IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

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

E. Ivanov
T. Ivanova

WPEC/Sg. 39 Meeting
Novembre 27-28, 2014
NEA, Issy-les-Moulineaux, France

General Remarks

- **Objective** of the exercise is to test continuous energy (CE) 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

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

Contributors

James Dyrda	AWE
Evgeny Ivanov, Maria Brovchenko	IRSN
Ian Hill	NEA
Mathieu Hursin, Sandro Pelloni	PSI
Brian Kiedrowski	LANL
Ivan Kodeli	IJS
Christopher Perfetti, Bradley Rearden	ORNL

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

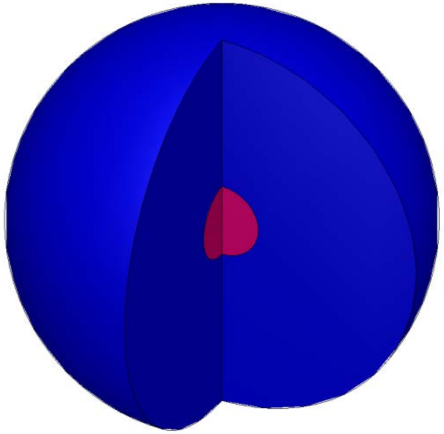
Participant	Tool	Model	Cross sections	Method	Output, groups
AWE	MONK	3D	CE ENDF/B-VII.0 JEFF3.1	MC	33
PSI	SERPENT v2	3D	CE ENDF/B-VII	MC	33
NEA, LANL, IRSN	MCNP6	3D	CE, ENDF/B-VII.1	MC	238, 33
IRSN	SCALE 6.1	1D	MG, ENDF/B-VII.0	SN	238
PSI, ORNL, IRSN	SCALE 6.2β	3D	CE, ENDF/B-VII.1, 0	MC	238
JSI	ANISN/PARTISN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

- **P**lutonium (94 wt ^{239}Pu) sphere surrounded by a thick reflector of natural uranium. Sensitive to scattering on heavy metals, and threshold reactions.

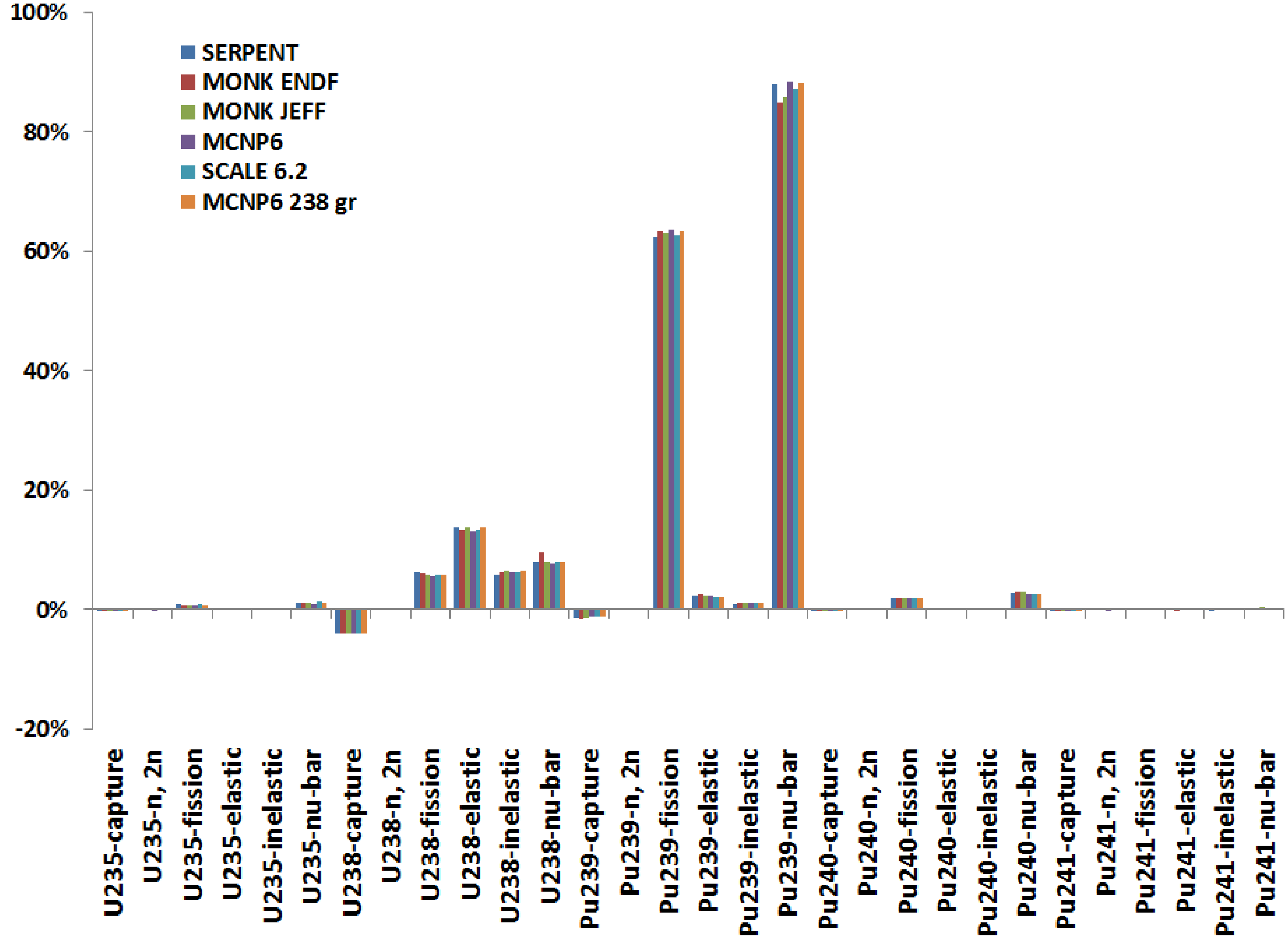
- k_{bench}=1.0000±0.0030



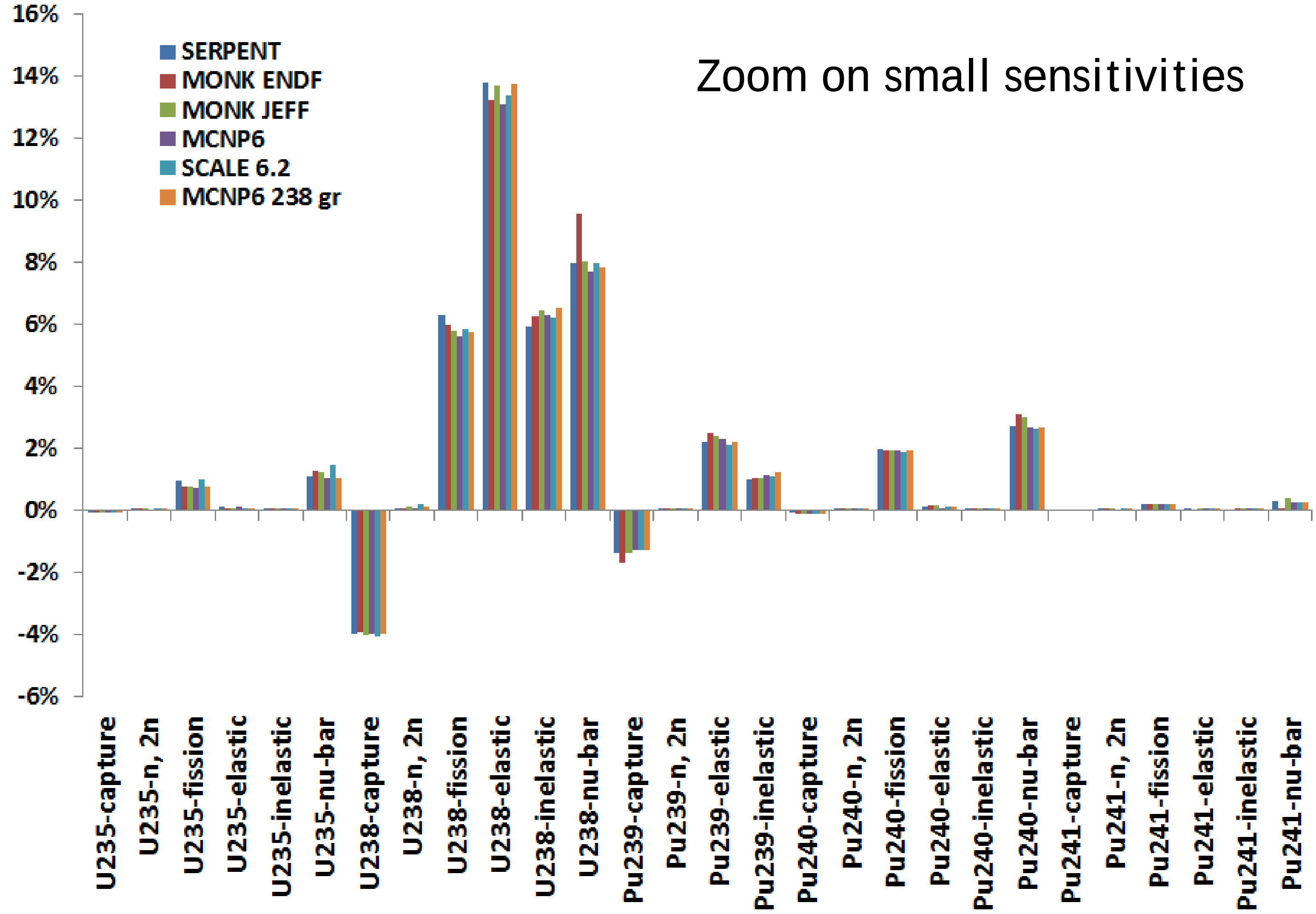
Popsy: Integrated Sensitivities (1/3)

	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

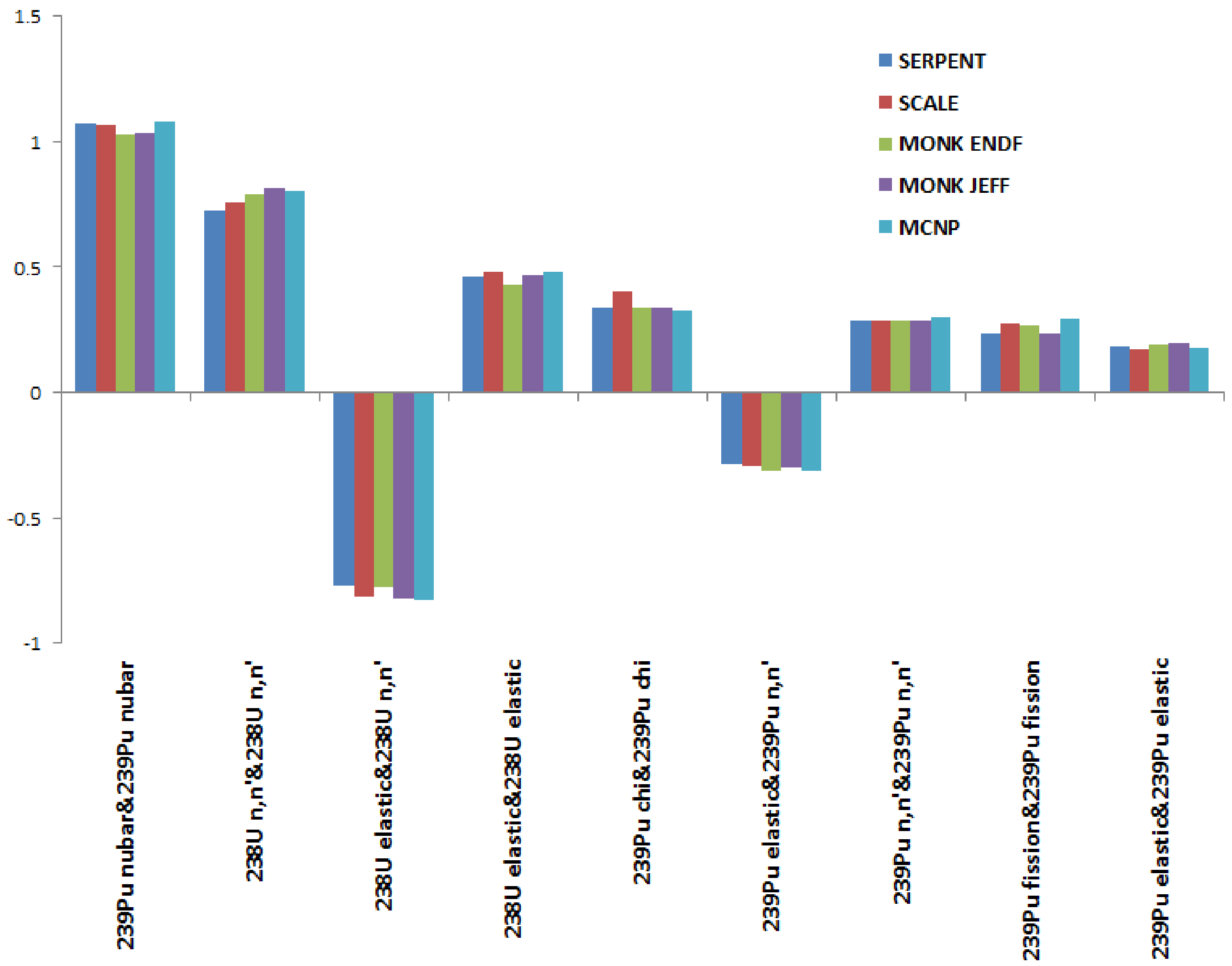
Popsy: Integrated Sensitivities (2/3)



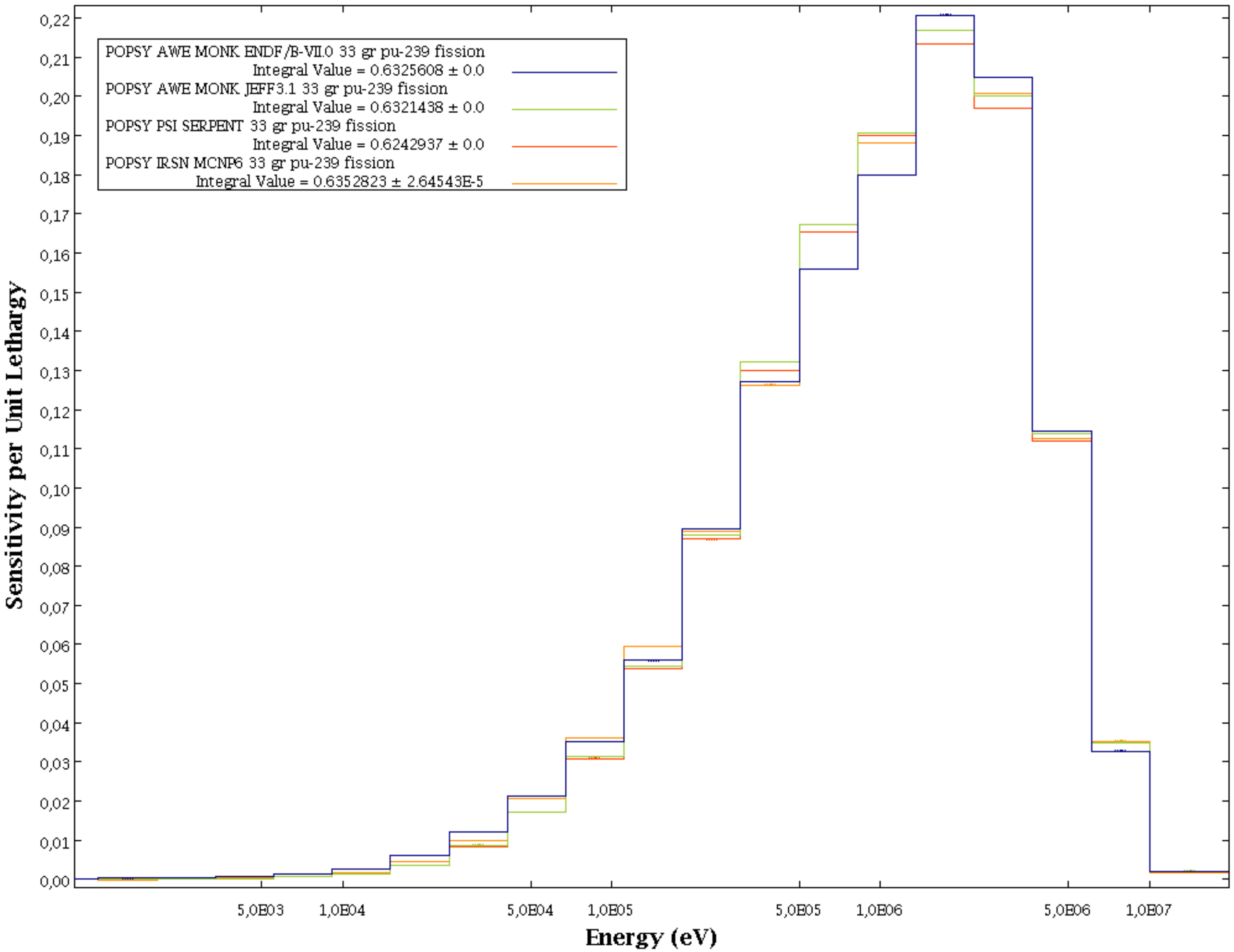
Popsy: Integrated Sensitivities (3/3)



