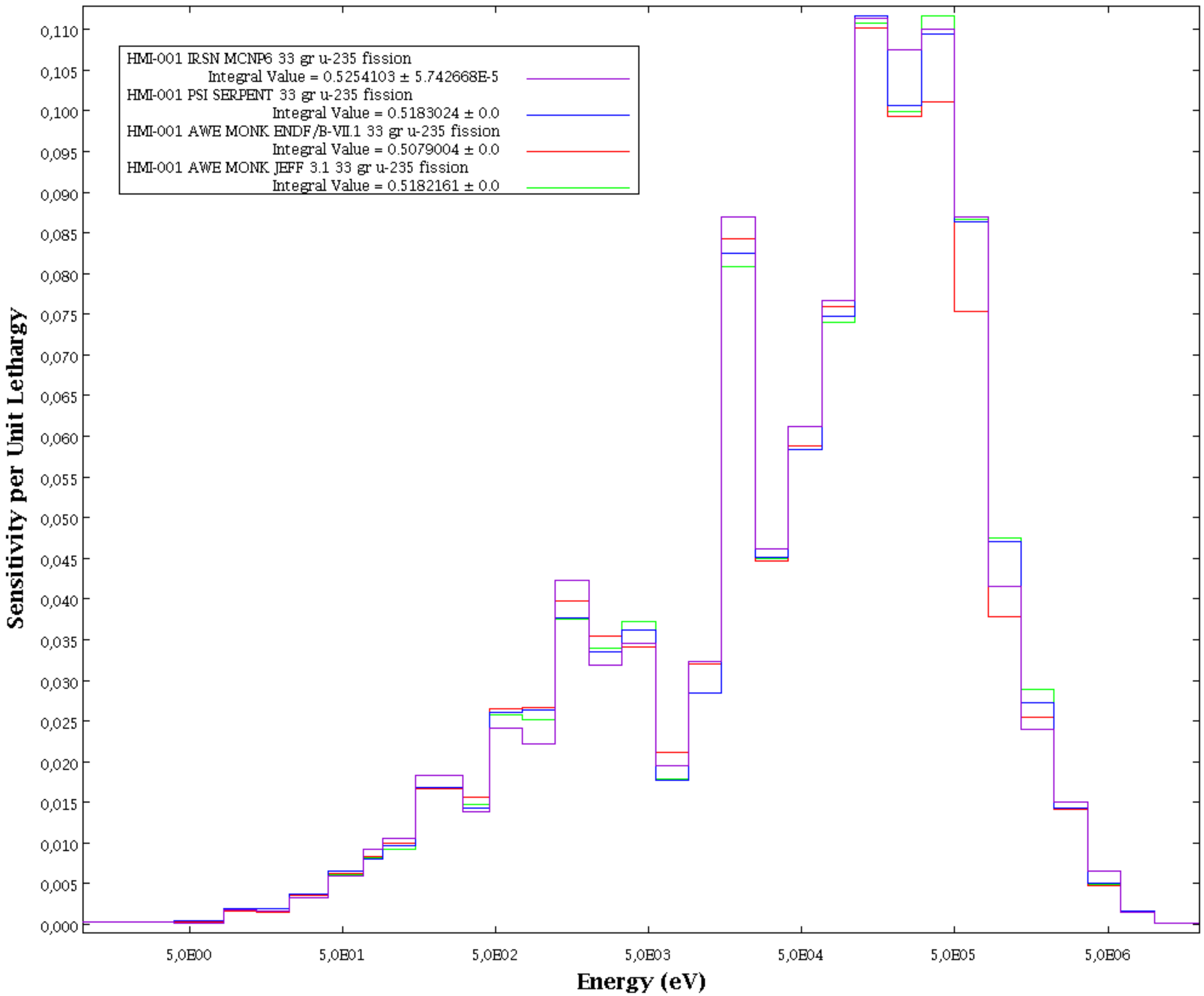
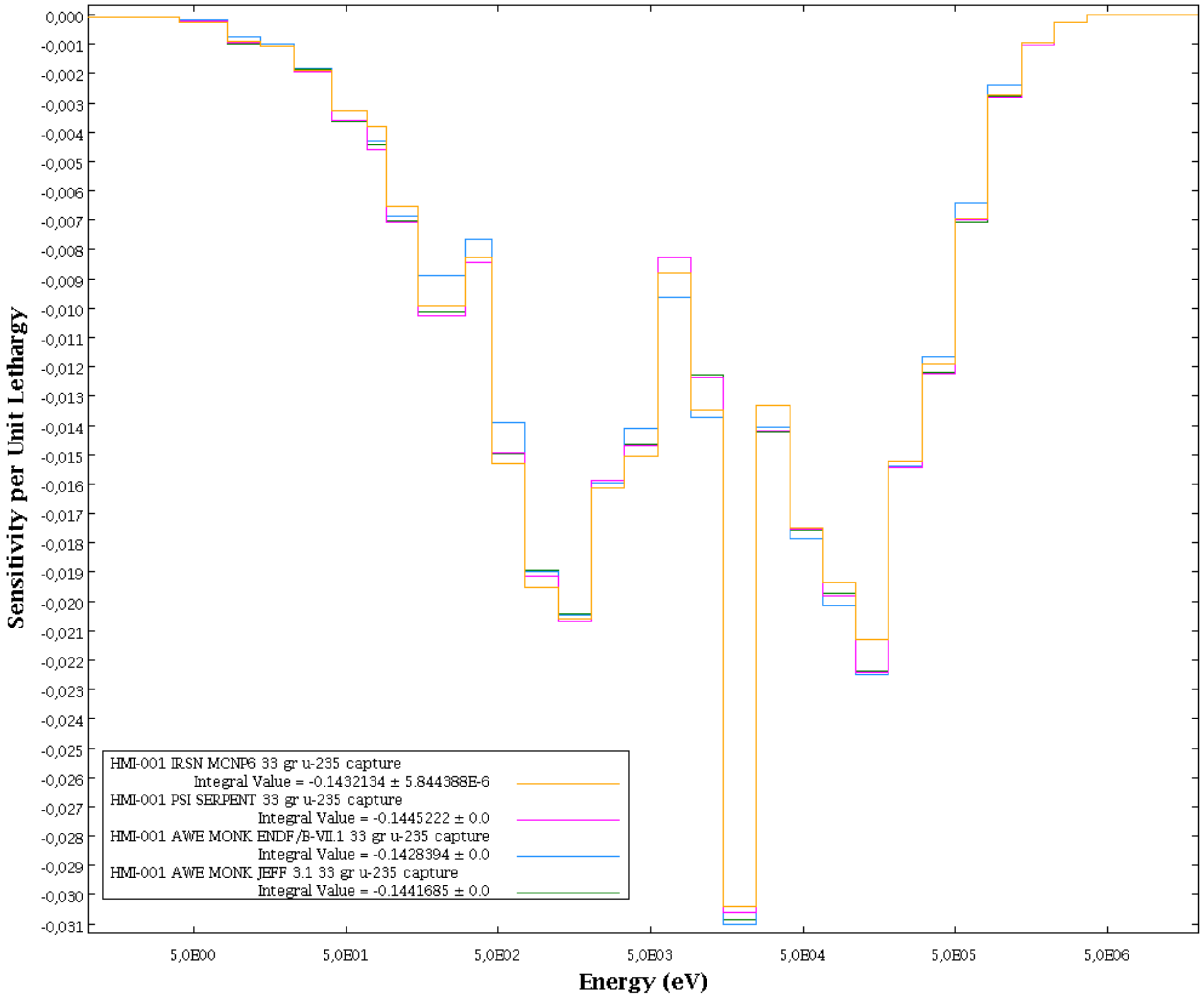
ZPR-9/34: Integrates Sensitivities (3/3)



