On the Use of Sensitivities to Identify Compensating Effects of Nuclear Data in Integral Benchmarks

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Background

The Working Party on Evaluation Cooperation of the OECD set up a subgroup WPEC-SG40 (alias CIELO) to focus on the evaluated nuclear data of the major nuclides in reactor technology, namely ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu. Different research groups in various parts of the world are working on improved evaluated nuclear data and their uncertainties for these nuclides; the ultimate test of improvement is the performance of the data in simulating integral experiments.

The Coordinated Research Project (CRP) was recently completed at the Nuclear Data Section (NDS) of the International Atomic Energy Agency (IAEA) with the objective to investigate the differential and integral experimental data on the prompt fission neutron spectra (PFNS) of actinides. Comprehensive results were submitted for publication in the special issue of the Nuclear Data Sheets Journal. Additionally, in the on-going neutron standard project it is planned to include ^{235}U PFNS induced by thermal neutrons as a reference neutron field. The overall conclusion of the projects is that the average neutron energies of the PFNS need to be reduced. This has severe impact on many criticality benchmarks. Compensating effects must be found based on better physics and supported by experimental evidence from differential data as much as possible.

The primary aim of the present investigation is to search for compensating effects, making use of the sensitivities included in the DICE package that was developed at the NEA Data Bank to support the ICSBEP Handbook of criticality benchmarks.

Sensitivities in the DICE package of ICSBEP

DICE search for the selected nuclide

The first step in the process is to identify benchmarks that are most sensitive to the reactions of the nuclide of interest (i.e. the ^{235}U in the present study) with the help of DICE. The process is as follows:

1. In the “Energy, spectra, sensitivities” select the Energy of average neutron causing fission, “Average fission group energy” and all sensitivities to k_eff.
2. Select the nuclide for which the sensitivities are required (e.g. ^{235}U)

3. Select reactions (e.g.: capture, elastic, fission inelastic; it is probably unnecessary to select nu-bar, since practically all benchmarks are directly sensitive to it. Likewise, it is not necessary to select the total, since all the major partial reactions are included).
4. Sort the selected benchmarks by thermal k_eff sensitivities, then by reaction.
5. Select six (or otherwise) benchmarks most sensitive to thermal capture of U-235; be careful not to double-count benchmarks with multiple entries in the database. Save the selection to an Excell spreadsheet (or otherwise).
6. Similarly, select six (or otherwise) benchmarks most sensitive to thermal scattering cross section; be sure to check the negative as well as positive sensitivities. Add the selection to an Excell spreadsheet (or otherwise).
7. Repeat the procedure for thermal fission cross section.
8. Repeat steps 4 to 7 for epithermal k_eff sensitivities, including the inelastic cross sections.
9. Repeat steps 4 to 7 for fast k_eff sensitivities, including the inelastic cross sections.

The result is a list of benchmarks about 50 to 60 benchmarks that are most sensitive to the major cross sections of ^{235}U. If any changes to the major reaction cross sections are made, the above-defined list of benchmarks should be checked to avoid unphysical changes.

The next step is to find the sensitivities of each of the above benchmarks to other materials. The procedure is very similar to the above, but with important small changes.

DICE search for sensitivities to materials for the selected benchmark

The procedure described below has to be applied for every benchmark identified in the previous section. The procedure is as follows:

1. In the “General Items” select “Identification”. To narrow down the search, define the “Fissile material”, “Physical form” and “Spectrum” appropriate for the selected benchmark. The “Search” button will result in the list of benchmarks.
2. In the “Energy, spectra, sensitivities” group, select “EALF”, “AFGE” and all Keff sensitivities and hit “Apply”.
3. Click on the selected benchmark in the top window to obtain the sensitivities for all the cases belonging to this benchmark.
4. Sort the selection by the “Total Keff sensitivity”.
5. Hide all entries with a total sensitivity less than 0.005 %/% (select the entries, right-click and chose “Hide selected” from the menu).
6. You may need to click on the selected benchmark in the top window and sort the cases in the “Case Identification” column. Select the entries for the chosen case, copy to clipboard and paste into a separate sheet in the Excell file. You may remove entries that are judged unnecessary.