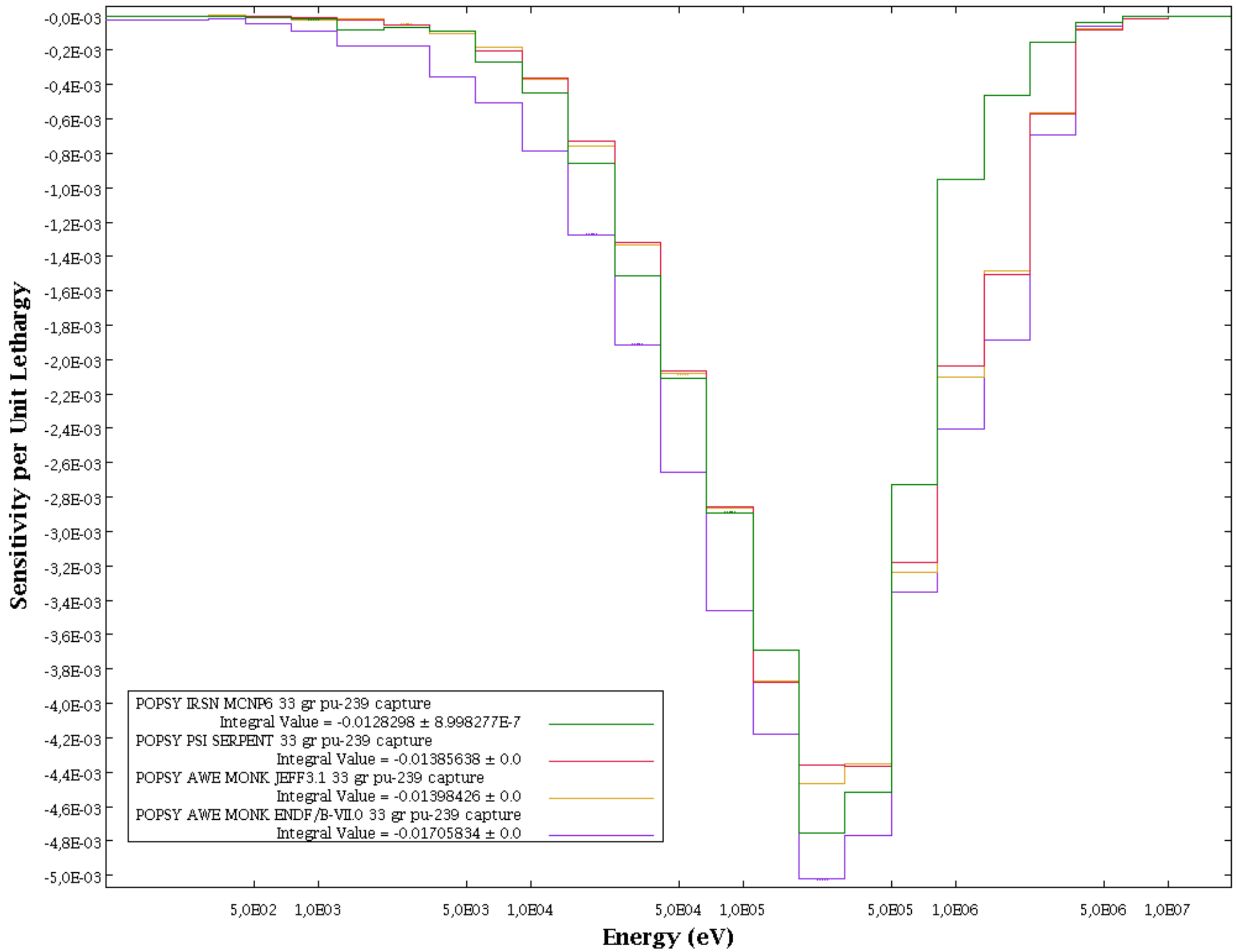
Popsy: Uncertainties by reactions



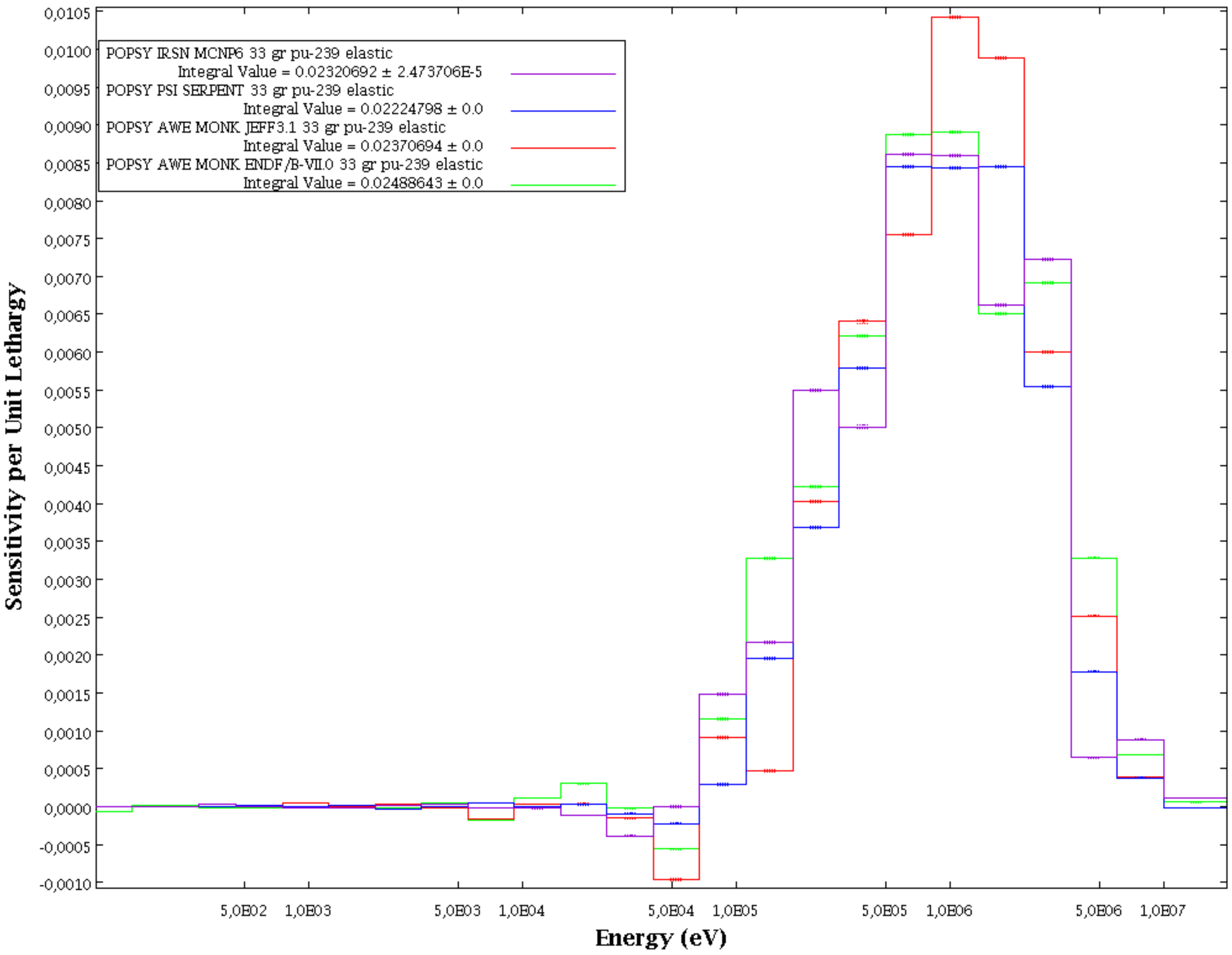
Popsy: Pu-239 Fission Profiles



Popsy: Pu-239 Capture Profiles

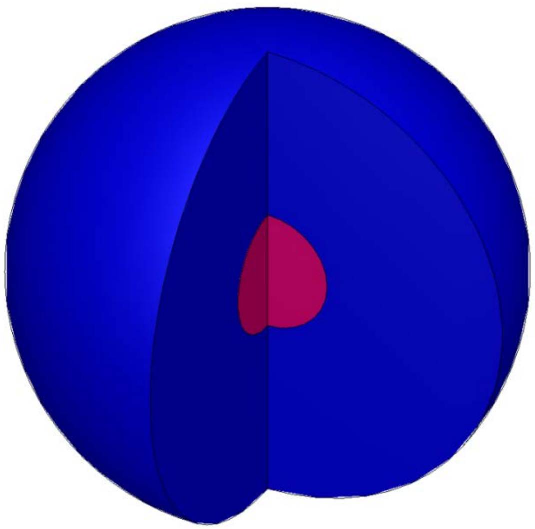


Popsy: Pu-239 Elastic Profiles



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



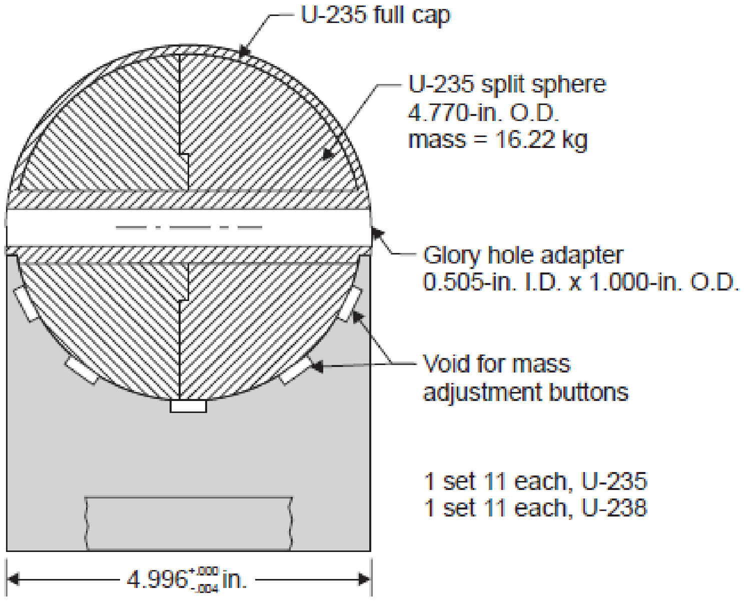
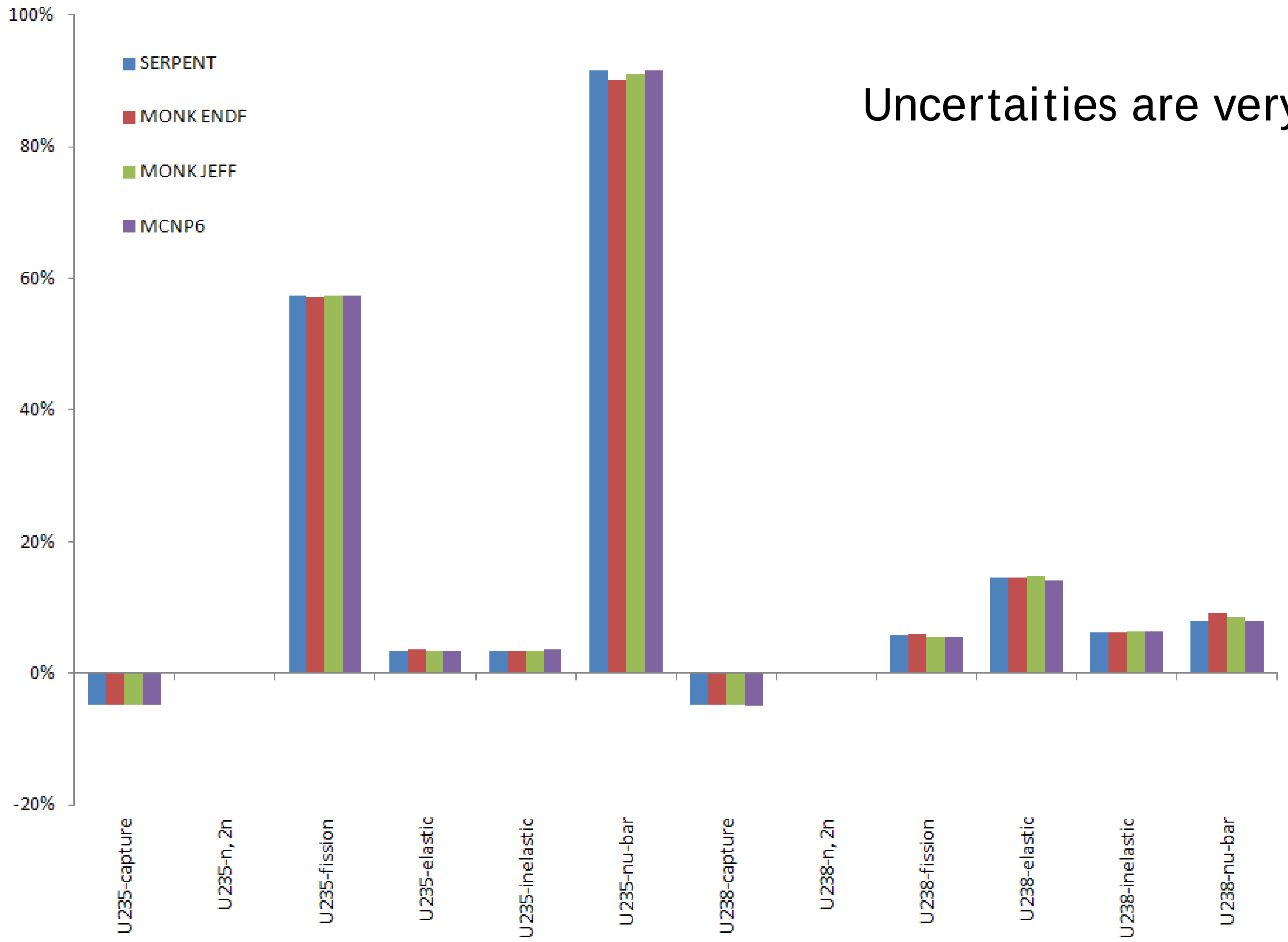


Figure 3. The HEU Sphere.