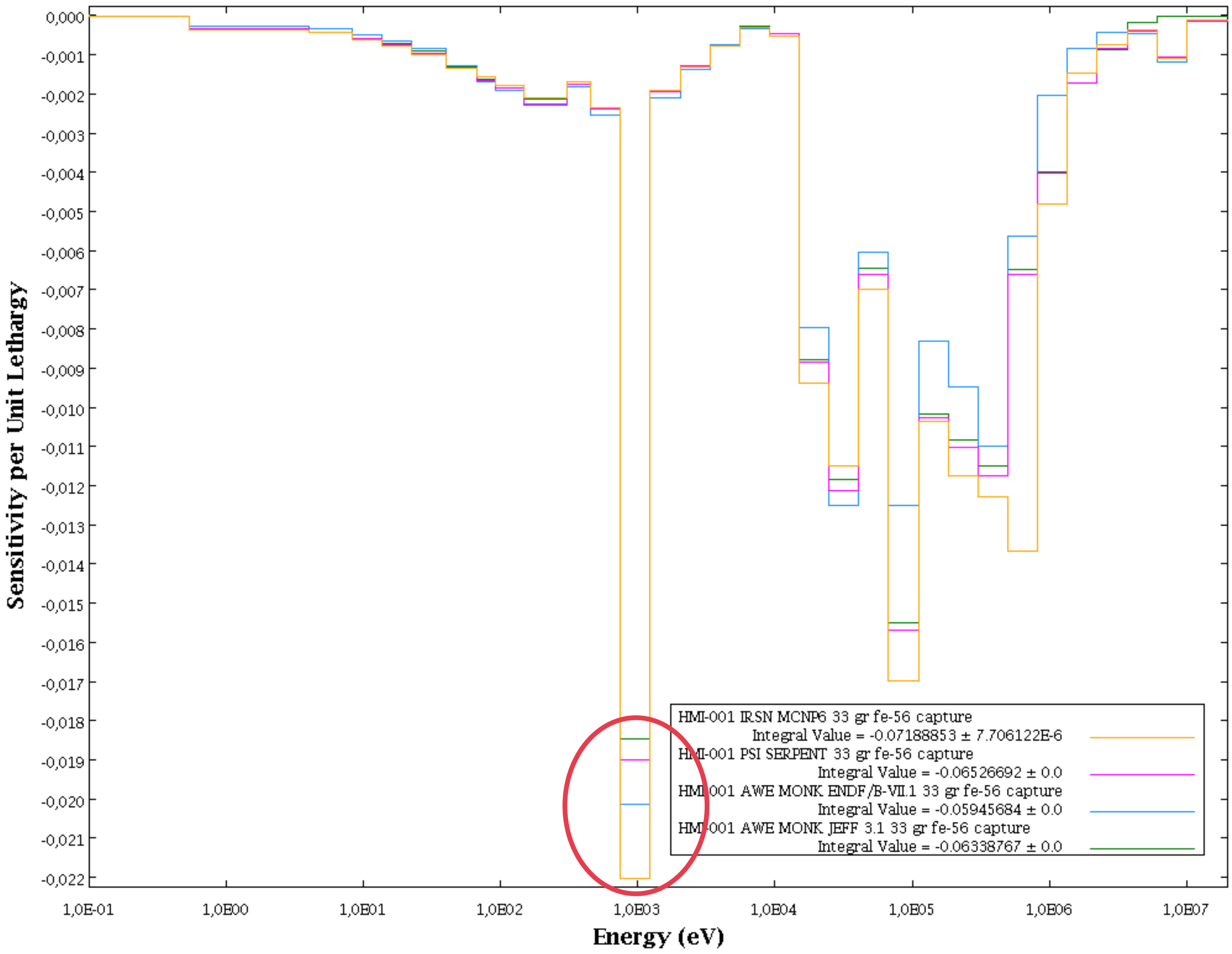
ZPR 9/34: U-235 Fission Profiles



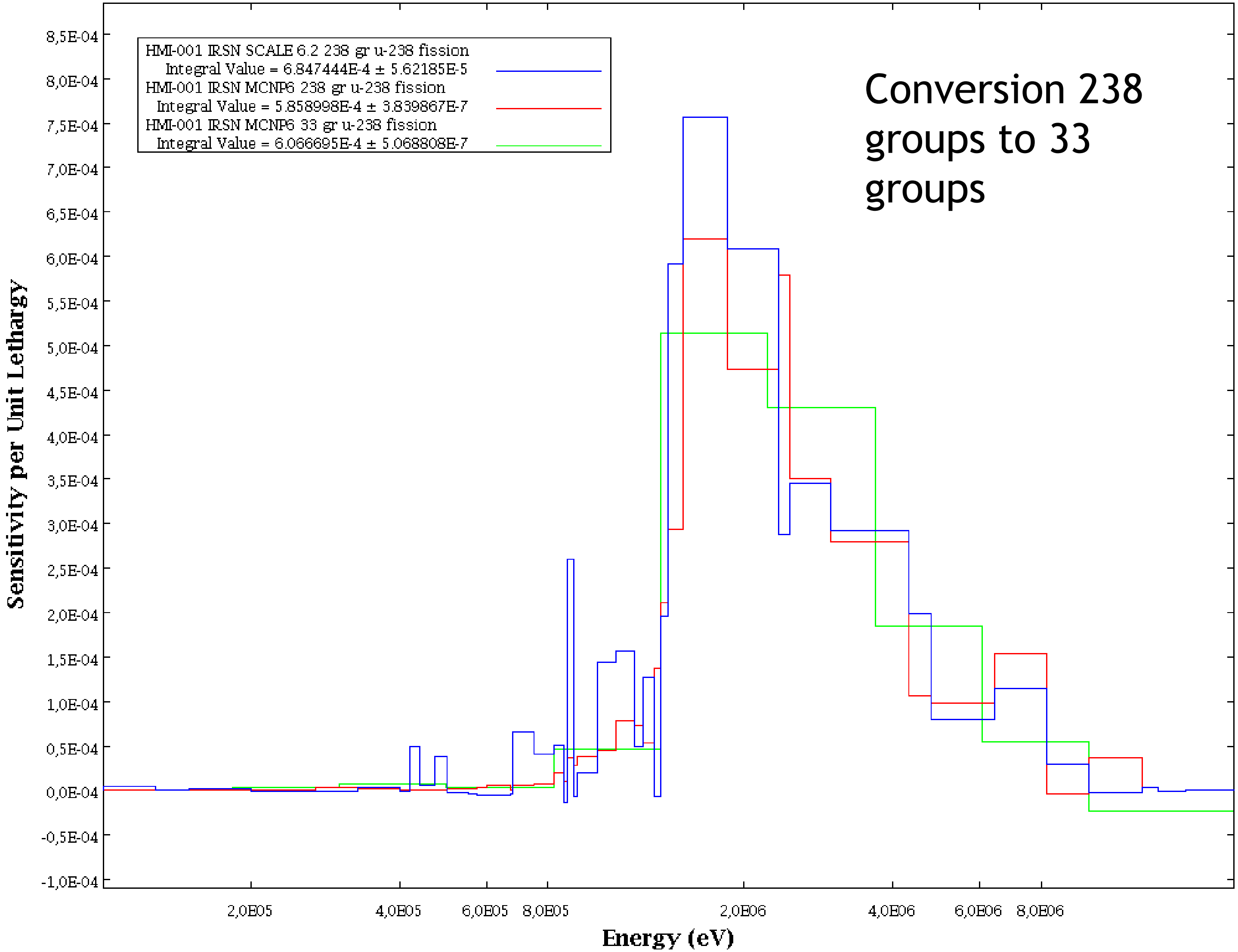
ZPR 9/34: U-235 Capture Profiles



ZPR 9/34: Fe-56 Capture Profiles

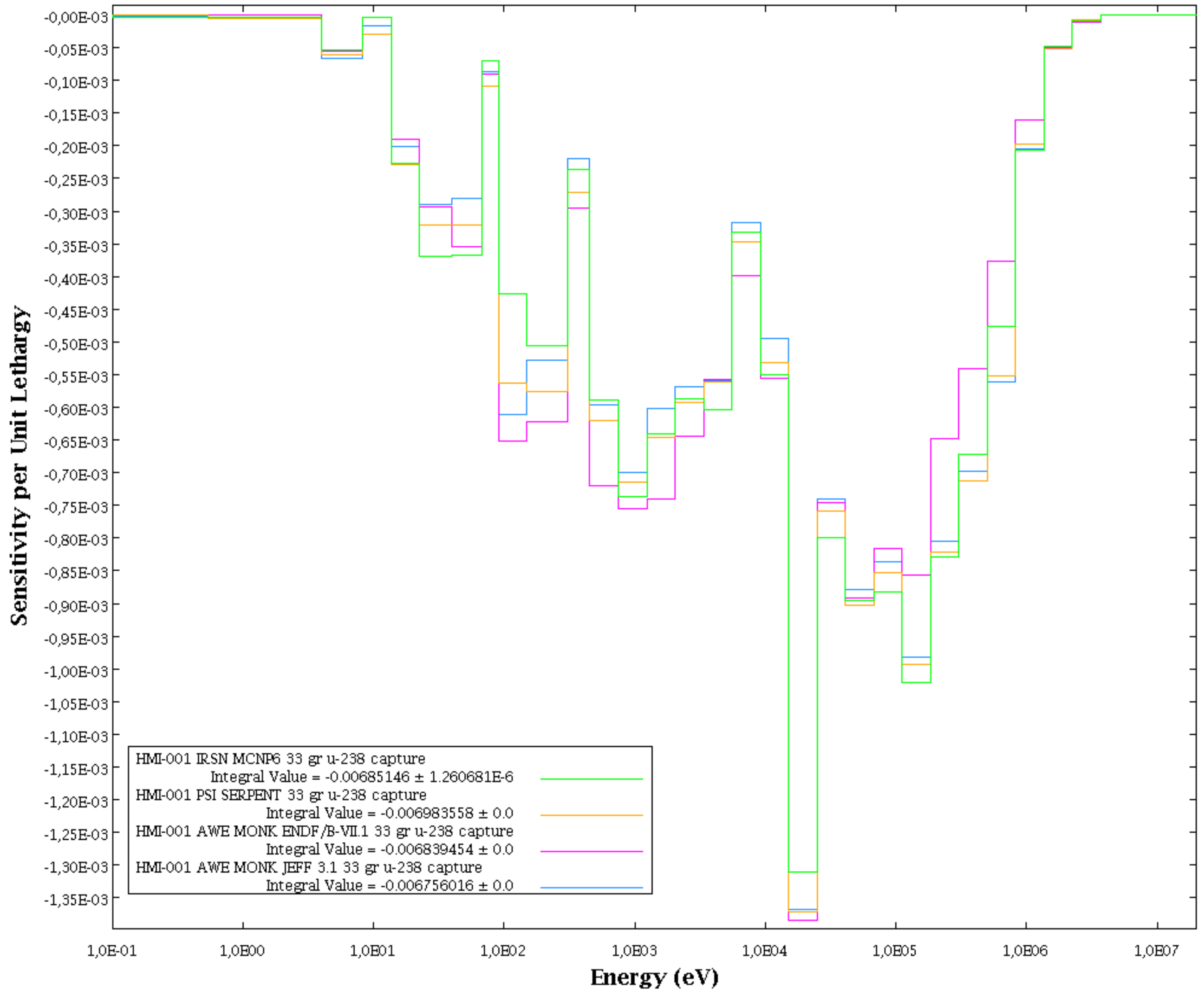


ZPR 9/34, U-238 Fission Profiles



Conversion 238 groups to 33 groups

ZPR 9/34, U-238 Capture Profiles



PMI-002 (ZPR 6/10 loading 24)