The information collected above has been stored in an Excell spreadsheet. A closer look at the sensitivities reveals that some of the benchmarks are highly sensitive to a broad variety of nuclides, some of which are known to have relatively poor nuclear data. For example, the tungsten data improved significantly in the latest ENDF/B-VII.1 library, but benchmarks containing tungsten are still among the biggest outliers. Similarly, benchmarks containing copper show significant discrepancies in comparison with integral measurements. The complete list of identified benchmarks for the thermal, the epithermal and the fast neutron energy range as it appears in the Excell spreadsheet is shown in the Appendix.

Benchmark Analysis

The benchmarks identified above have been analysed using the MCNP-6.1 Monte Carlo transport code with the following data libraries:

“e71”	Original ENDF/B-VII.1 data library
“u238ib44ur”	^{238}U evaluation for CIELO with IRMM data for the unresolved resonance region.
“o16haleadx”	^{16}O evaluation by G. Hale from Los Alamos National Laboratory.
“u235ib02o4g6a”	^{235}U evaluation “ib02” from the IAEA in the fast energy range and “ornl4” evaluation
“o16u5u8”	Calculation combining evaluations “o16haleadx” for ^{16}O, “u238ib44ur” for ^{238}U and “u235ib02o4cWg6aNu” for ^{235}U; in the later the capture cross section around 25 keV was reduced by 3 % and around 426 keV by 10 %. A decrease is supported by the mass spectrometry measurement by Wallner and was adopted to restore agreement with fast benchmarks. In addition, the nu-bar at thermal energies was decreased by 0.34 % to undo the fix introduced in the ENDF/B-VII.1 library, in order to restore criticality prediction for thermal solution benchmarks.

The adjustments in the “u235ib02o4cWg6aNu” evaluation are not unique, but they perform well compared to ENDF/B-VII.1 data for thermal solution benchmarks as seen from Figure 1.

The situation is less clear for the fast benchmarks. The ZPR-9 series of benchmarks are strongly sensitive to the tungsten data and the Zeus benchmarks are strongly sensitive to copper data, which overshadow the effects of the major nuclides. For this reason a number of fast assembly benchmarks were added to the analysis. The ^{235}U data with a PFNS having a lower average energy tends to decrease reactivity. The reduction of the capture cross section generally restores the agreement with measurements. The majority of benchmarks seem to be predicted at least as well compared to ENDF/B-VII.1 data, as seen from Figure 3.

Benchmarks sensitive to the epithermal data seem to be systematically overpredicted, as shown in Figure 2. This could be an indication that a decrease of the capture cross section of ^{235}U is not justified and alternative compensations need to be introduced.