Topsy: Integrated Sensitivities (1/3)

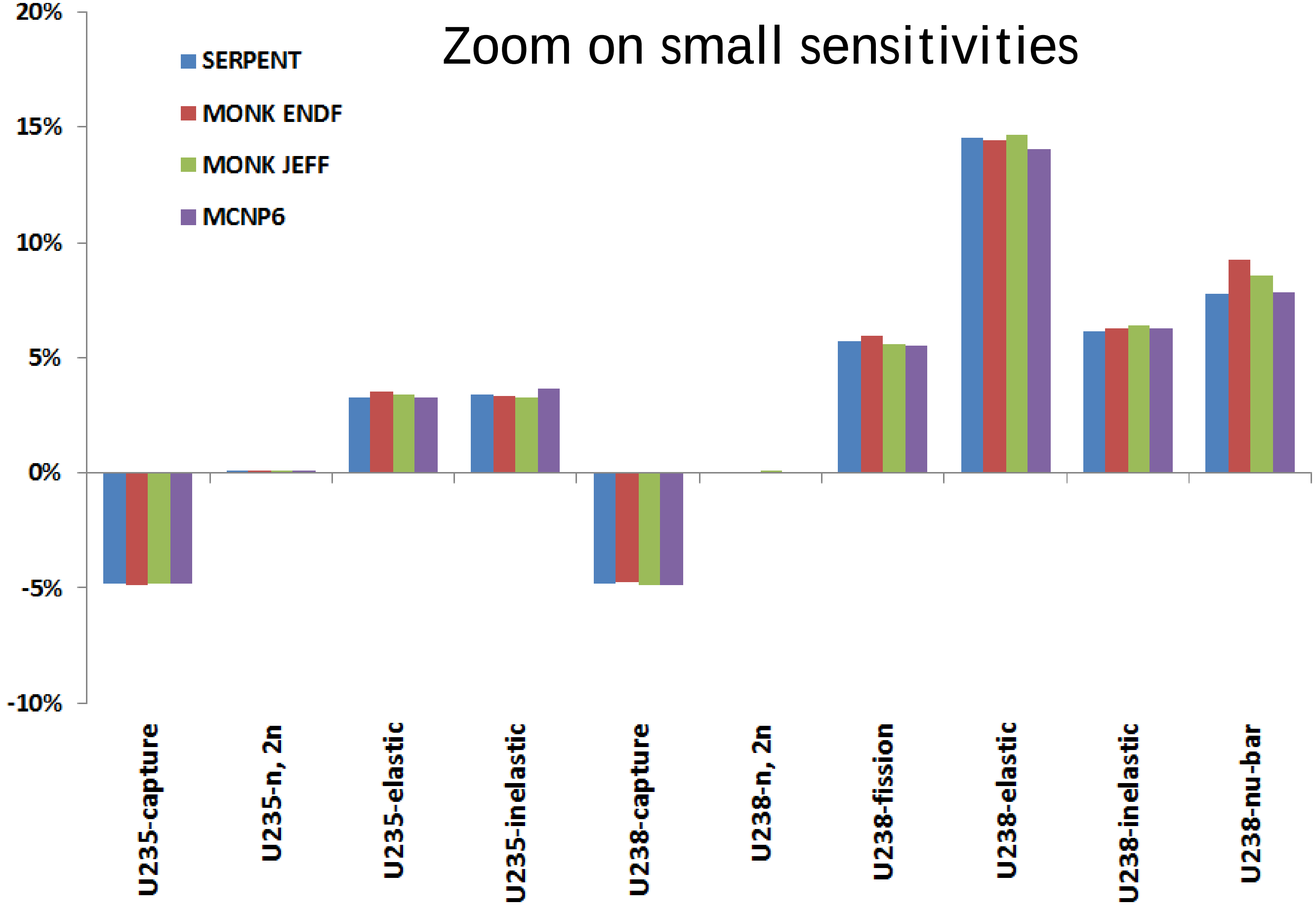
	SERPENT	MONK ENDF	MONK JEFF	MCNP6
U235-capture	-4,79	-4,87	-4,82	-4,84
U235-n, 2n	0,11	0,12	0,12	0,12
U235-fission	57,37	57,17	57,32	57,41
U235-elastic	3,30	3,54	3,43	3,30
U235-inelastic	3,39	3,34	3,28	3,63
U235-nu-bar	91,56	90,10	90,88	91,53
U238-capture	-4,83	-4,74	-4,88	-4,90
U238-n, 2n	0,07	0,05	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)

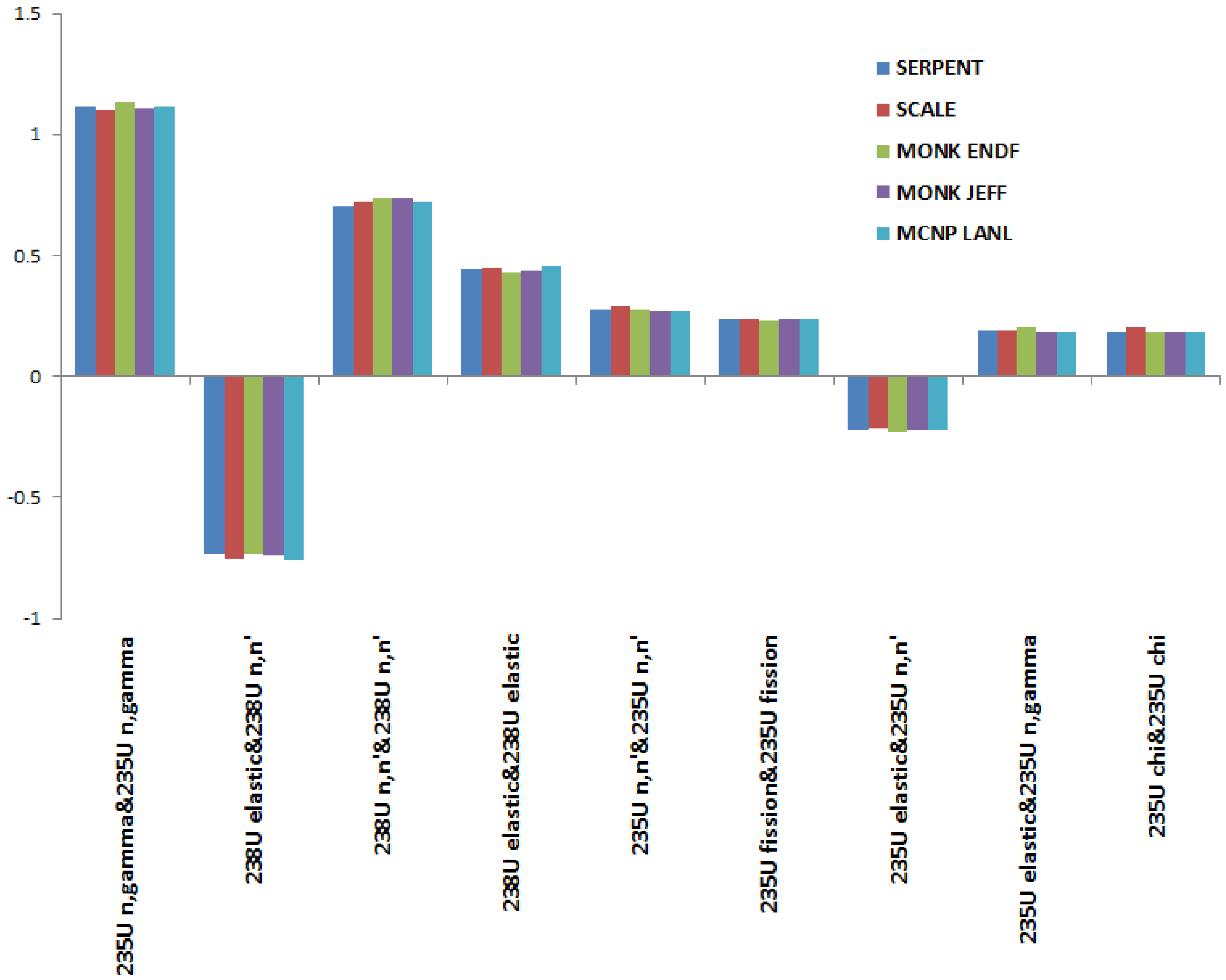


Uncertaities are very small

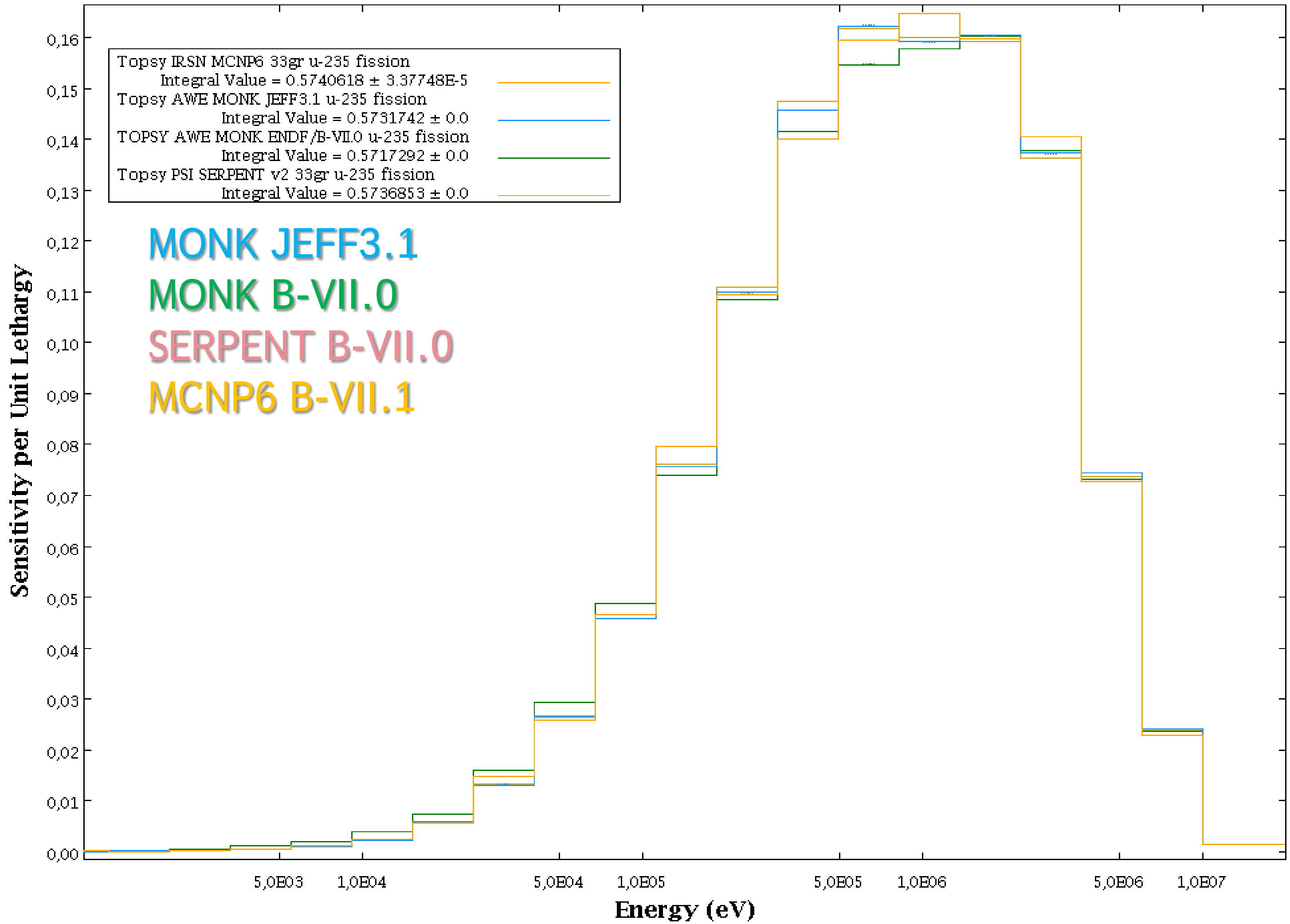
Topsy: Integrated Sensitivities (3/3)



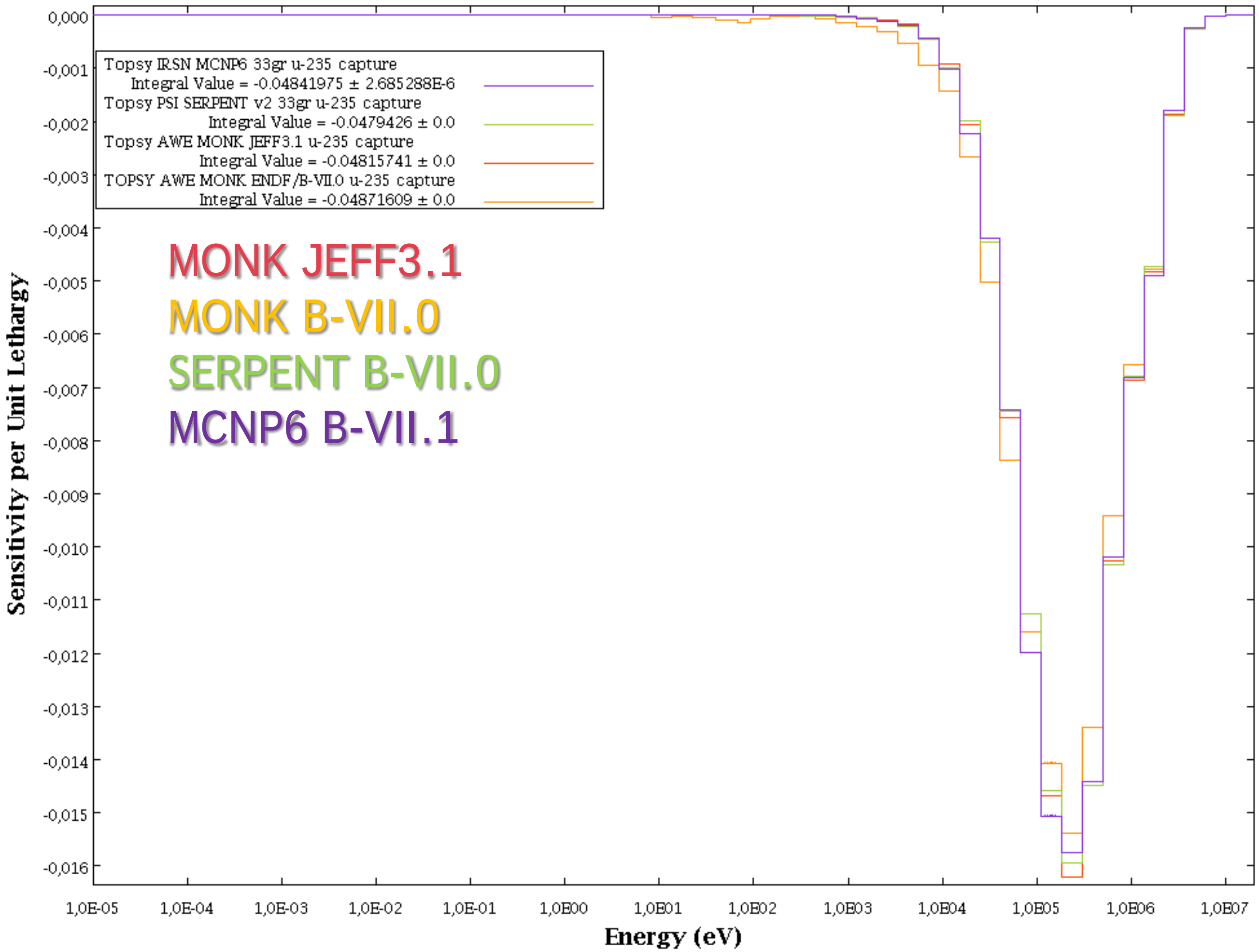
Topsy: Uncertainties by reactions



Topsy: U-235 Fission Profile



Topsy: U-235 Capture Profile



HMI-001 (ZPR 9/34 loading 303)

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

- k_{bench}=0.9966±0.0026

- ^{56}Fe-tot sensitivity in core = 0.0785, in reflector = 0.0166(0.015)