- Core with heterogeneous plutonium metal fuel with carbon/stainless steel dilutions, and a steel reflector.

- k_{bench}=0.9862±0.0005 ($k_{ZPR6/10}$=1.0009±0.0007)

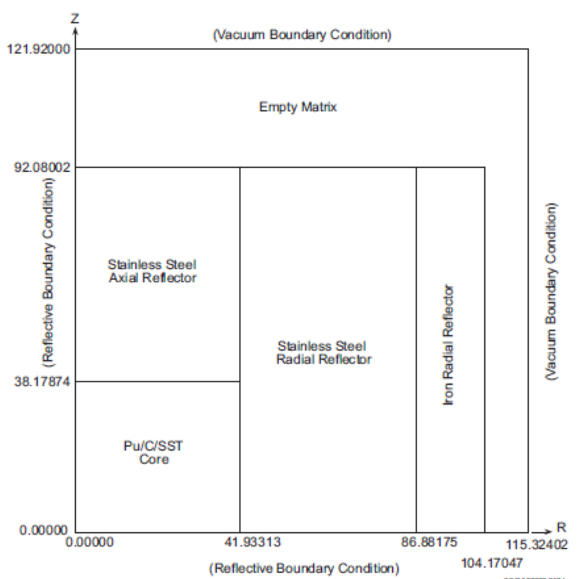
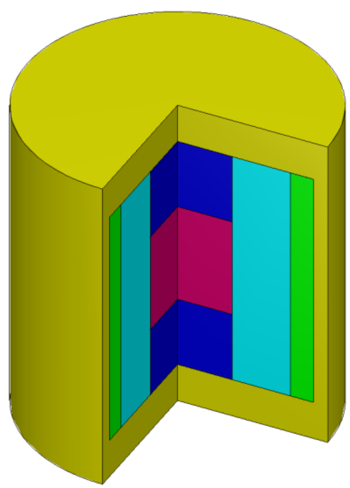
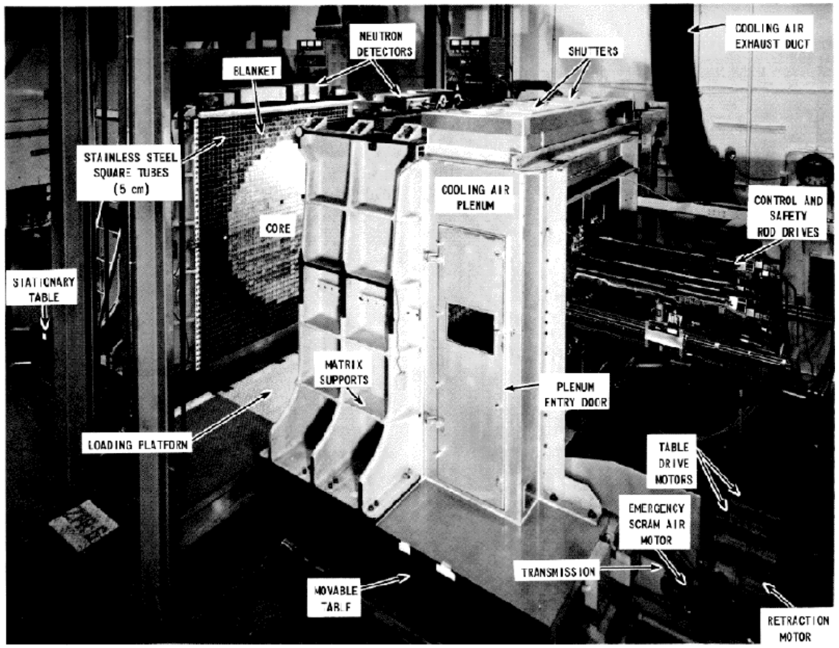


Figure 6. Benchmark-Model Geometry for ZPR-6/10.