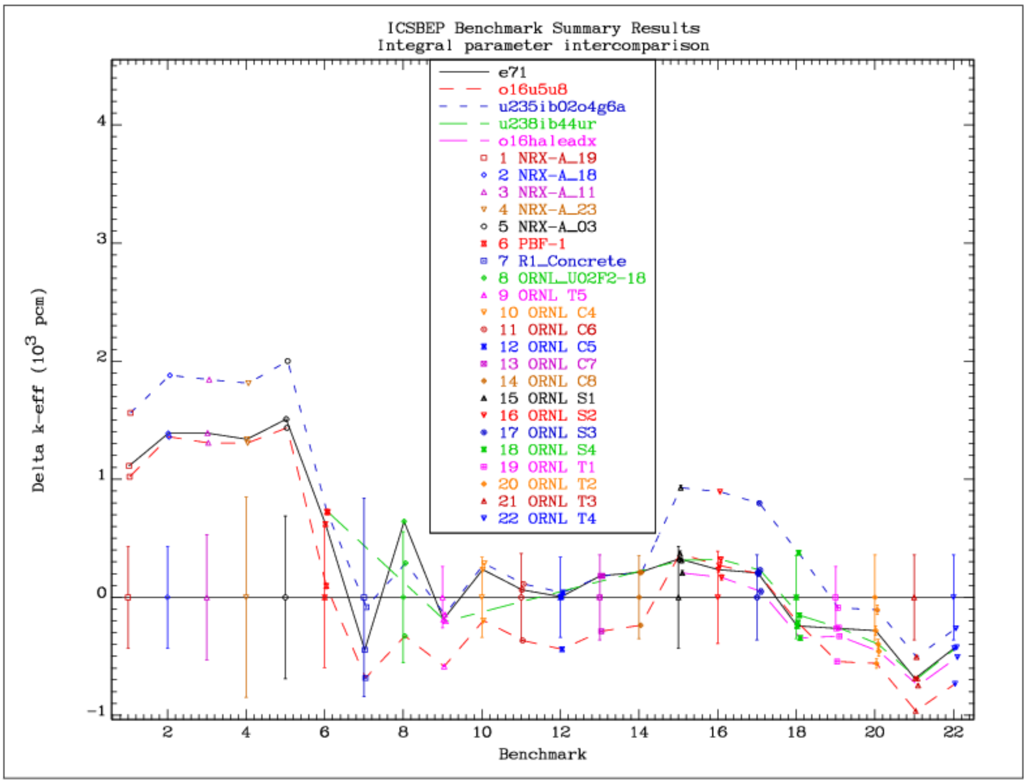

Figure 1: Results for thermal benchmarks.

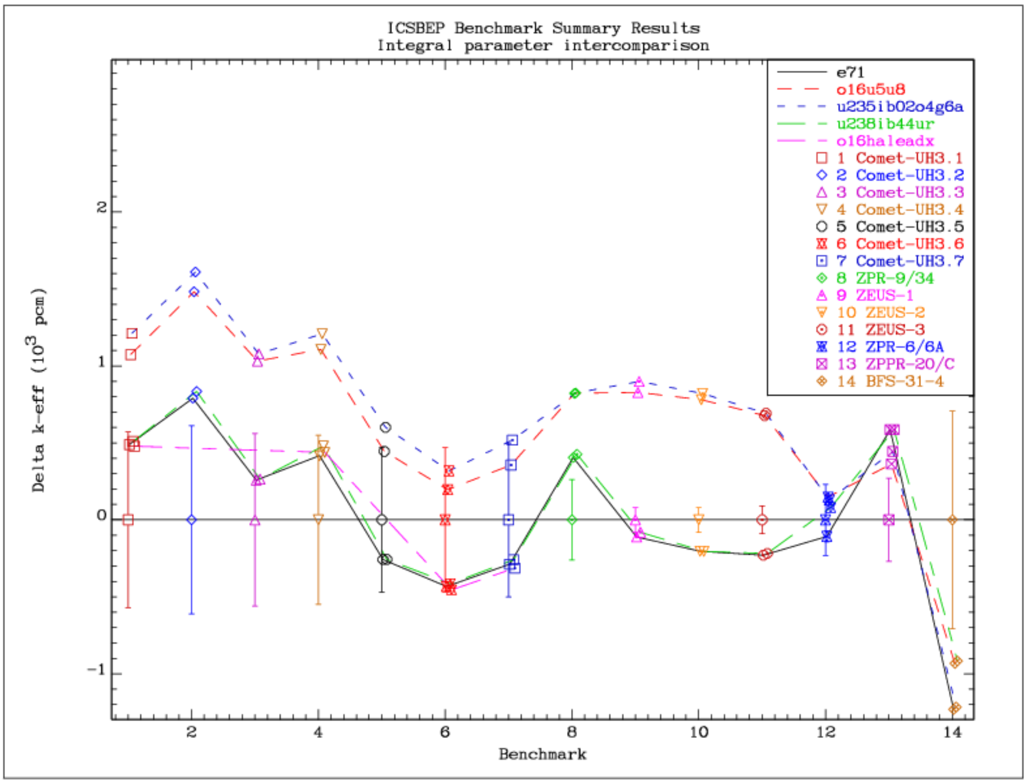

Figure 2: Results for benchmarks sensitive to the epithermal data.