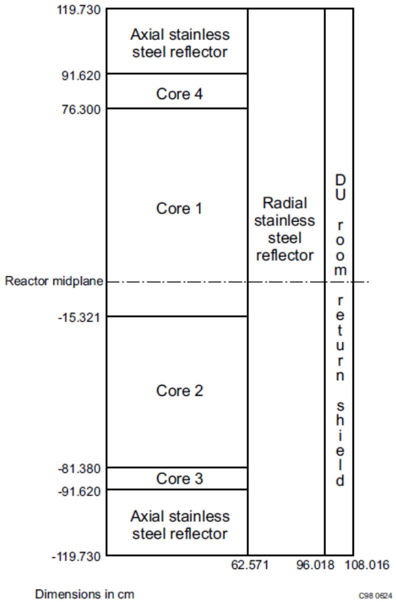
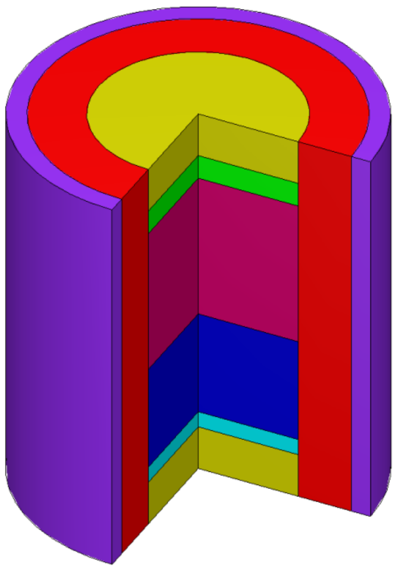
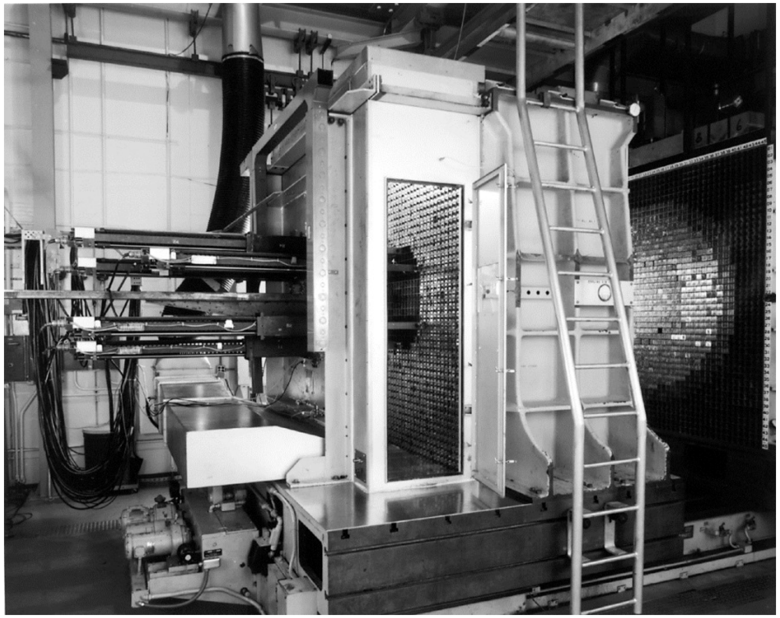


Figure 12. Benchmark Model Geometry.

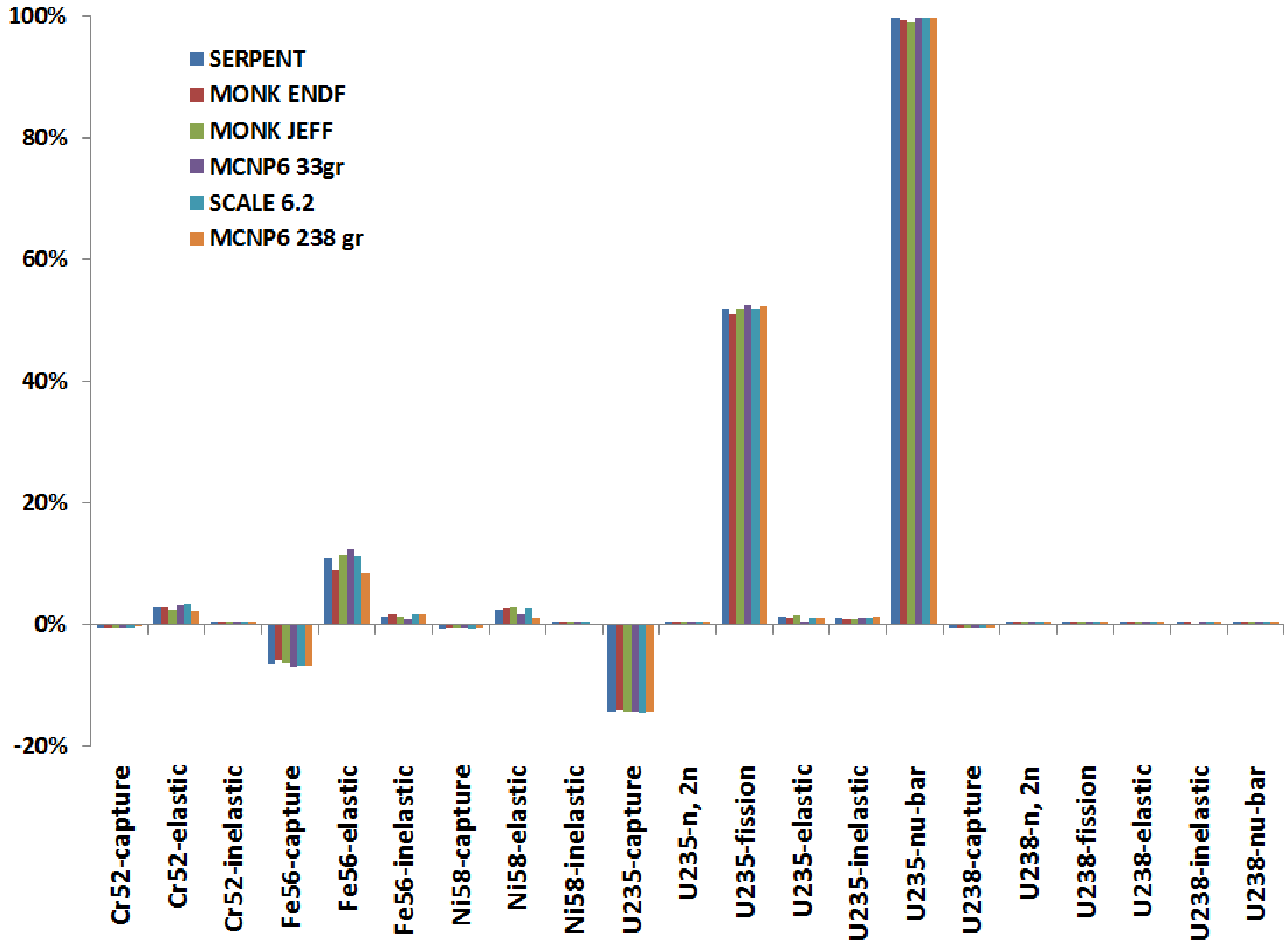




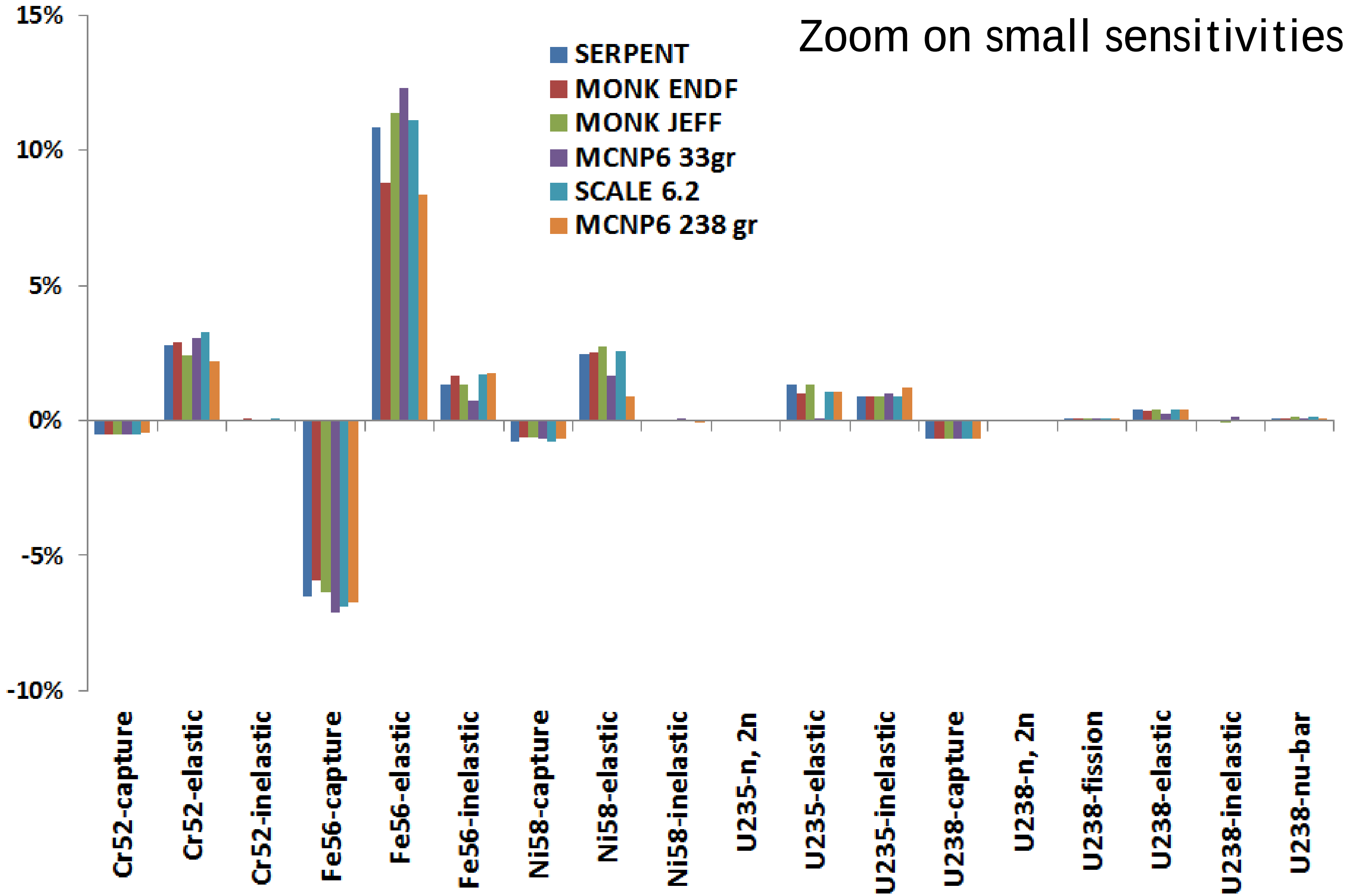
ZPR-9/34: Integrates Sensitivities (1/3)

	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

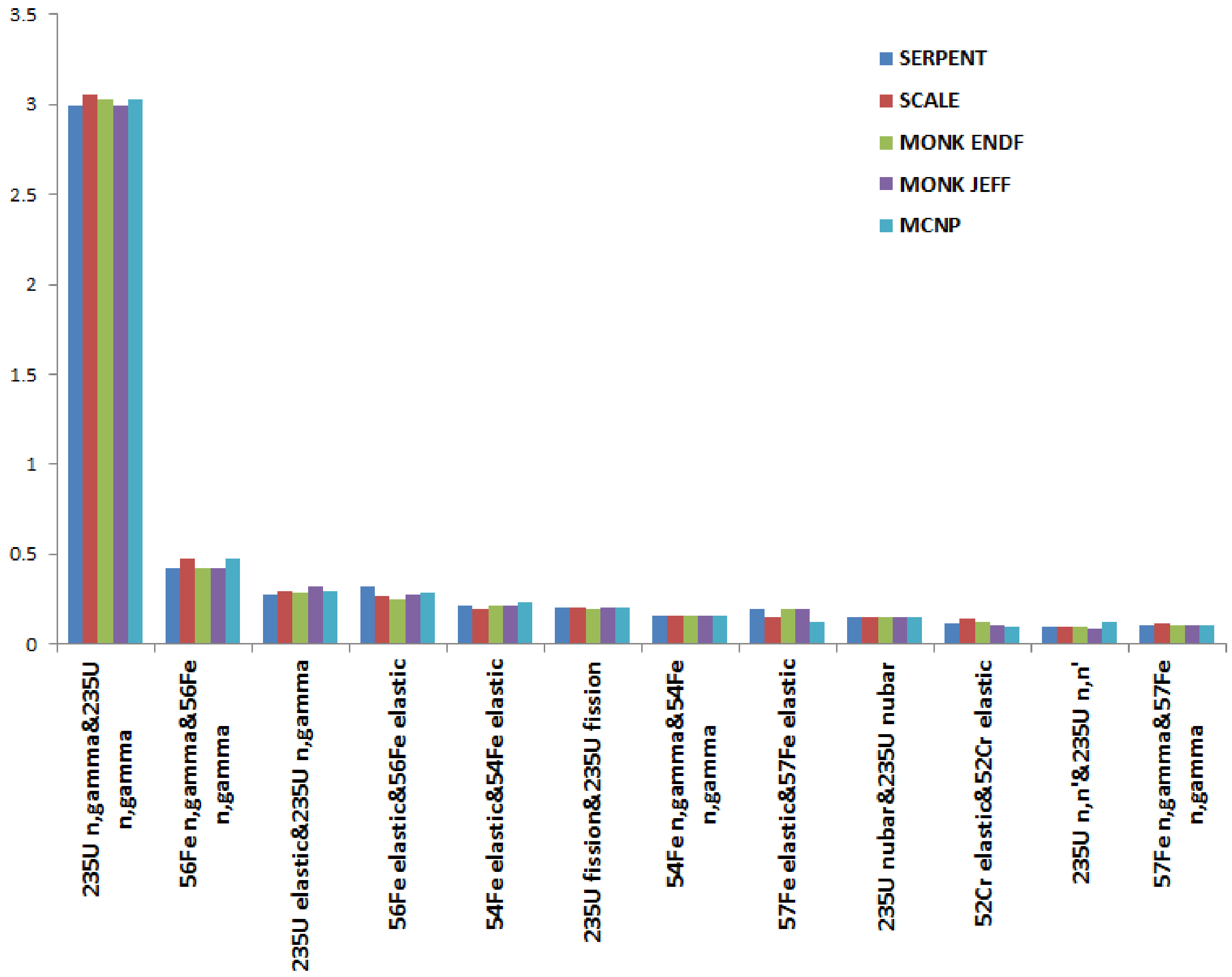
ZPR-9/34: Integrates Sensitivities (2/3)