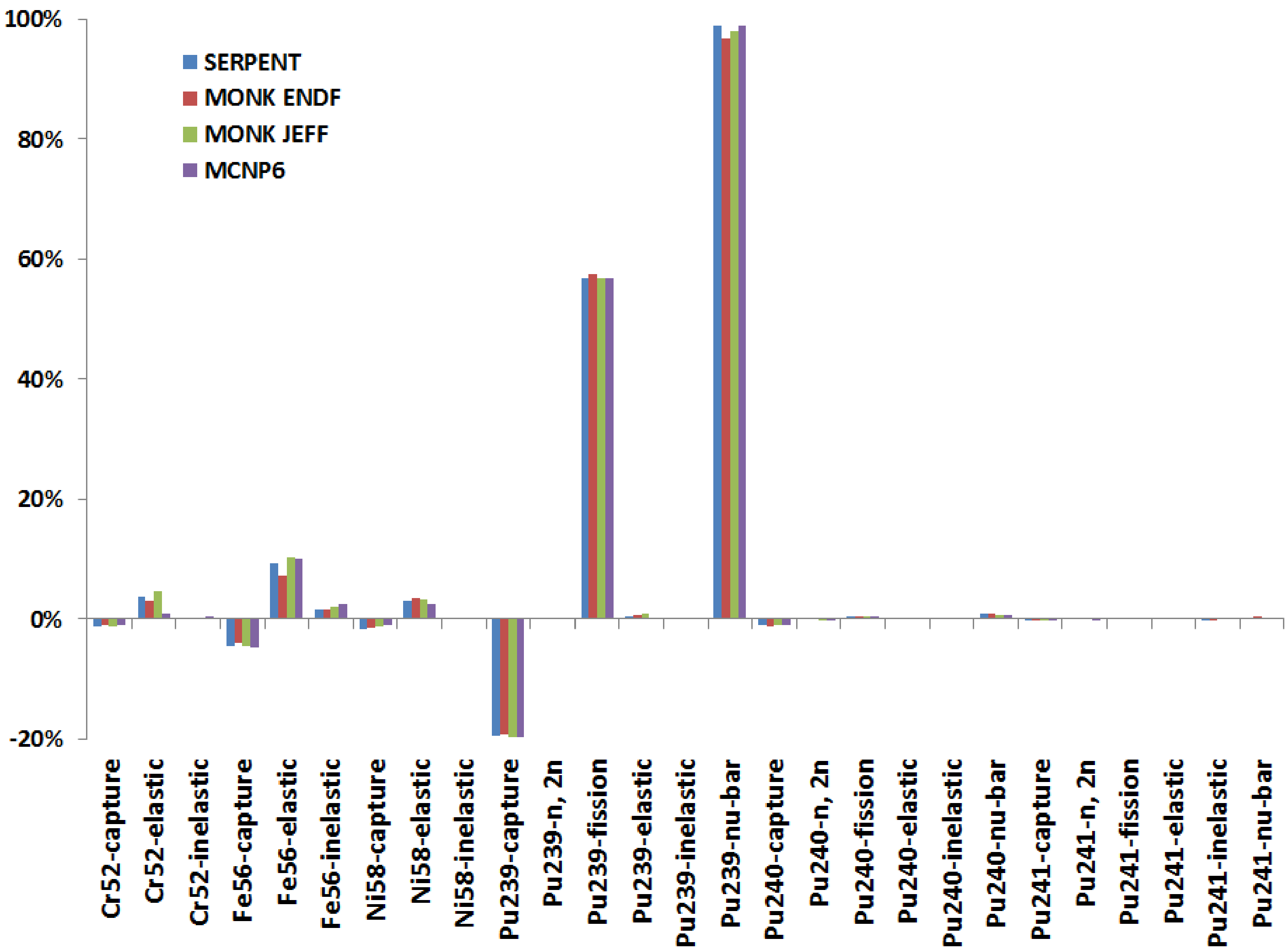




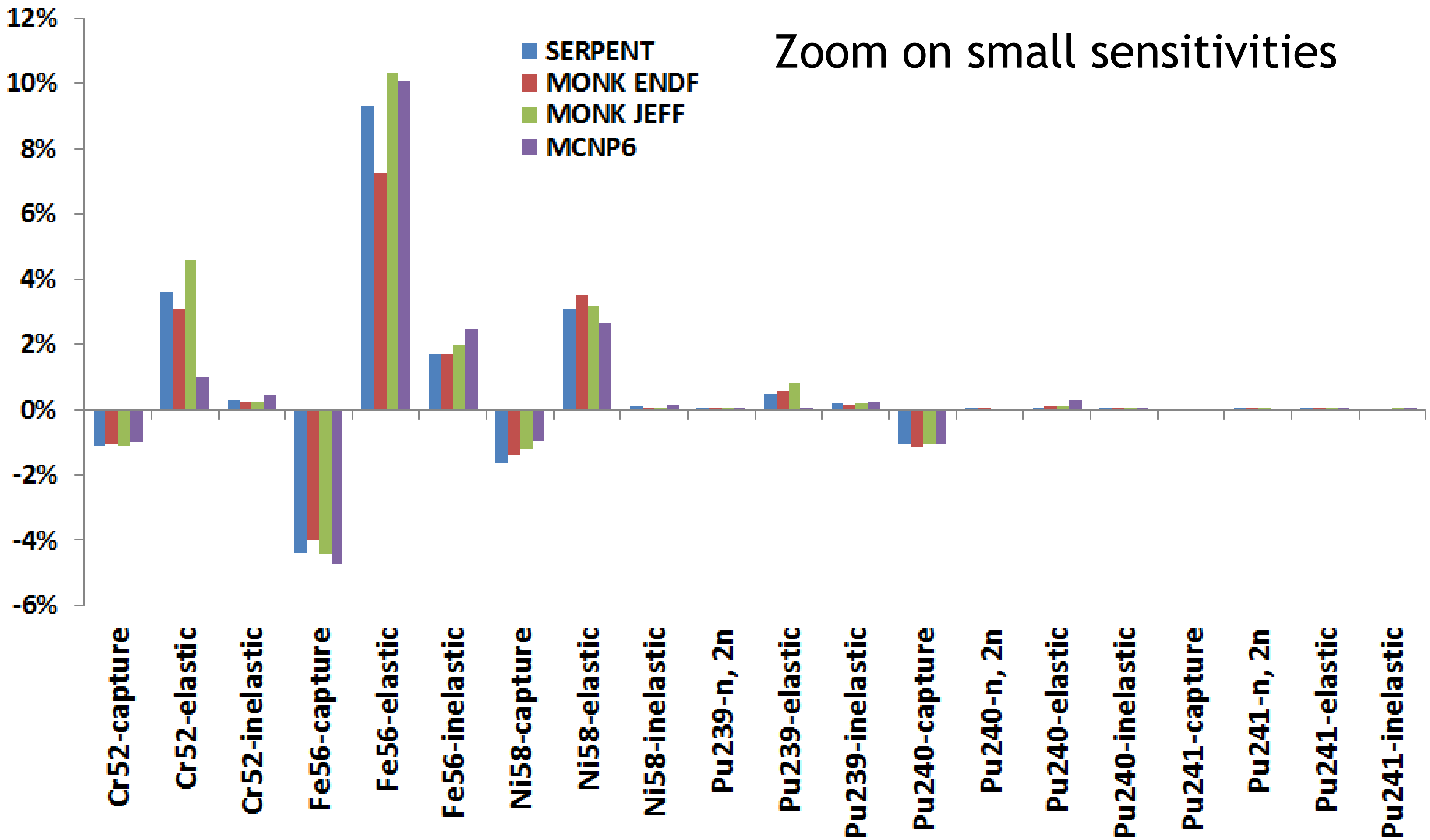
ZPR 6/10: Integrated Sensitivities (1/3)

	SERPENT	MONK ENDF	MONK JEFF	MCNP6
Cr52-capture	-1,10	-1,06	-1,11	-0,99
Cr52-elastic	3,61	3,09	4,57	1,02
Cr52-inelastic	0,30	0,26	0,23	0,46
Fe56-capture	-4,39	-4,00	-4,45	-4,72
Fe56-elastic	9,33	7,24	10,34	10,11
Fe56-inelastic	1,69	1,72	1,99	2,46
Ni58-capture	-1,63	-1,37	-1,18	-0,98
Ni58-elastic	3,08	3,51	3,18	2,65
Ni58-inelastic	0,09	0,05	0,04	0,13
Pu239-capture	-19,42	-19,17	-19,58	-19,78
Pu239-n, 2n	0,01	0,00	0,01	0,01
Pu239-fission	56,78	57,41	56,82	56,81
Pu239-elastic	0,50	0,60	0,84	0,03