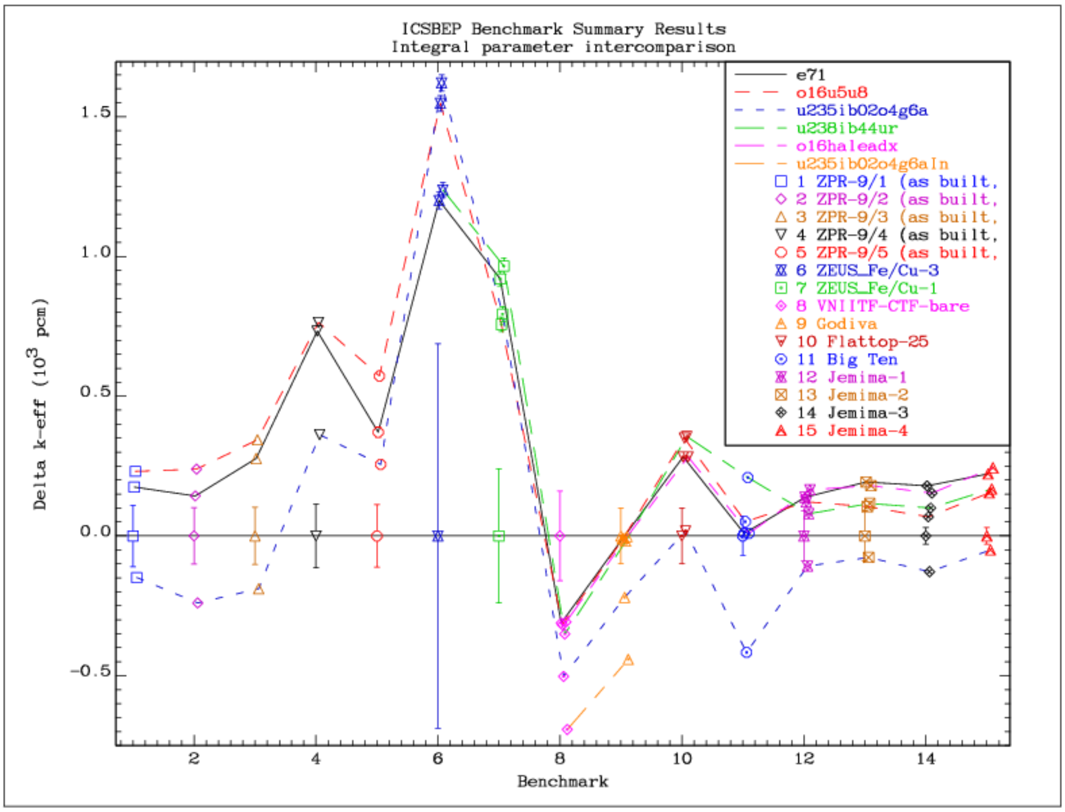

Figure 3: Results for fast benchmarks.

Application of sensitivities in search of improved cross sections

In the WPEC SG-39 the covariance data and the calculated sensitivities were used in a purely mathematical way on a pre-selected set of benchmarks to obtain adjusted multigroup cross sections. The basic principle tested in the present work is to use the sensitivities for orientation as to which reactions might need special attention and then seek a solution constrained by "best" physical models in nuclear model calculations, supported as much as possible by measured differential cross sections.

A convenient example seem to be the bare ^{235}U sphere benchmarks Godiva (HEU-MET-FAST-001) and the Russian equivalent VNIITF-CTF-bare (HEU-MET-FAST-008), the latter being underpredicted in reactivity using ENDF/B-VII.1 data by 312 pcm (*parts per 100 000*) compared to the benchmark value, while the experimental uncertainty is 160 pcm. On the contrary, Godiva is in agreement to within 12 pcm with a statistical uncertainty of 8 pcm, while the experimental uncertainty is 100 pcm.