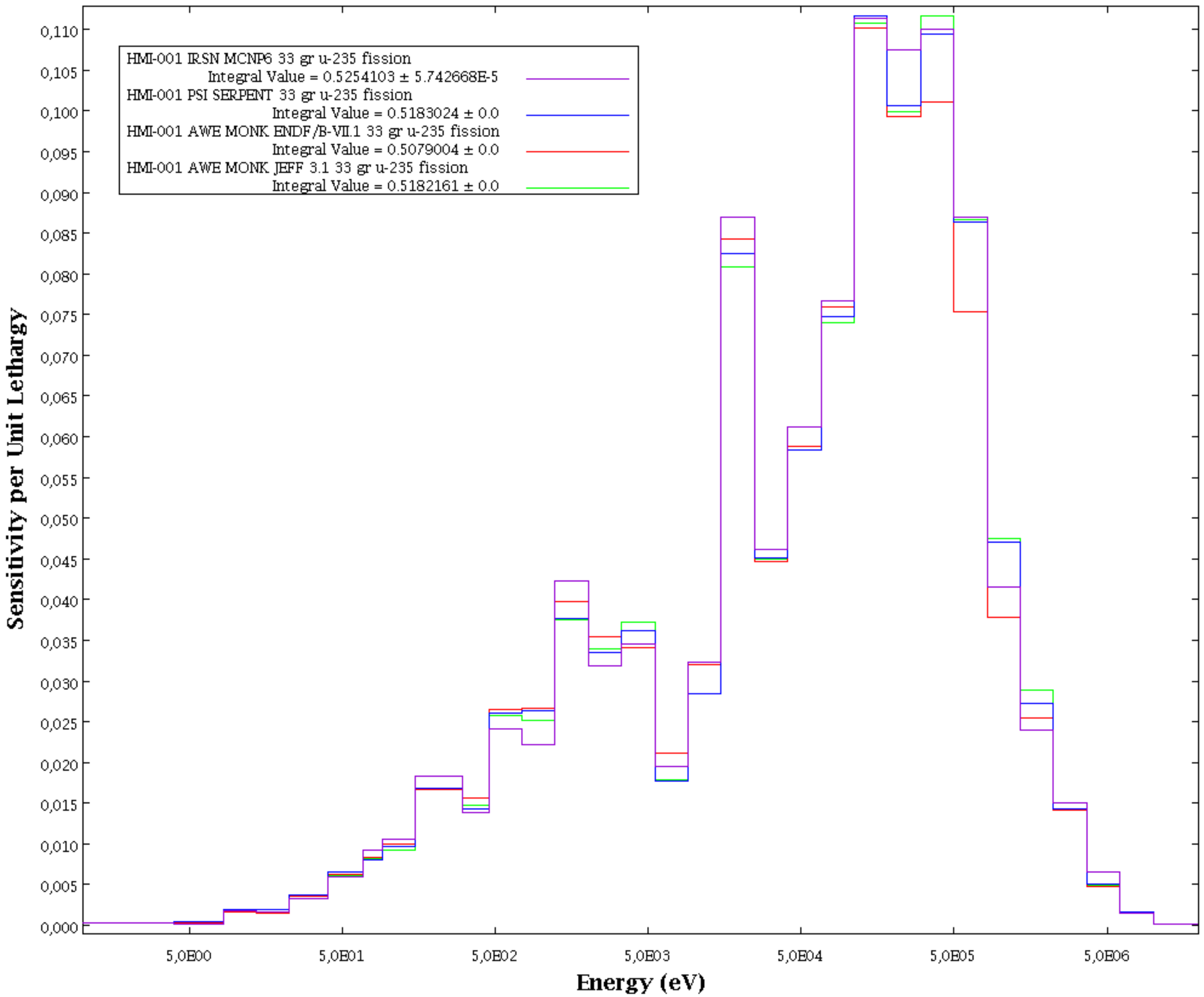
ZPR-9/34: Integrates Sensitivities (3/3)



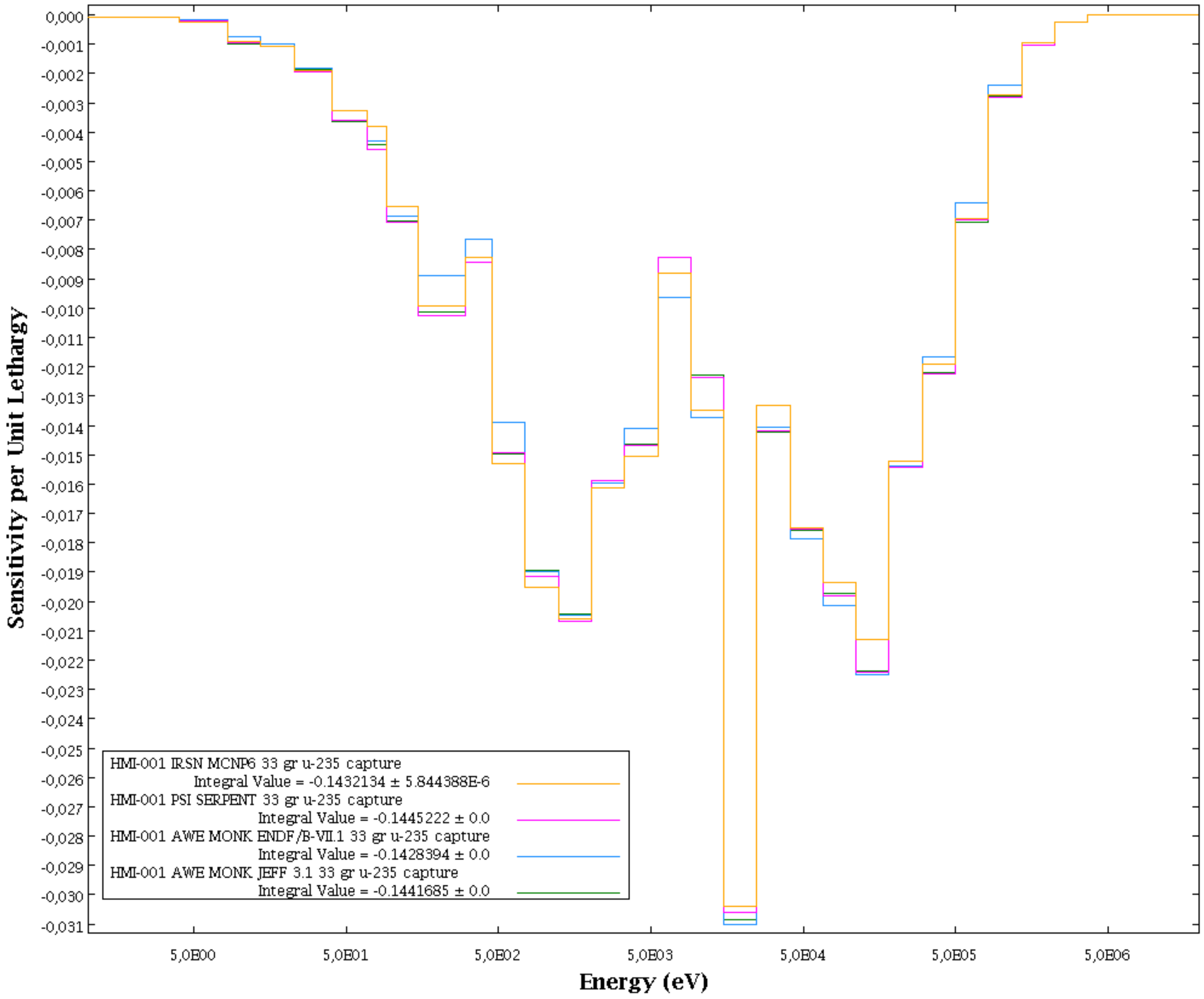
ZPR 9/34: Uncertainties by reactions



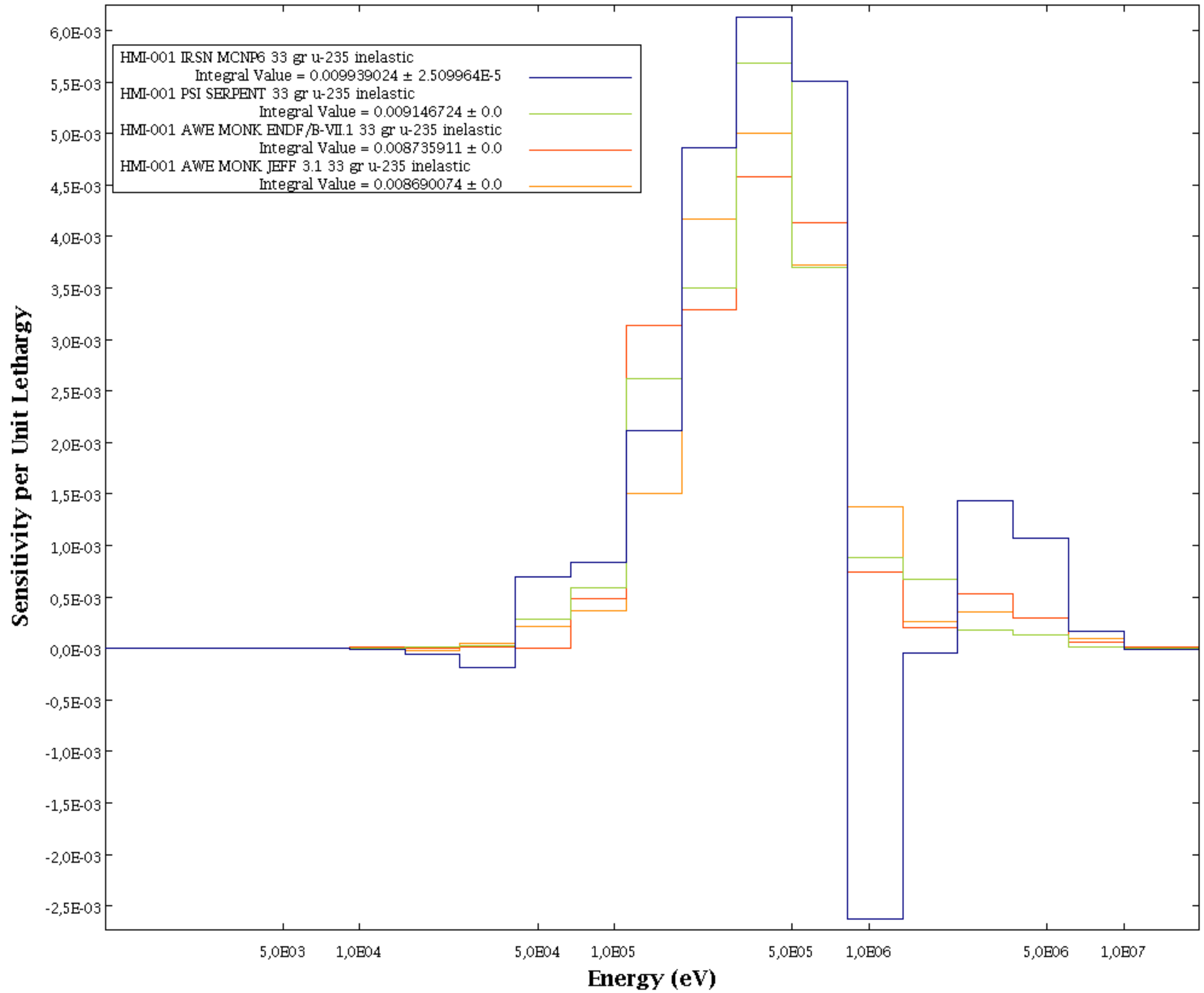
ZPR 9/34: U-235 Fission Profiles



ZPR 9/34: U-235 Capture Profiles



ZPR 9/34: U-235 Inelastic Profiles



PMI-002 (ZPR 6/10 loading 24)

- **C**ore 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)

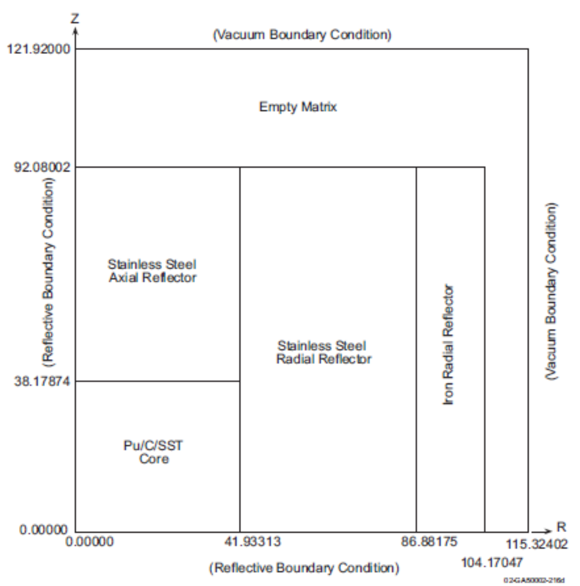
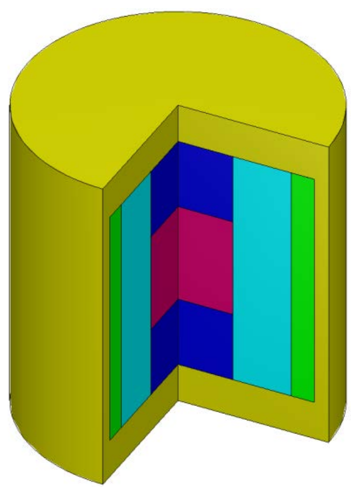
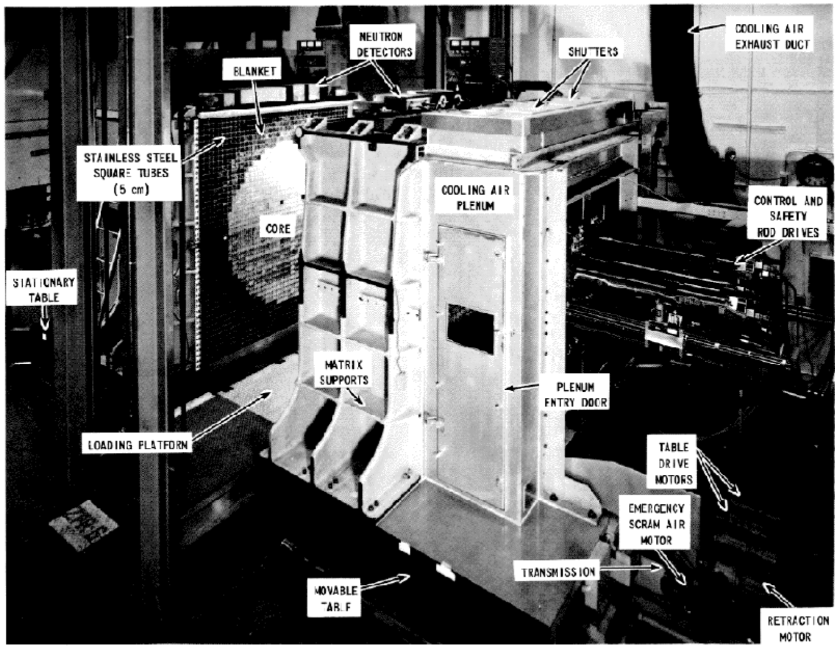


Figure 6. Benchmark-Model Geometry for ZPR-6/10.