Pu239-inelastic	0,18	0,15	0,20	0,25
Pu239-nu-bar	98,91	96,80	97,98	98,93
Pu240-capture	-1,04	-1,14	-1,05	-1,05
Pu240-n, 2n	0,00	0,00	0,00	0,00
Pu240-fission	0,53	0,49	0,51	0,52
Pu240-elastic	0,05	0,11	0,10	0,28
Pu240-inelastic	0,00	0,04	0,03	0,01
Pu240-nu-bar	0,80	0,93	0,73	0,79
Pu241-capture	-0,03	-0,02	-0,03	-0,02
Pu241-n, 2n	0,00	0,00	0,00	0,00
Pu241-fission	0,14	0,14	0,15	0,14
Pu241-elastic	0,00	0,01	0,00	0,00
Pu241-inelastic	0,00	-0,01	0,00	0,01
Pu241-nu-bar	0,25	0,38	0,25	0,24

ZPR 6/10: Integrated Sensitivities (2/3)

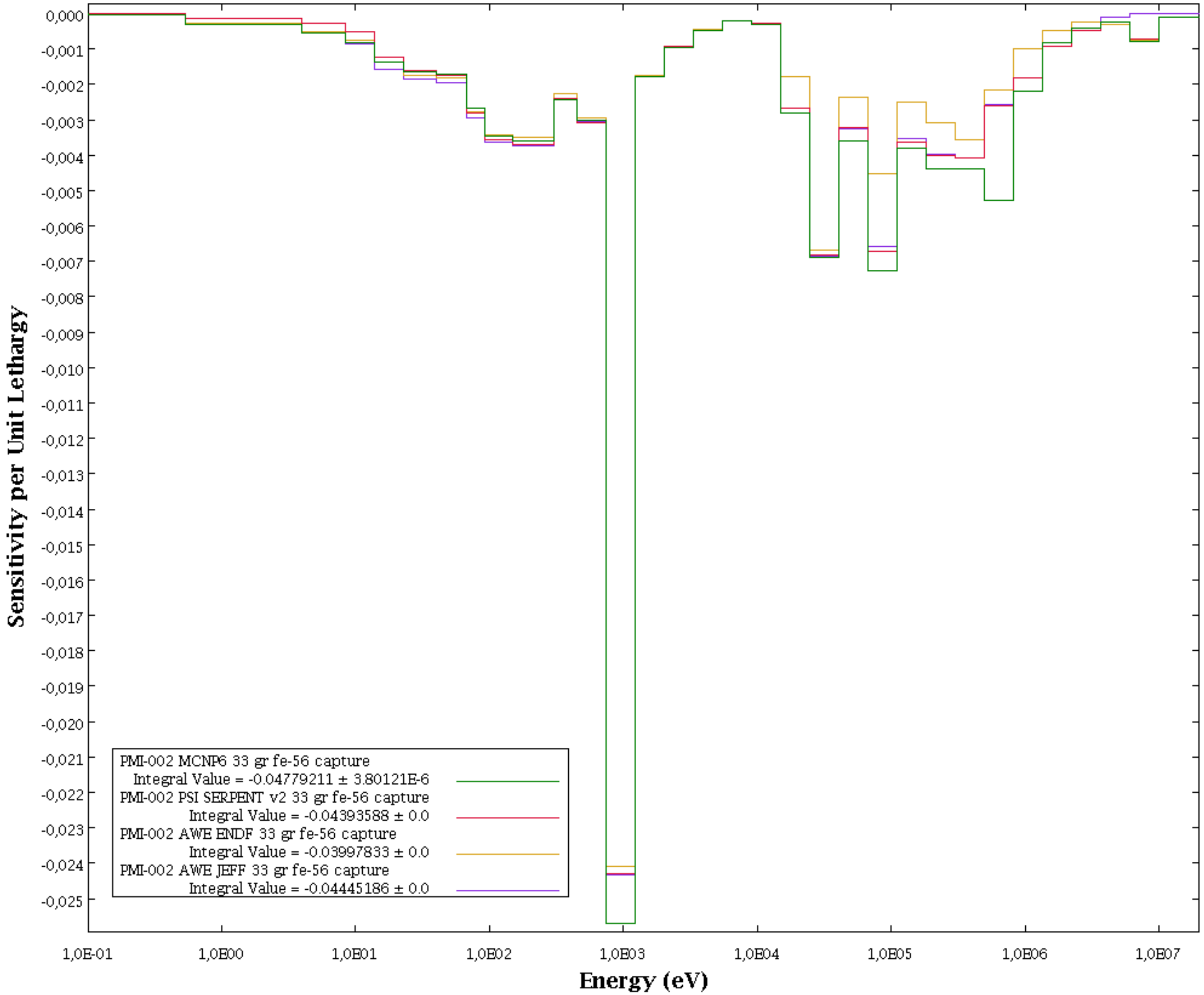


ZPR 6/10: Integrated Sensitivities (3/3)

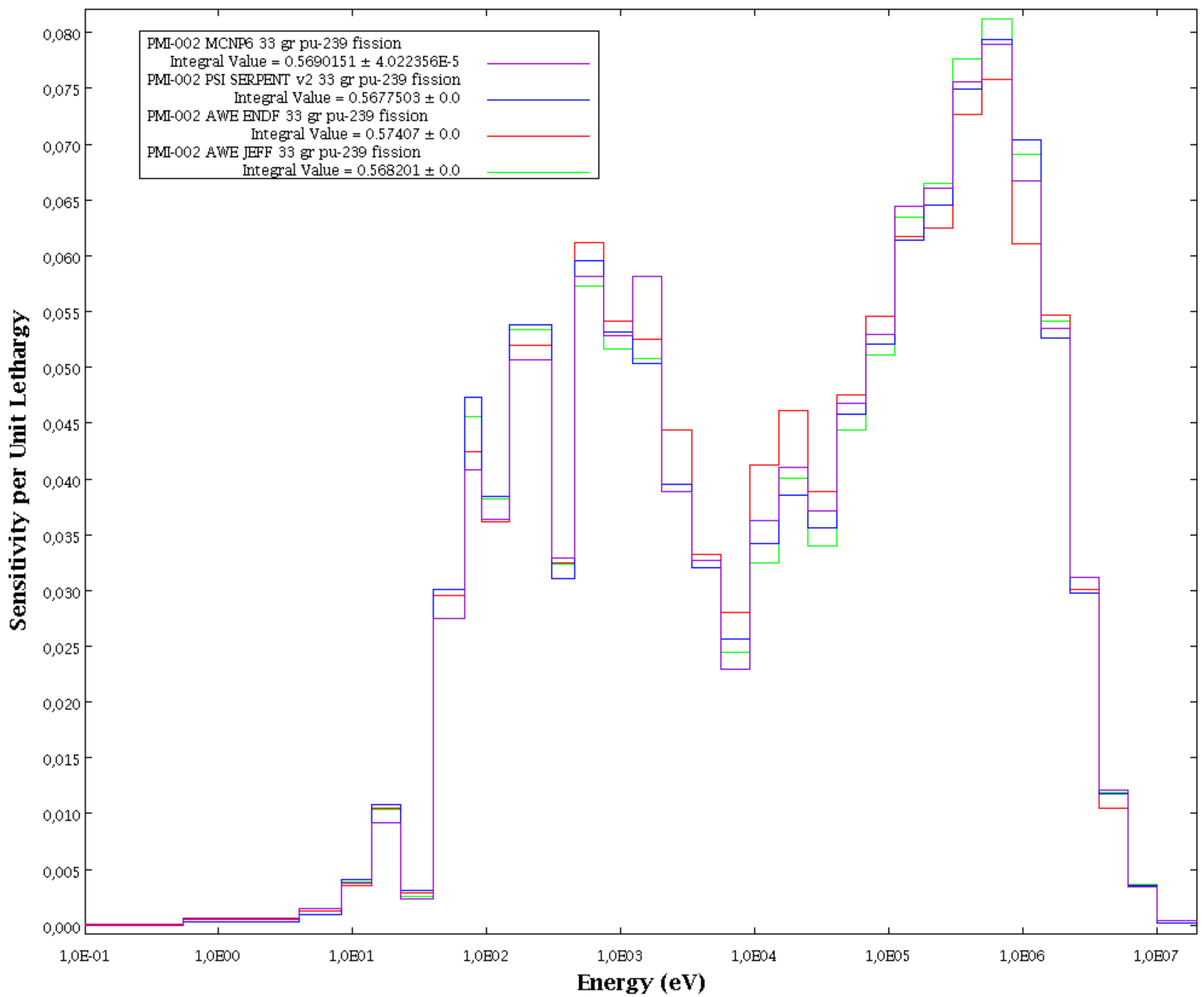


Zoom on small sensitivities

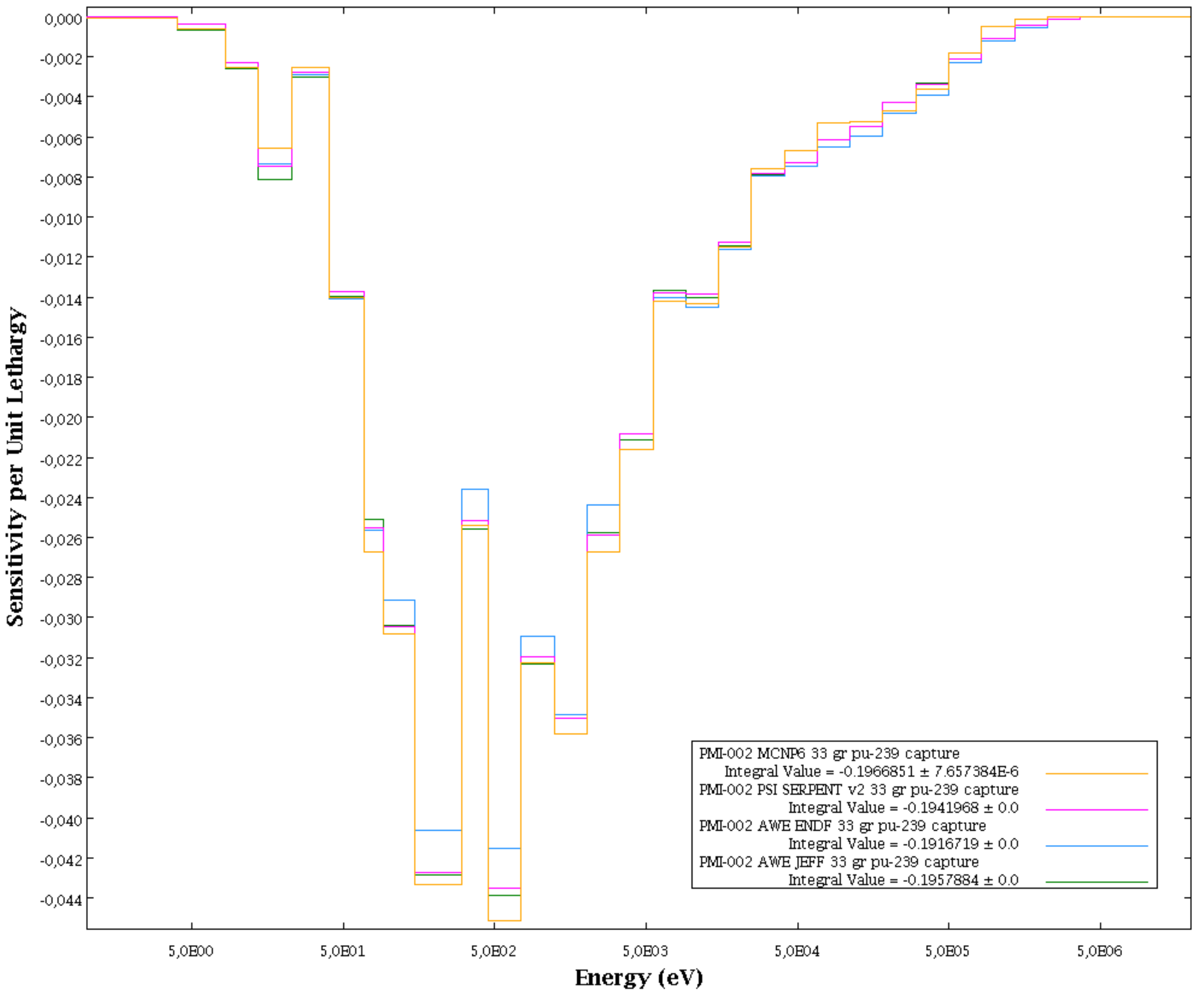
ZPR 6/10: Fe-56 Capture Profiles



ZPR 6/10: Pu-239 Fission Profiles



ZPR 6/10: Pu-239 Capture Profiles



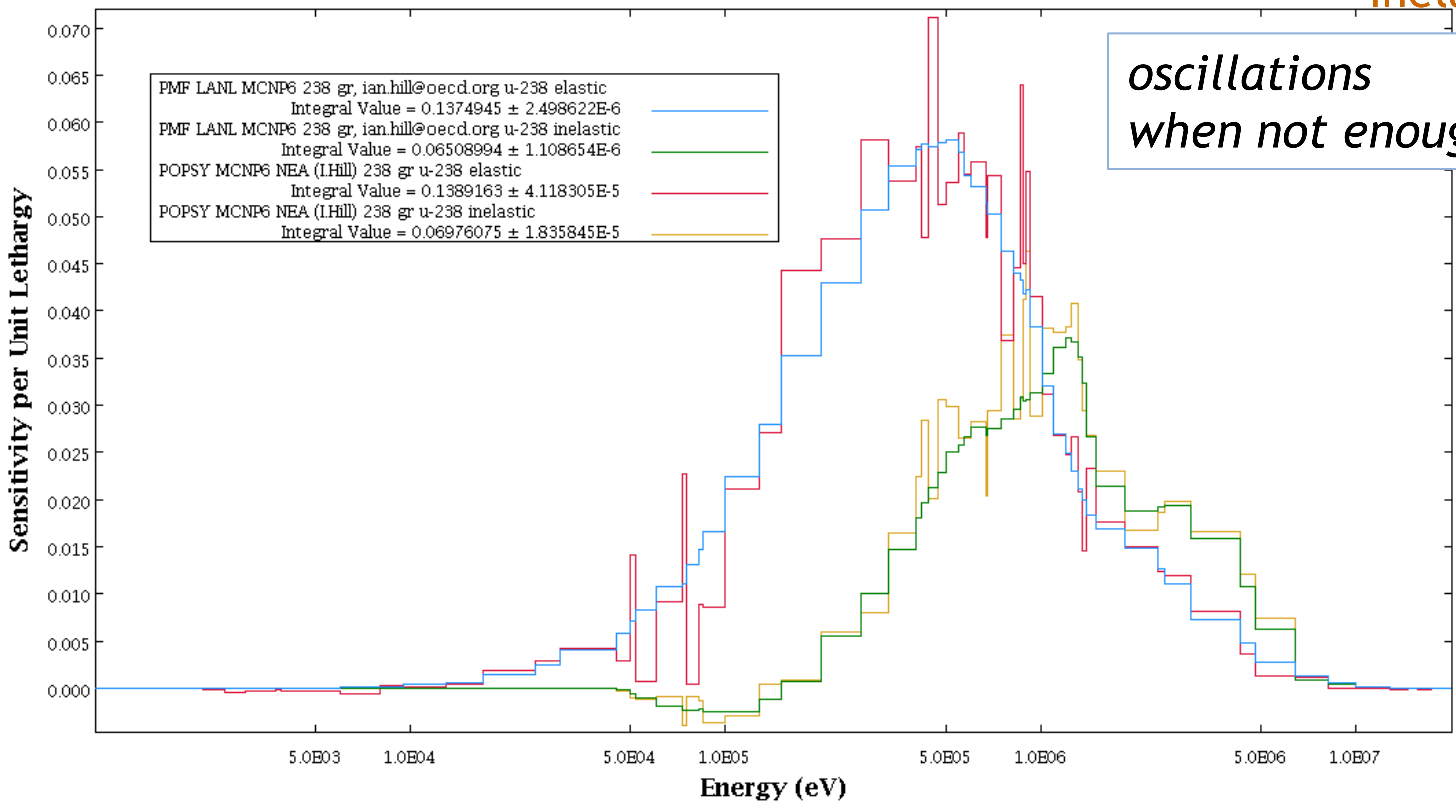
Convergence Issues

- Oscillations in sensitivity profiles (MCNP6 example) - addressed
- Optimization of sensitivity algorithms acceleration (CLUTCH example) - addressed
- Negative n,2n contributions

Popsy: MCNP6 Convergence

MCNP6/ENDF/B-VII.1 5B histories (500000×10000) u-238 elastic
(Results provided by B. Kiedrowski) inelastic