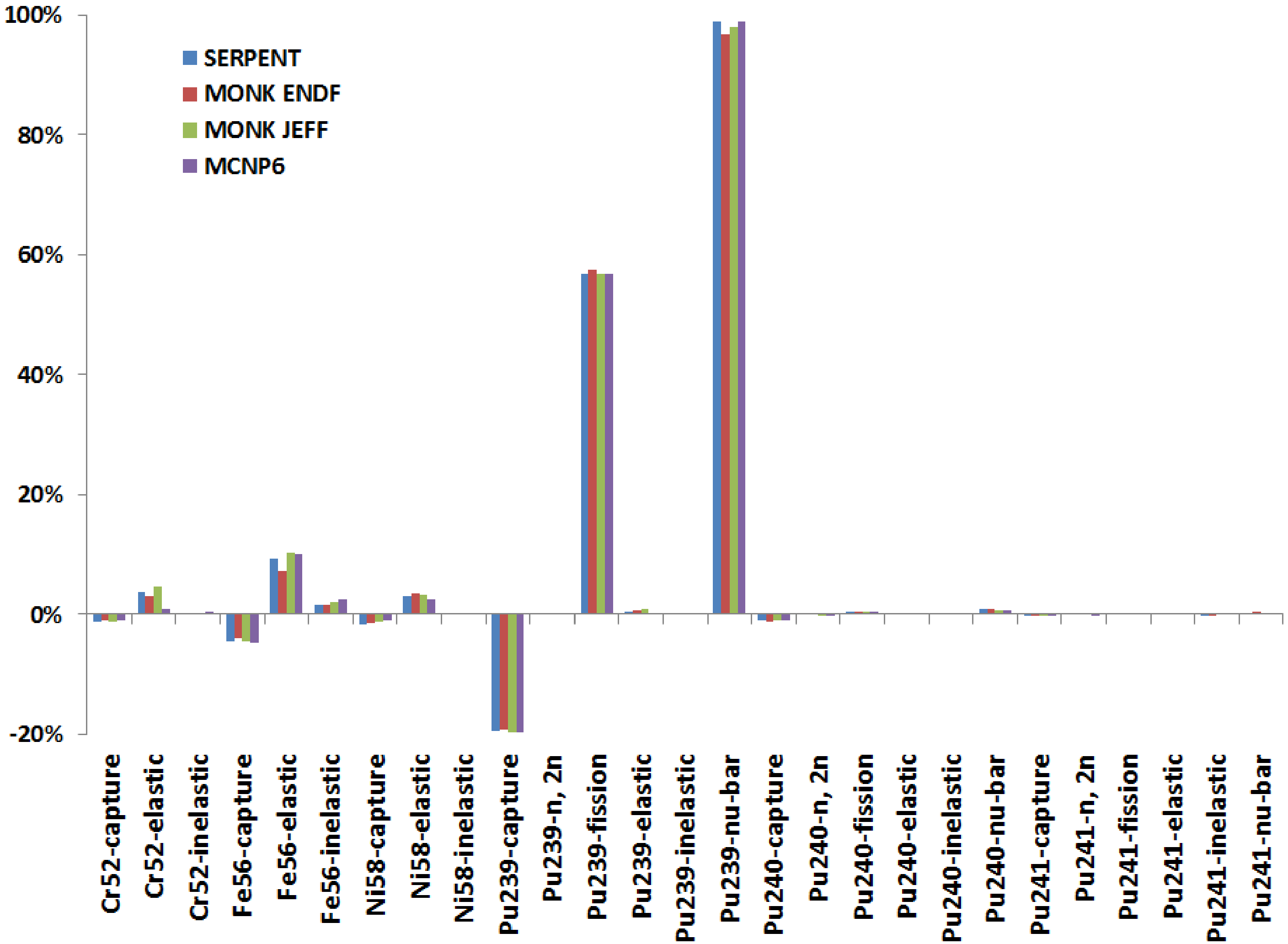




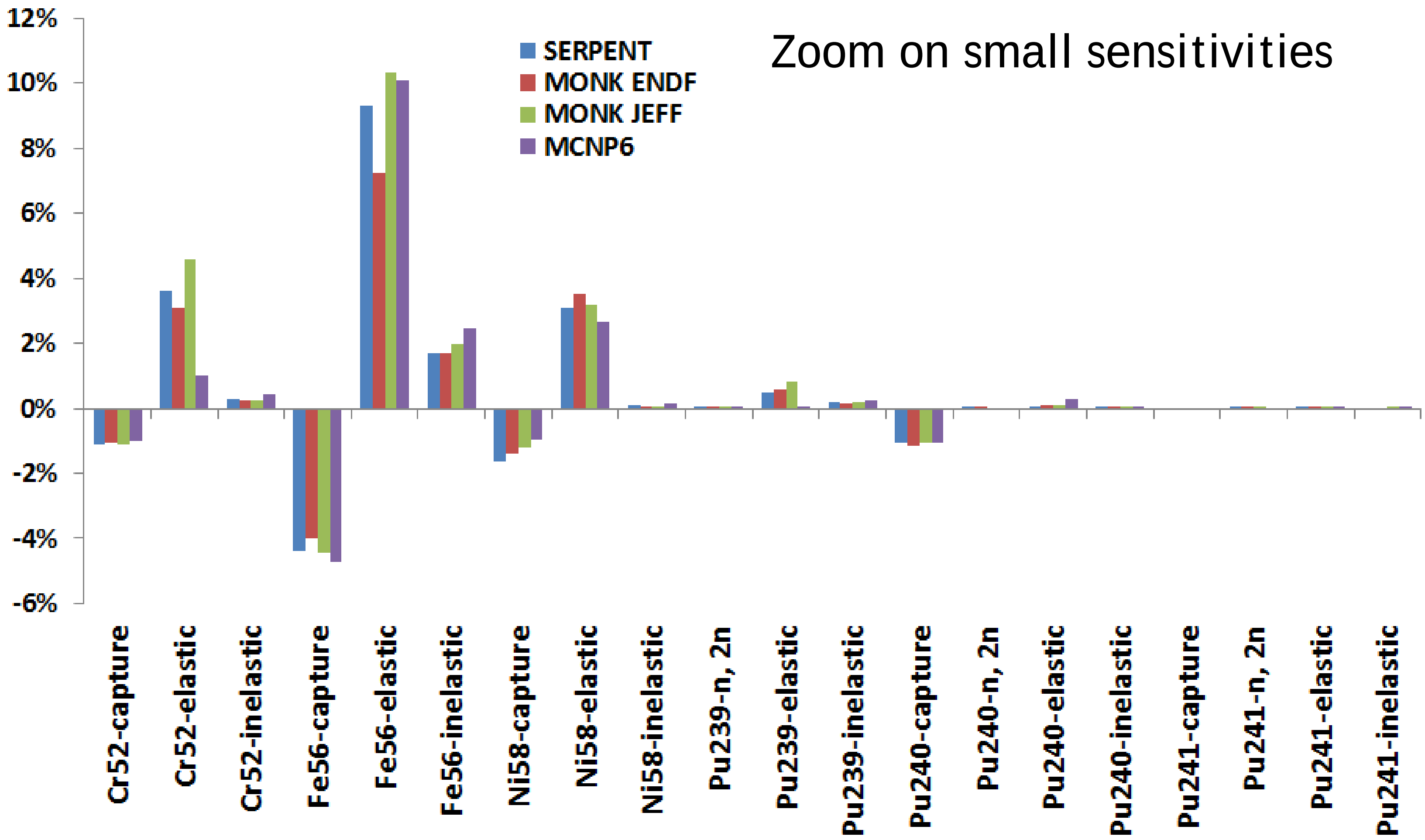
ZPR 6/10: Integrated Sensitivities (1/3)

	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

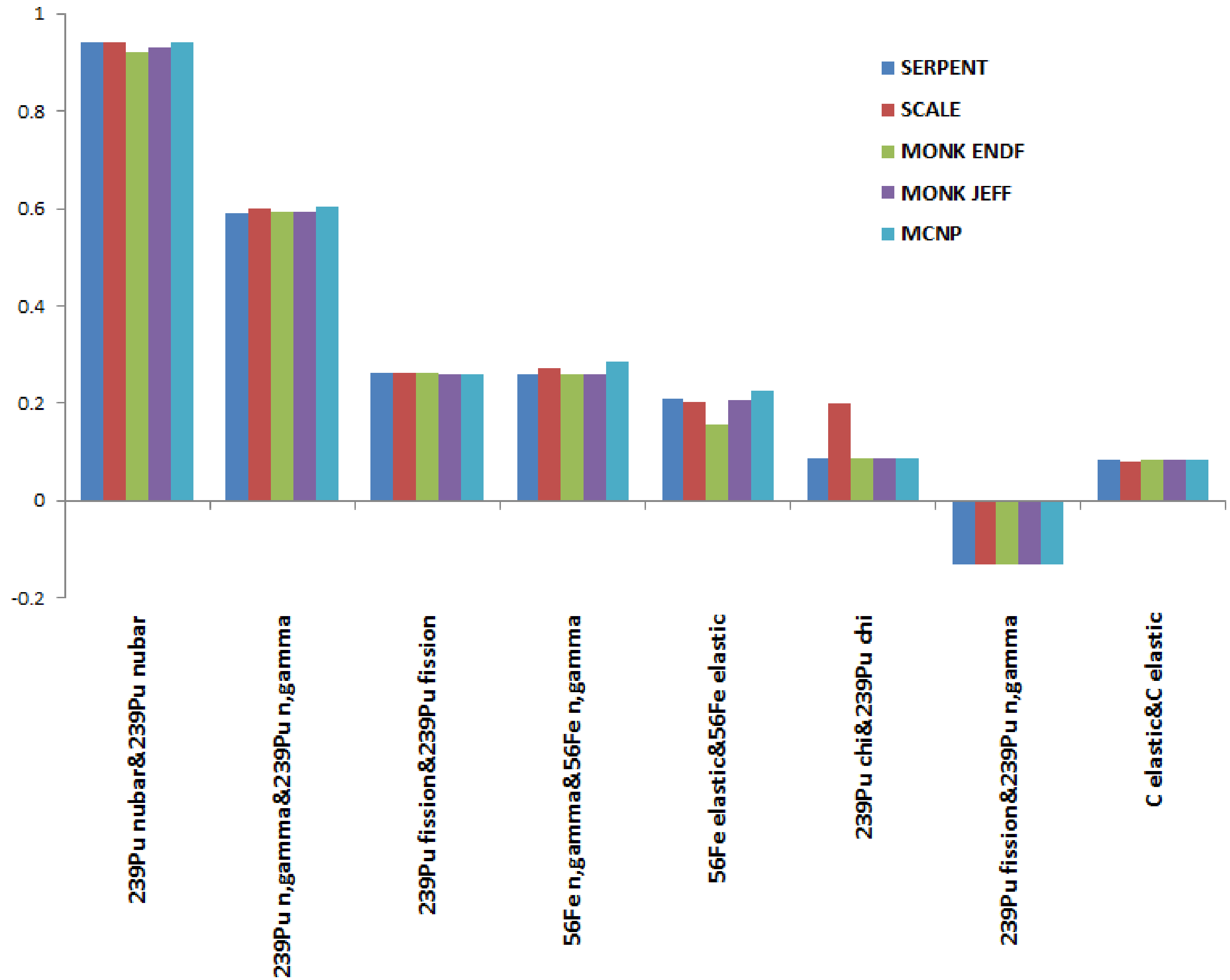
ZPR 6/10: Integrated Sensitivities (2/3)



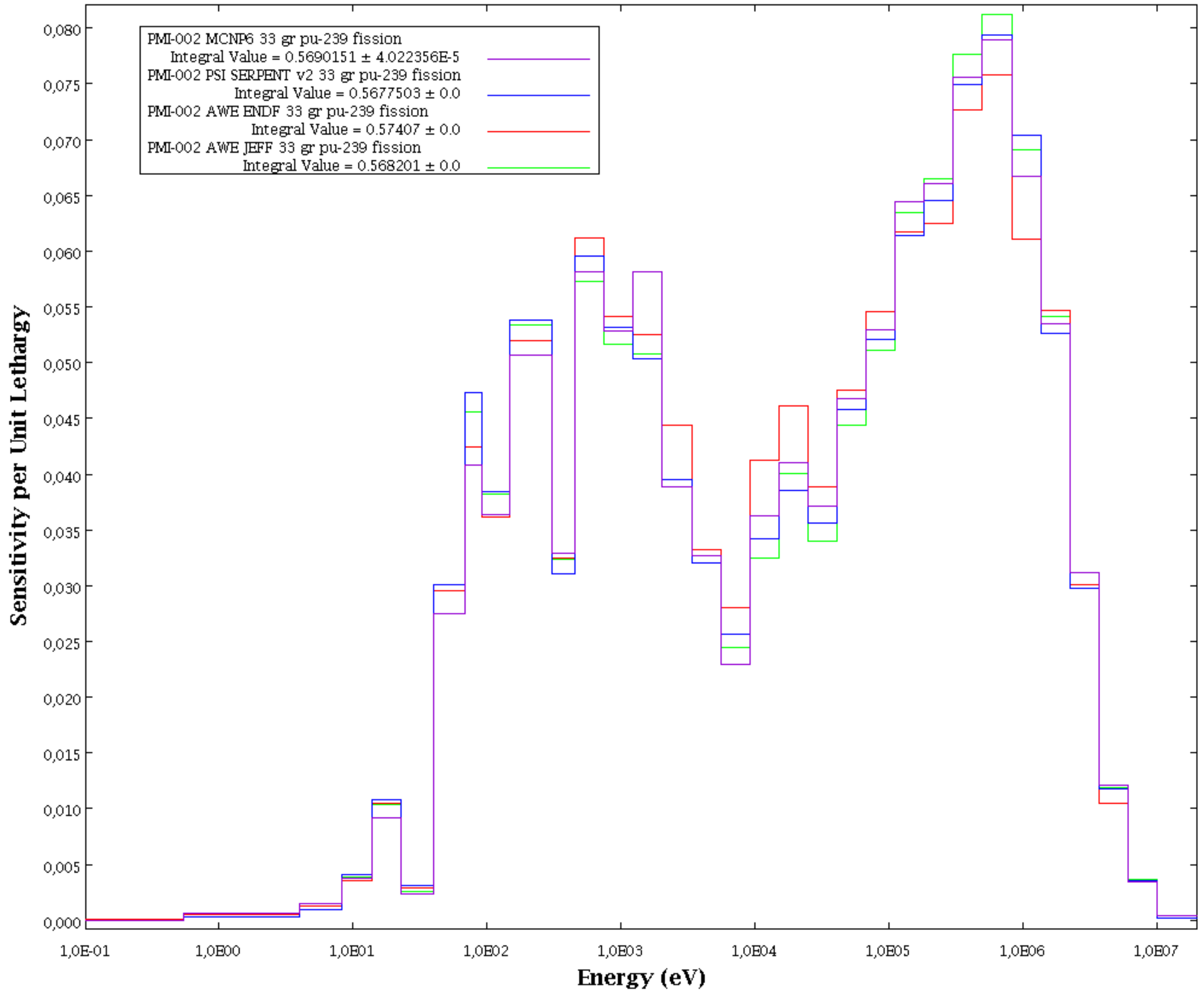
ZPR 6/10: Integrated Sensitivities (3/3)