MCNP6/ENDF/B-VII.1 1.2M histories (2000×600) u-238 elastic
inelastic



oscillations
when not enough statistics

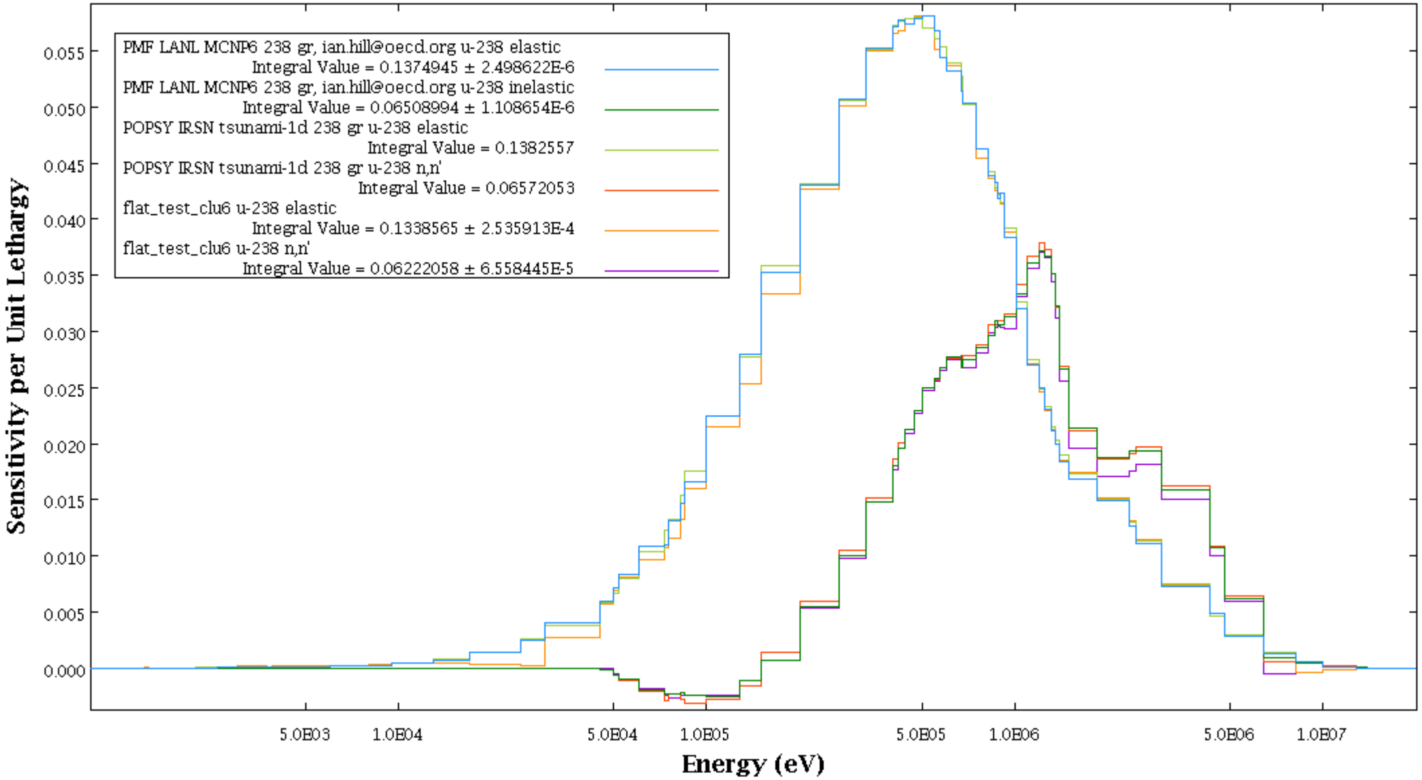
IRSN

Popsy: SCALE Convergence

MCNP6/ENDF/B-VII.1 5B histories (500000×10000) u-238 elastic inelastic

SCALE 6.1/TSUNAMI-1D/ENDF/B-VII u-238 elastic inelastic

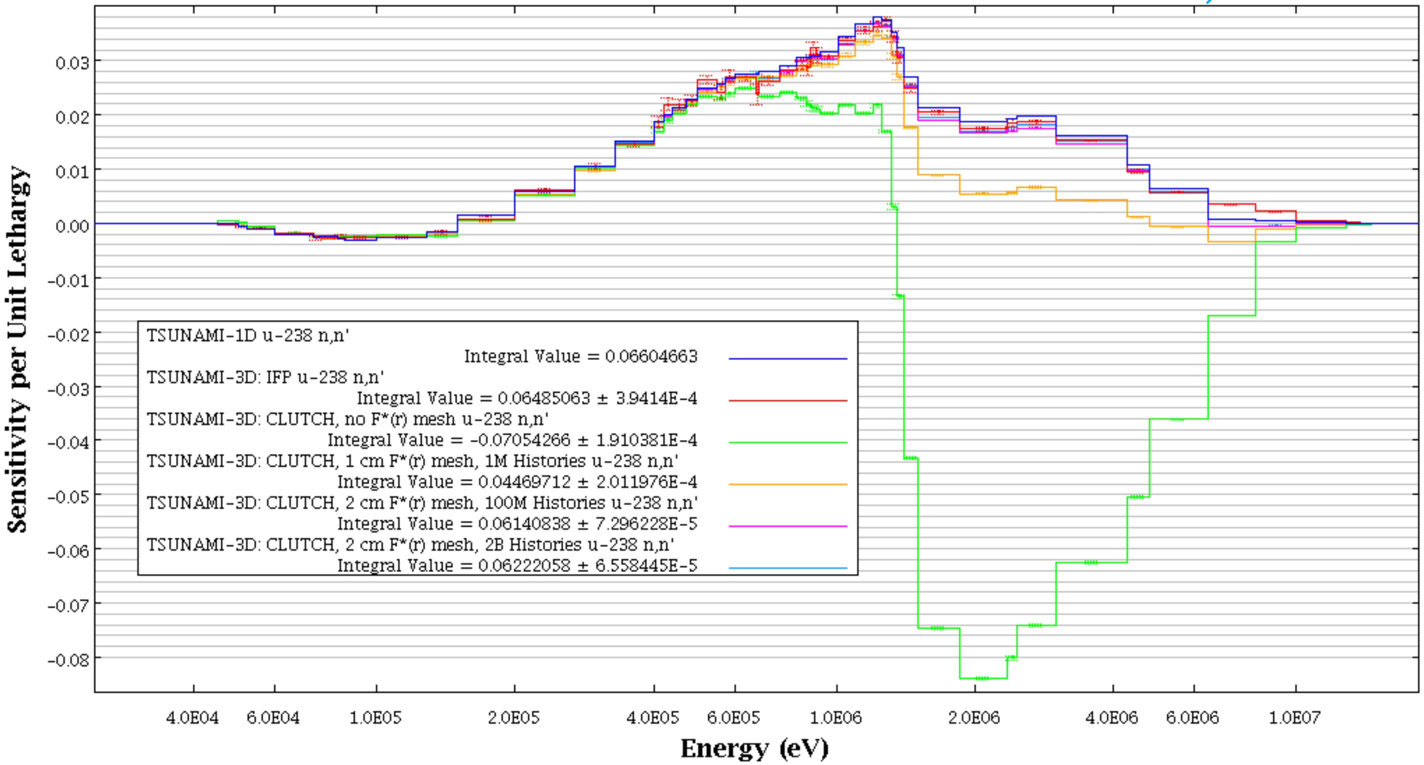
SCALE 6.2β/CLUTCH/ENDF/B-VII u-238 elastic inelastic



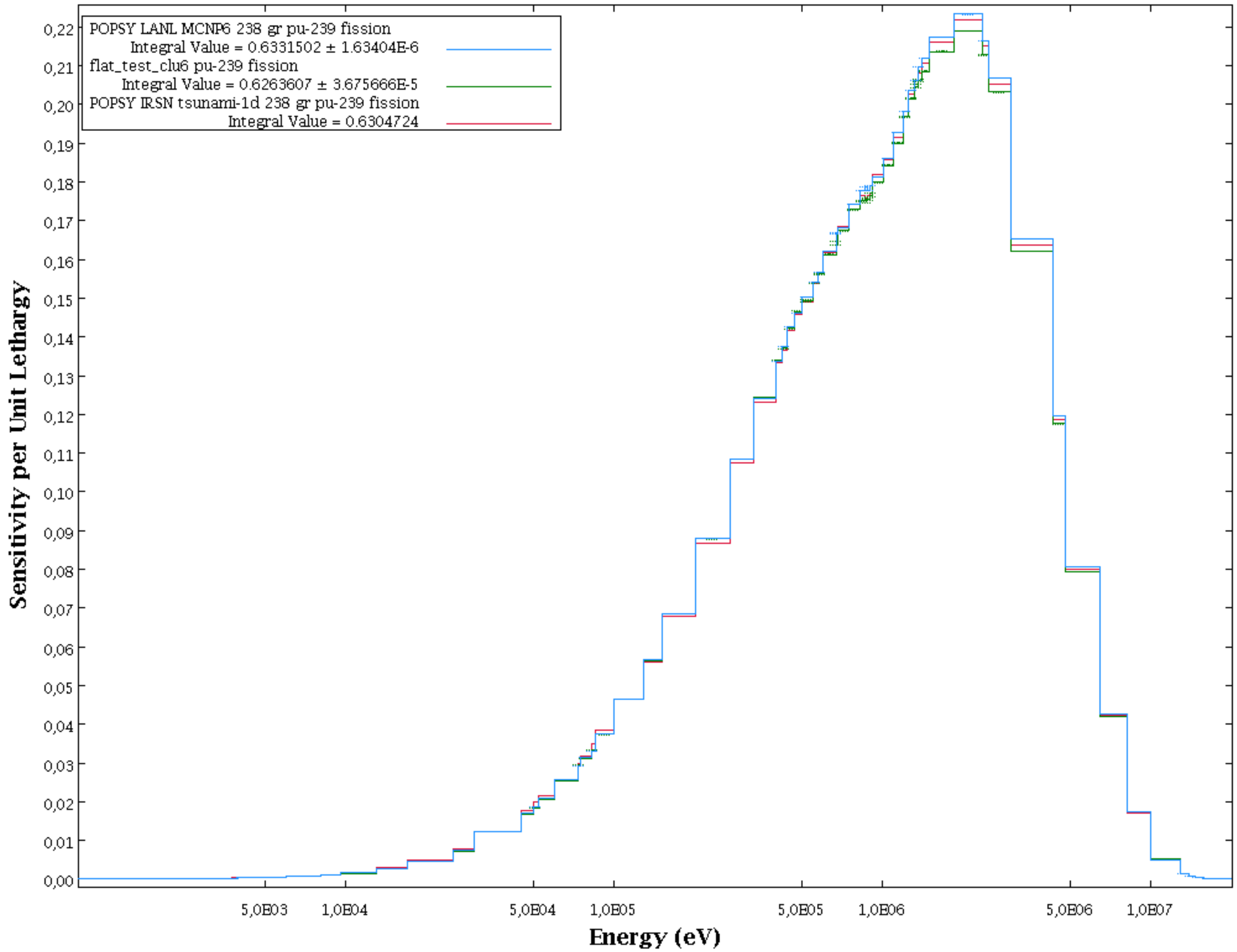
Popsy: SCALE/CLUTCH Convergence

TSUNAMI-1D	U-238	inelastic
SCALE 6.2β IFP	U-238	inelastic
SCALE 6.2β CLUTCH	U-238	inelastic no mesh
		inelastic mesh 1cm, 1M
		inelastic mesh 2cm, 100M
		inelastic mesh 2cm, 2B

C.Perfetti/ ORNL



Popsy: Pu-239 Capture MCNP6 vs TSUNAMI-1D and ANISN



Notes on MC Sensitivity Theory

$$k_{ef}\cdot Q(\mathbf{r})=\int Q(\mathbf{r}')\cdot P(\mathbf{r}'\to\mathbf{r})\cdot d\mathbf{r}'$$

$$k^{+}_{ef}\cdot Q^{+}(\mathbf{r})=\int Q^{+}(\mathbf{r}')\cdot P(\mathbf{r}\to\mathbf{r}')\cdot d\mathbf{r}'$$

$$k^{+}_{ef}=k_{ef}$$

$$P(\mathbf{r}'\to\mathbf{r})$$

is a number of particles appeared in the point *r* being born in fissions caused by neutron emitted in the point *r'*

$$\frac{\partial k_{ef}}{\partial\alpha}=\frac{\iint Q^{+}(\mathbf{r})\cdot Q(\mathbf{r}')\cdot\frac{\partial}{\partial\alpha}P(\mathbf{r}'\to\mathbf{r})\cdot d\mathbf{r}'\cdot d\mathbf{r}}{\int Q^{+}(\mathbf{r})\cdot Q(\mathbf{r})\cdot d\mathbf{r}}$$

Formally any infinitely derivable function can be taken instead of ajoint source density, but normalization factor might be unknown if it will be another spatially distributed function.

$$F(x)=\frac{\nu\Sigma_f(\mathbf{r},E)}{k_{эф}\Sigma_a(\mathbf{r},E)}Q^{+}(\mathbf{r})$$

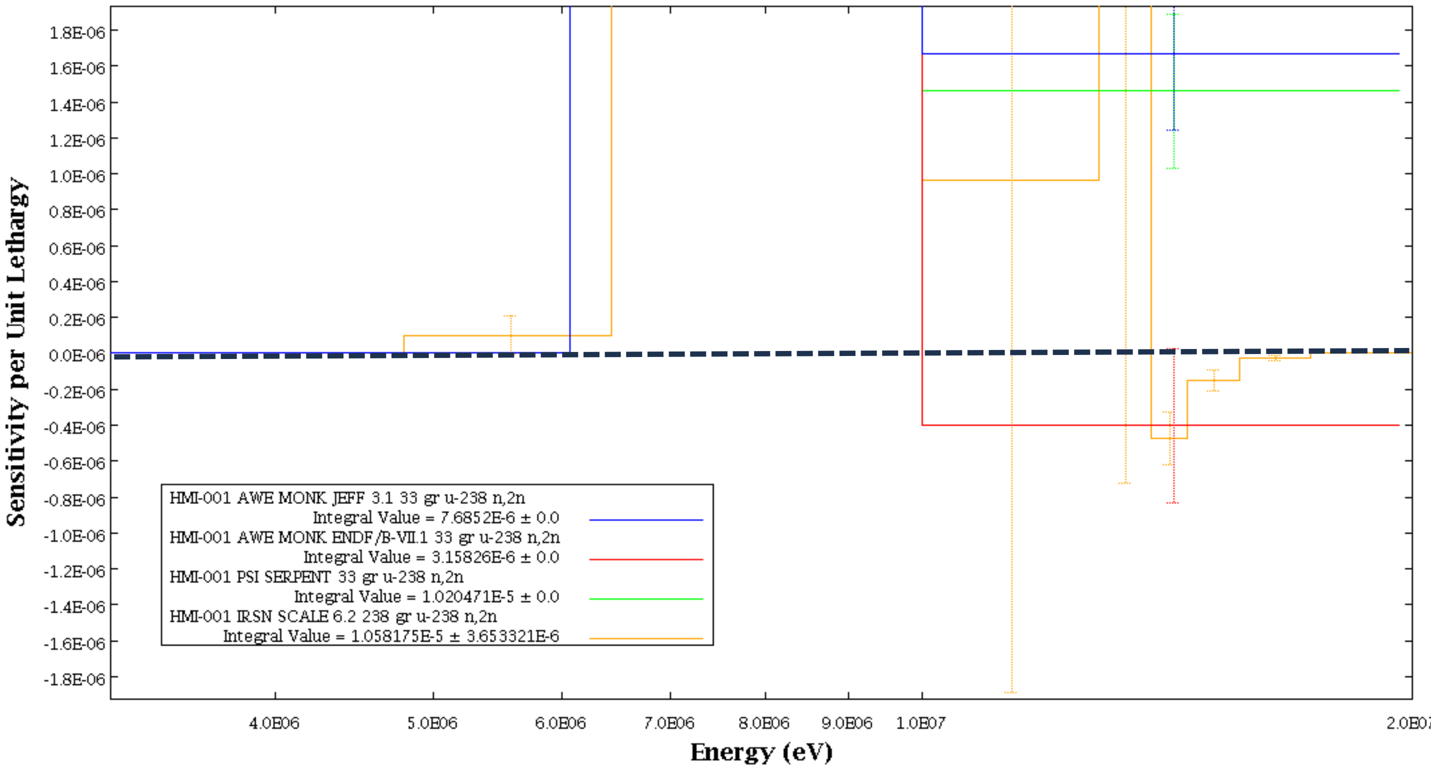
$$\left\langle\lambda_i\cdot\hat{\mathbf{F}}\cdot\vec{\mathbf{\Phi}}_i,\vec{\mathbf{\Psi}}_j\right\rangle=\left\langle\lambda_j\cdot\hat{\mathbf{F}}^{+}\vec{\mathbf{\Psi}}_j,\vec{\mathbf{\Phi}}_i\right\rangle=a_{i,j}\cdot\delta_{ij}$$

$$\frac{1}{k_{эф}}\frac{\partial k_{эф}}{\partial\alpha}=\frac{\int F(x)\left\{\frac{\Sigma_a(\mathbf{r},E)}{\nu\Sigma_f(\mathbf{r},E)}\Psi(x)\frac{\partial}{\partial\alpha}\left[\frac{\nu\Sigma_f(\mathbf{r},E)}{\Sigma_t(\mathbf{r},E)}\right]+\frac{\Sigma_a(\mathbf{r},E)}{\Sigma_t(\mathbf{r},E)}\frac{\partial}{\partial\alpha}\Psi(x)\right\}dx}{\int F(x)\frac{\Sigma_a(\mathbf{r},E)}{\Sigma_t(\mathbf{r},E)}\Psi(x)dx}$$

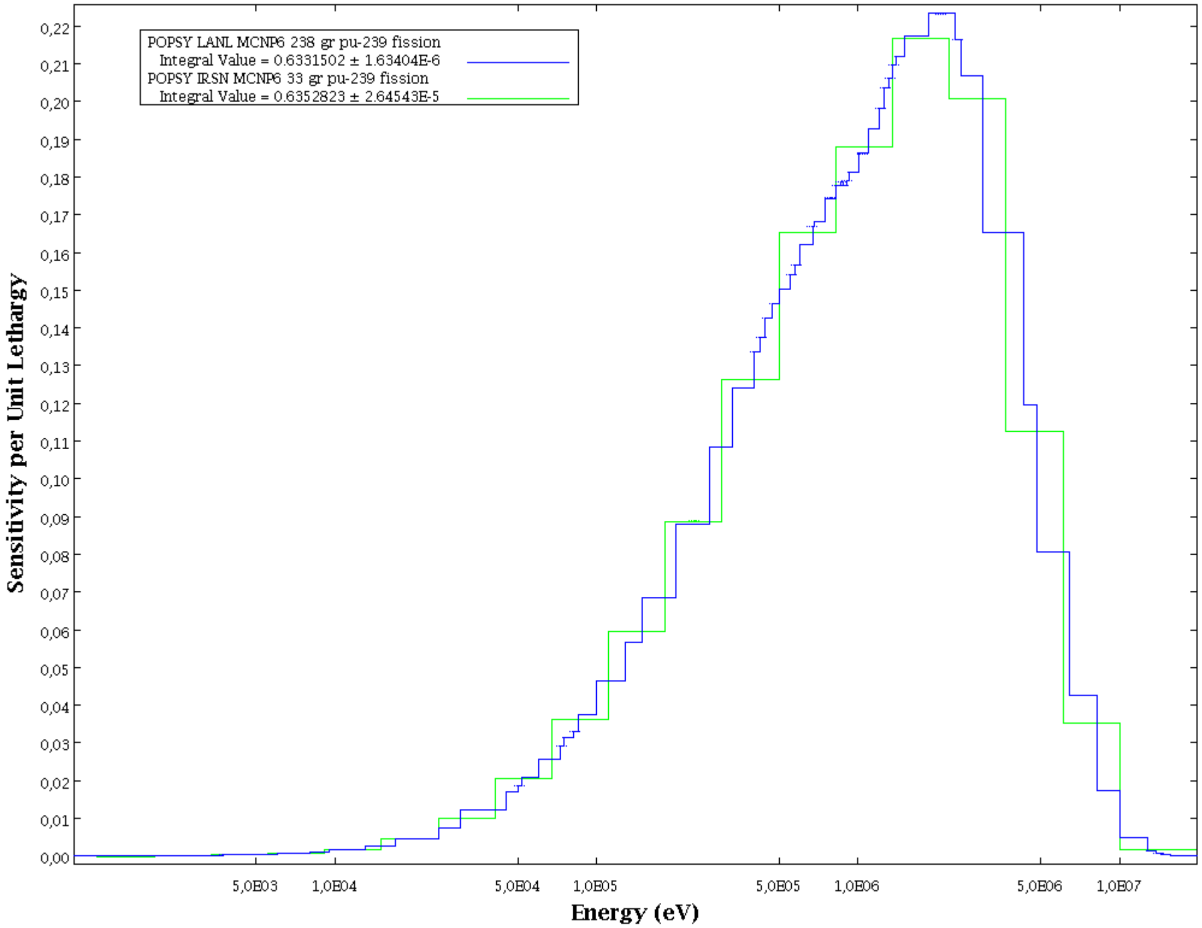
Note It has been proven that the bias of the of the sensitivity sampling estimator equals zero; e.g. asymptotical convergence of statistical integration to mathematical expectation exists. However there is no one theory to prove the rate of convergence - how many particles are needed to converge the sensitivities, as well there is no proven procedure to associate sampling dispersion with sensitivity profiles parameters.

ZPR9/34: Negative $S_{n,2n}$ Example

MONK with JEFF	U-238	n,2n reaction
MONK with ENDF	U-238	n,2n reaction
SERPENT	U-238	n,2n reaction
SCALE 6.2β	U-238	n,2n reaction
		Zero level



Popsy: Pu-239 Fission, MCNP6 238 gr. vs 33 gr.



Summary and Conclusions (1/2)

- Selected tree additional physically complex benchmarks, sensitive to neutron albedo, enable to highlight angular related issues in sensitivity calculations, if any

- Collected results from 7 organizations that generated sensitivities using 8 codes/methods (6 MC codes and 3 deterministic SN codes)

- All sensitivity profiles are converted to 33-gr. structure and then to SCALE/sdf format

Summary and Conclusions (2/2)

- Good agreement between deterministic and all MC sensitivities is observed for nu-bar, fission, and capture profiles
- MC scattering sensitivities depends on statistical options
- Statistics issues are addressed and statistic options are recommended for scattering sensitivity calculations
- 3D MC modelling allows using geometrically complex models for the adjustment, avoiding modeling correction factor
- MC sensitivity capabilities results in modeling flexibility. This fits the CIELO objectives but requires some more time to provides results of adjustment

Further Steps (TBD)

- Complete the analysis
- Check impact of model simplification on sensitivity results (1-2 configurations)
- Test MCNP6 eigenvalue sensitivities for angular distributions
- Extend sensitivity study to thermal and epithermal spectra benchmarks (in connection with UACSA benchmark Phase-III)
- Publish lessons learnt