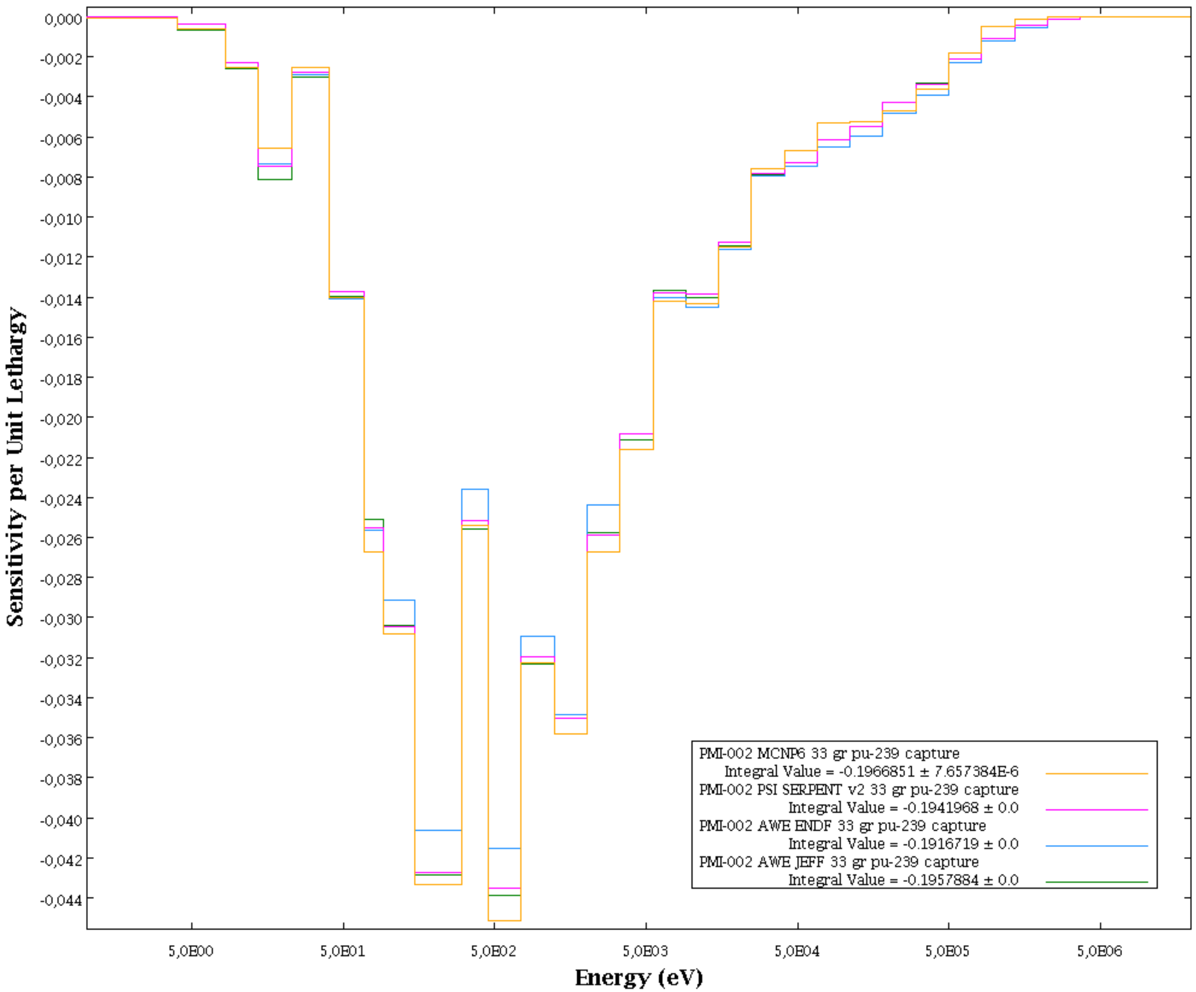
ZPR 6/10: Uncertainties by reactions



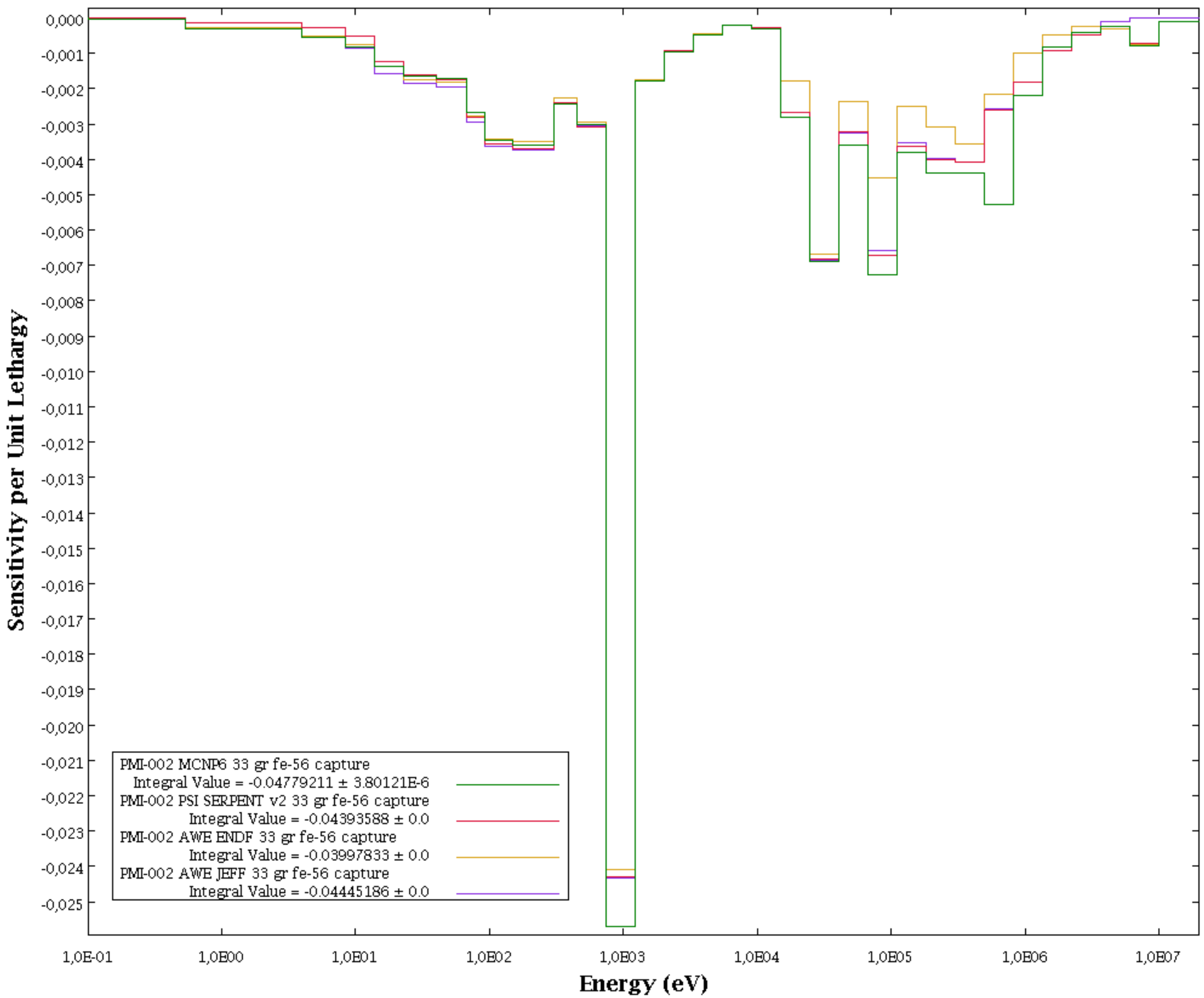
ZPR 6/10: Pu-239 Fission Profiles



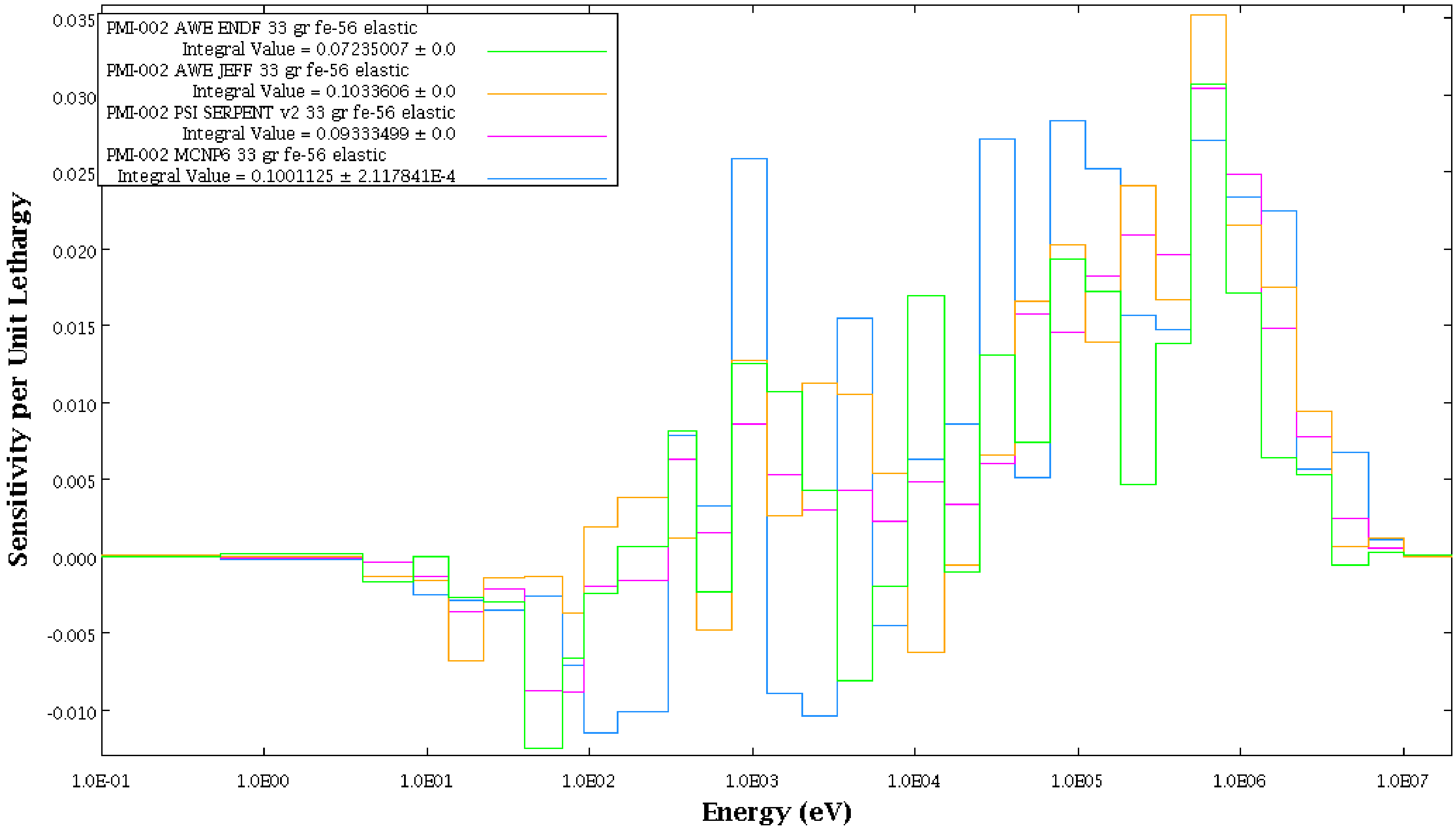
ZPR 6/10: Pu-239 Capture Profiles



ZPR 6/10: Fe-56 Capture Profiles



ZPR 6/10: Fe-56 Elastic Profiles



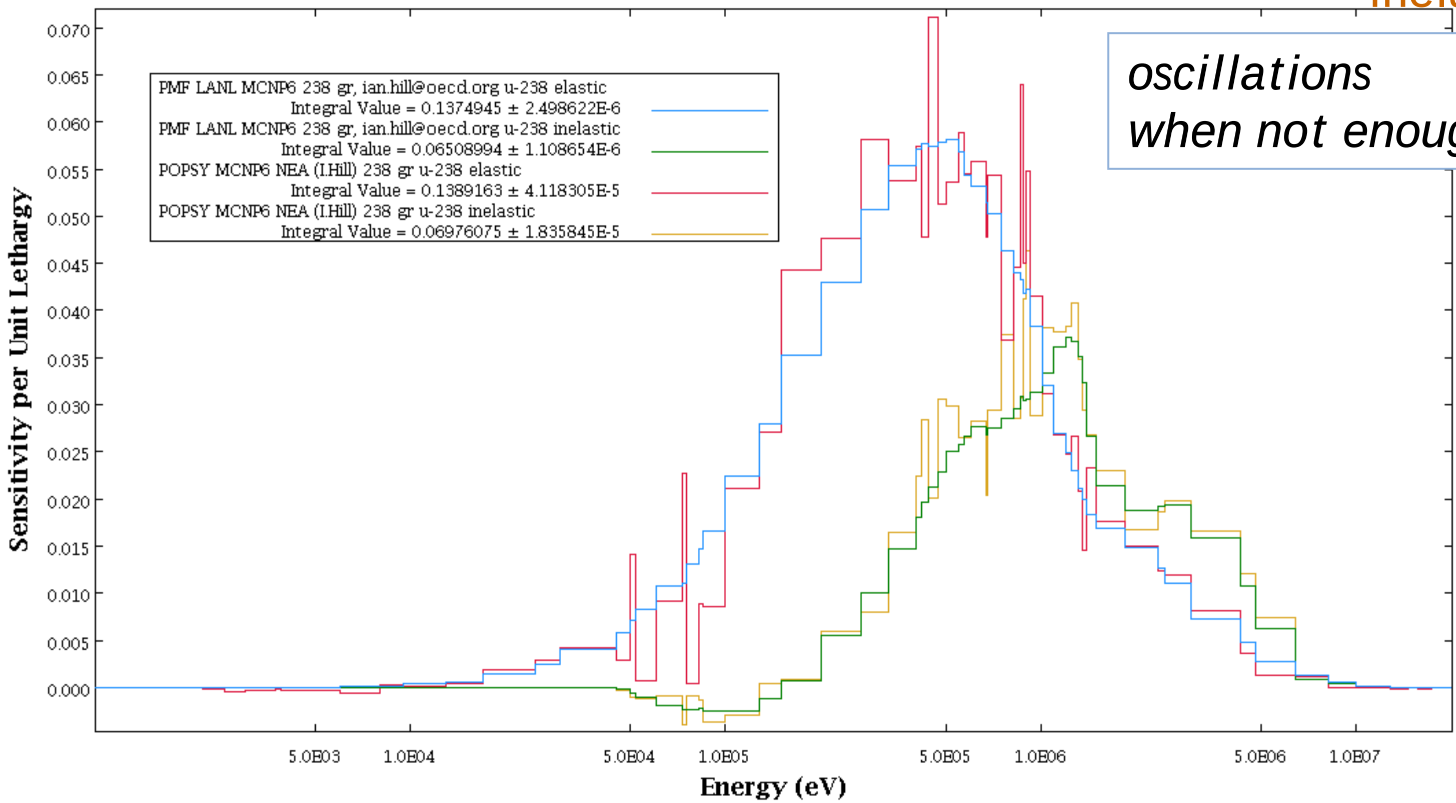
Convergence Issues

- 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

E. Tsvetkov EMPIRICAL TESTING OF SOME PSEUDO-RANDOM NUMBERS GENERATORS/ Mathematical Modeling, v 23, #5, pp.81-94, 2011

- Empirical testing of statistical properties of some pseudo-random numbers generators based on a partition of the unit hypercube with dimension from 1 to 15 was performed. Some CLHEP library pseudo-random numbers generators, Mersenne Twister generator and MCNP generator were tested. The results of tests allowed to determine the parts of the pseudo-random numbers sequences with bad statistical properties. The easy recoverable defects of two CLHEP generators were found.

$$I = \lim_{n\to\infty} S_n, \qquad \mathbf{r}_1 = (x_1, x_2, \ldots, x_k), \mathbf{r}_2 = (x_{K+1}, x_{K+2}, \ldots, x_{K+k}), \ \ldots,$$

$$S_n = \frac{V}{n}\sum_{i=1}^{n} f(\mathbf{r}_i), \qquad \mathbf{r}_n = \left(x_{(n-1)K+1}, x_{(n-1)K+2}, \ldots, x_{(n-1)\cdot K+k}\right), \ \ldots,$$

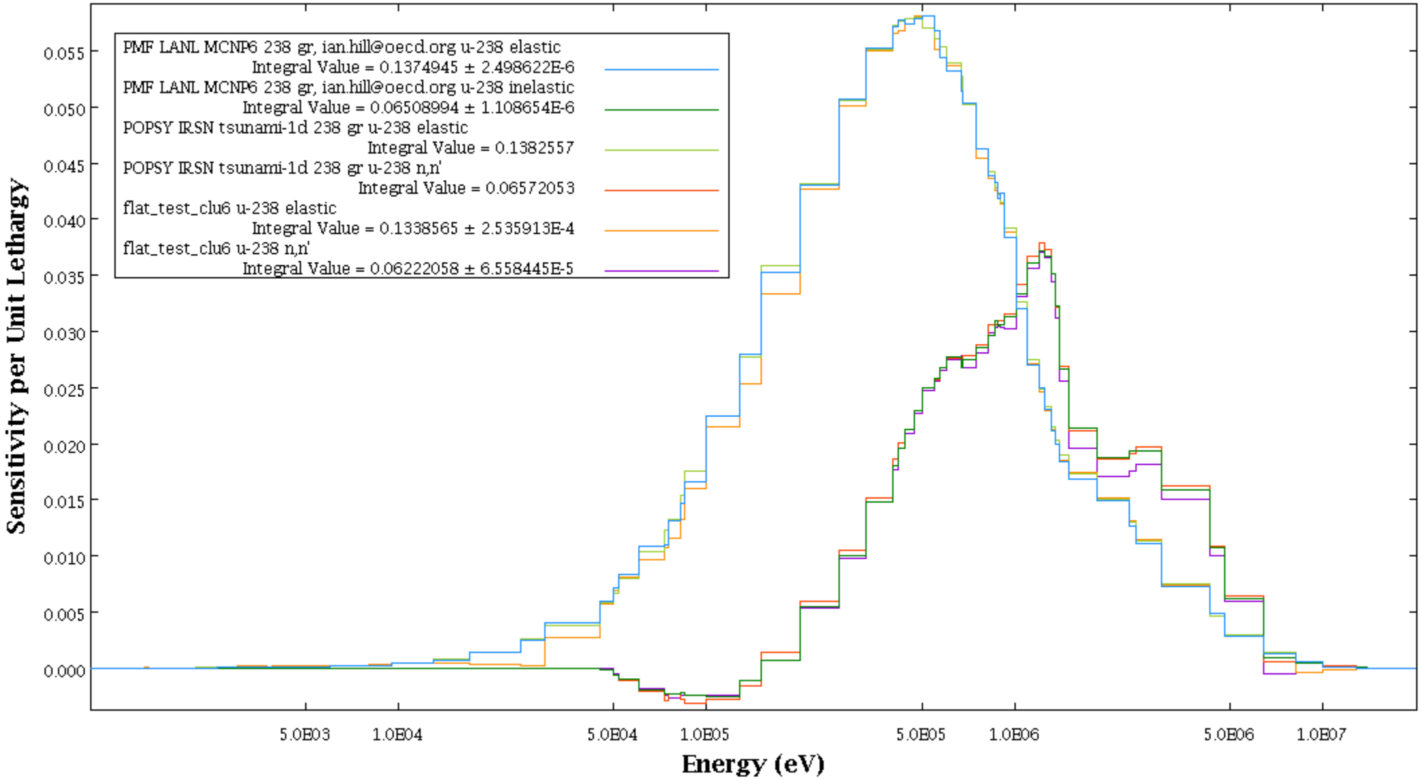
$$\chi^2 = \frac{1}{MX}\sum_{i=1}^{S^k}(X_i - MX)^2$$

E. Tsvetkov EMPIRICAL TESTING OF SOME PSEUDO-RANDOM NUMBERS GENERATORS/ Mathematical Modeling, v 23, #5, pp.81-94, 2011

	1	2	3	4	5	6	7	8	9	10
CLHEP::DualRand	**0.995323**	0.948053	0.340351	0.768940	0.987268	**0.998447**	0.947438	0.794921	0.865710	0.981127
CLHEP::HepJamesRandom	**1.000000**	0.699740	0.936632	0.966977	0.886762	0.928390	0.948037	0.874440	0.531962	0.831159
CLHEP::Hurd160Engine	0.981242	0.971623	0.958399	0.631339	0.863938	0.867428	0.974473	0.694394	0.906157	0.928675
CLHEP::Hurd288Engine	0.559912	0.792181	0.509890	0.757253	**0.999971**	0.976666	0.931154	**0.994599**	0.953089	0.946499
CLHEP::MTwistEngine	**0.994270**	0.946652	0.974972	0.899679	0.752039	0.944401	0.947856	0.951318	0.878380	0.871078
CLHEP::RanecuEngine	**0.998975**	**0.996958**	0.346334	0.709779	0.679632	0.900535	0.870693	0.705390	0.773634	0.619596
CLHEP::Ranlux64Engine	0.933658	0.874168	0.850137	0.974327	0.737928	0.960292	**0.997410**	0.917534	0.810551	**0.990689**
CLHEP::RanluxEngine	**1.000000**	0.642228	0.777547	0.841973	0.988477	0.908988	0.740307	0.493492	**0.999962**	0.937359
CLHEP::RanshiEngine	**0.993416**	0.707369	0.972229	0.910035	0.679360	0.921317	0.978640	0.977095	0.904776	0.934596
CLHEP::TripleRand	**0.995091**	0.398372	0.577427	**0.993931**	0.968364	0.962025	0.975680	0.988473	0.876030	0.983850
Matlab::twister	0.959231	0.702784	0.810525	0.569543	0.781814	0.982808	0.892043	0.864386	0.758089	0.882524
MersenneTwister	0.906981	0.939482	0.924331	0.906341	0.931654	0.652740	0.972370	0.123699	0.954542	0.881406
MCNP::rang	0.709312	**0.000000**	**1.000000**	**0.000000**	**0.000000**	**0.000000**	0.686396	**0.000000**	0.966349	**1.000000**
MCNP::rang, форм. (4), табл	0.887875	**0.000000**	**1.000000**	**0.000000**	0.000240	0.000170	0.716351	**0.000000**	0.447955	0.000460
MCNP::rang, форм. (4), табл	**0.992192**	0.895684	0.405542	0.701091	0.956045	0.970338	0.554682	0.974754	**0.997694**	0.809440

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

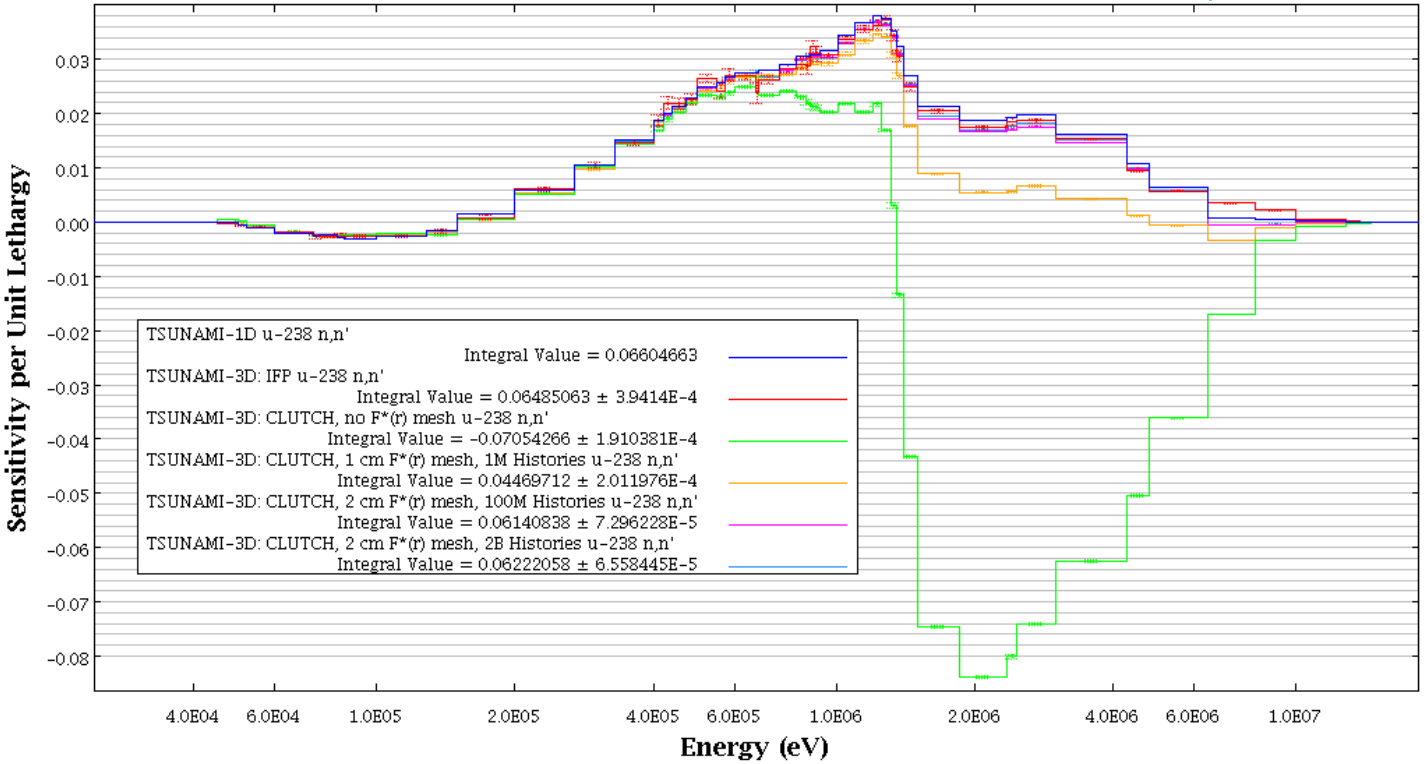


IRSN

Popsy: SCALE/CLUTCH Convergence

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

C.Perfetti/ ORNL



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.

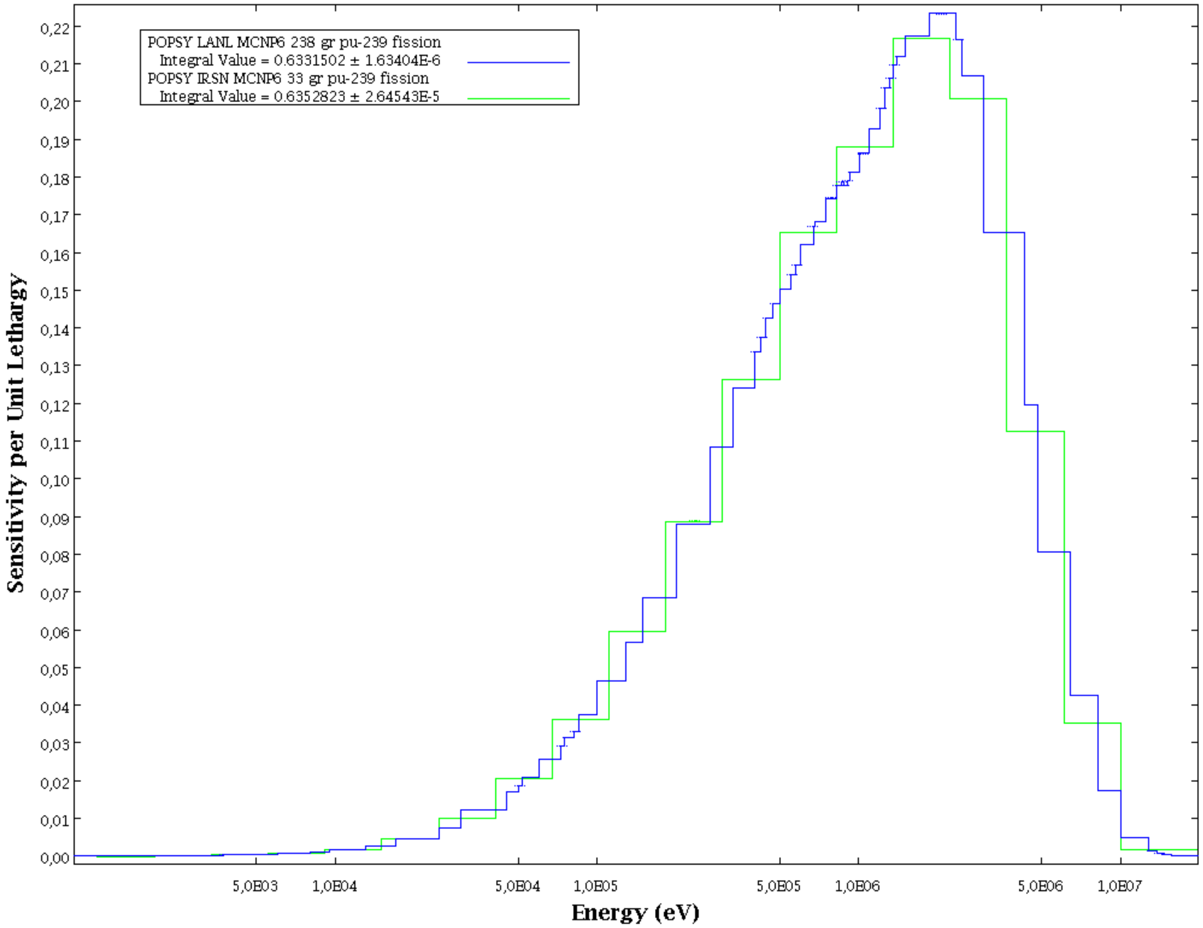
$$F(x) = \frac{\nu\Sigma_f(\mathbf{r},E)}{k_{эф}\Sigma_a(\mathbf{r},E)} Q^{+}(\mathbf{r})$$

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

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

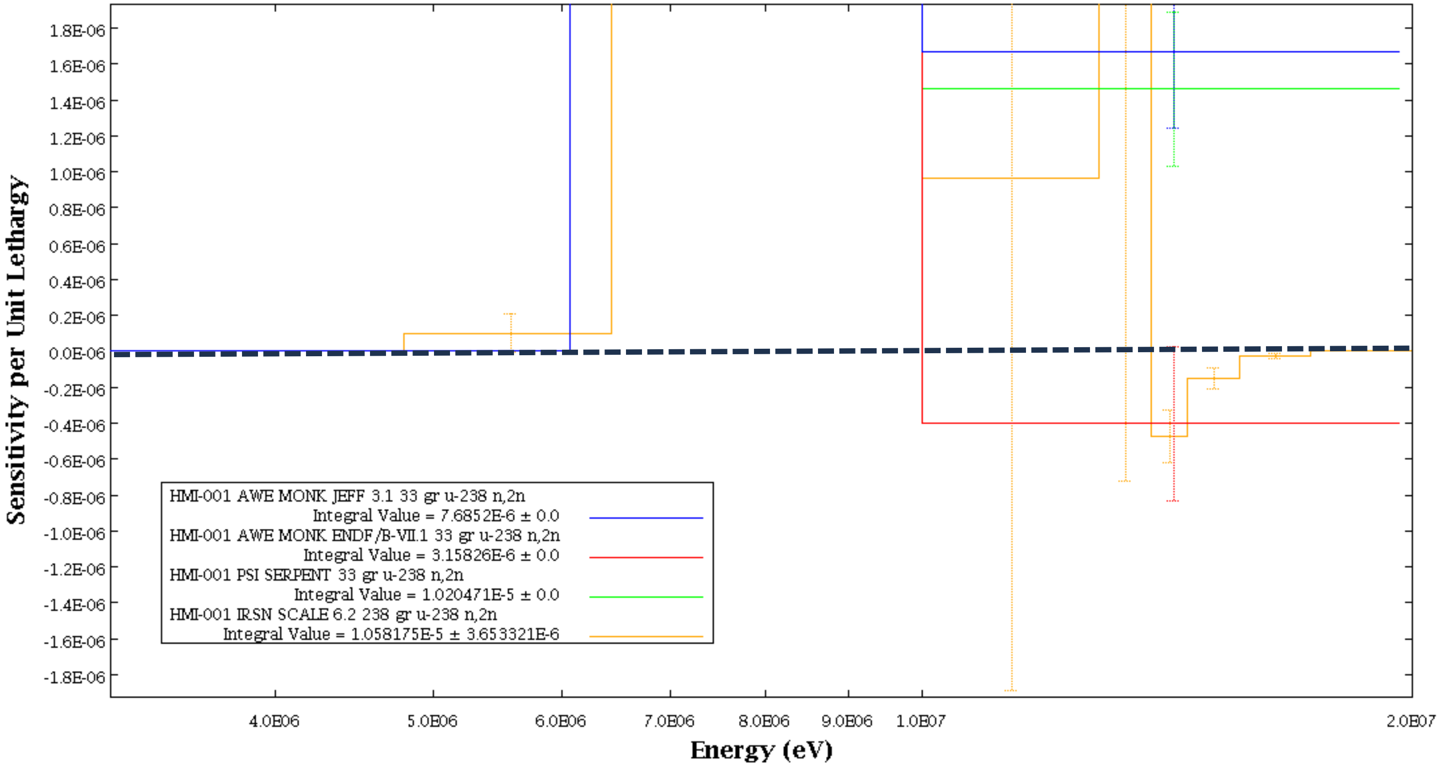
Note It has been proven that the bias of the of the sensitivity sampling estimator equals zero; e.g. asymptotical convergence of statistical integration to mathematical expectation exists. However there is no one theory to prove the rate of convergence - how many particles are needed to converge the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

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



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 6.2ß	U-238	n,2n reaction
		Zero level



Summary and Conclusions

- Selected four 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)

- Good agreement between deterministic and all MC sensitivities is observed for nu-bar, fission, and capture profiles

- MC scattering sensitivities depends on statistical options

- In general, all tested MC methods and codes demonstrate consistency in the results that confirms the methods maturity

Other experimental data: SNEAK 7A β_{eff} uncertainties