The ^{235}U cross sections were averaged in the Godiva neutron spectrum from the core centre. The sensitivities from DICE and the averaged cross sections are shown in Table 1. The sensitivities to the capture and fission cross sections of ^{235}U are practically the same; therefore they cannot be used to introduce differential changes in reactivity to the two benchmarks. The sensitivities to the fission cross sections of ^{238}U differ, but this cross section is a standard and there is little flexibility to adjust it. The remaining sensitivities are for the elastic and the inelastic cross sections. The sensitivity to the inelastic cross section of ^{238}U is an order of magnitude smaller than that of ^{235}U, hence it is sensible to perturb the cross sections of this isotope. Arbitrarily, the inelastic continuum cross section of ^{235}U is reduced by 10 %, giving an overall decrease of the inelastic cross section of about 9 %. To compensate this decrease, the elastic cross section is increased by about 3 % to keep the total cross section unchanged. Based on the sensitivities, the expected changes in reactivities for the two benchmarks are shown in the last two columns in Table 1. The expected net decrease in reactivity is bigger for the Russian VNIITF-CTF benchmark by 73 pcm, which should bring the two benchmarks closer together (although another compensating effect is then needed to uniformly increase the reactivity). The cross section changes were introduced into a test ENDF file and the MCNP calculations were repeated. The observed changes in reactivities were much smaller and the difference in reactivity changes for the two benchmarks were only 32 pcm, which is by far insufficient to align the predicted reactivities.

Table 1: Estimates of changes in k-eff due to relative changes in cross sections (green fields)

Isotope	Reaction	Godiva k_eff %/%	Russian k_eff %/%	x.s. [mbarns]	Δ x.s. [mbarns]	Δ x.s. [%]	Godiva Δ keff [pcm]	Russian Δ keff [pcm]
U235	capture	-.03973	-.04003	0.6869	0.0000	0.0%	0	0
U238	elastic	0.00744	0.01168	29.5400	0.0000	0.0%	0	0
U235	elastic	0.10175	0.0957	26.5380	0.8043	3.0%	308	290
U234	fission	0.00576	0.00642					
U238	fission	0.00637	0.01116	0.9894	0.0000	0.0%	0	0
U235	fission	0.64438	0.64578	6.2572	0.0000	0.0%	0	0
U238	inelastic	0.00521	0.00908	11.3180	0.0000	0.0%	0	0
U235	inelastic	0.08545	0.07632	8.0430	-0.8043	-10.0%	-855	-763
						Expected	-546	-473
						Observed	-222	-190

Conclusions

A scheme is proposed based on sensitivities retrieved with the DICE package for the ICSBEP benchmarks to search of compensating effects in reactivity prediction in criticality benchmarks. To test the scheme the adjustment of ^{235}U scattering cross sections was attempted to align the predicted reactivities for two bare critical assemblies of highly-enriched uranium, namely the GODIVA (HEU-MET-FAST-001) and the Russian VNIITF-CTF (HEU-MET-FAST-0008) benchmarks from the ICSBEP compilation. The following conclusions can be drawn:

- Strong non-linearities appear in the sensitivity coefficients, particularly when scattering data are in question.
- The predicted criticalities of bare highly-enriched uranium spheres Godiva and VNIITF-CTF cannot be aligned by changing the cross section data, judging by the sensitivity coefficients. It appears that a bias is introduced in at least one of the benchmarks in the modelling of the experiment.
- Nevertheless, the scheme is useful for identifying possible interferences from other constituents in the assembly. The scheme does not provide the solution, but points in the direction in which to search for compensating effects that would eventually lead to better evaluated nuclear data sets.

Appendix

Thermal benchmarks

HEU-COMP-THERM-002-019		0.0777	0.162	U235	capture	-0.11878	-0.02287	-0.00039	-0.14204
HEU-COMP-THERM-002-018		0.12	0.26	U235	capture	-0.11838	-0.03865	-0.00062	-0.15764
HEU-COMP-THERM-002-011		0.108	0.232	U235	capture	-0.11825	-0.03199	-0.00055	-0.15079
HEU-COMP-THERM-002-023		0.0818	0.174	U235	capture	-0.11815	-0.02605	-0.00041	-0.14461
HEU-COMP-THERM-002-003		0.085	0.176	U235	capture	-0.11798	-0.02375	-0.00043	-0.14216
HEU-MET-THERM-011-042	27 B	0.0888	0.195	U235	capture	-0.11756	-0.02288	-0.00048	-0.14092
IEU-COMP-THERM-009-001				U235	elastic	-0.00211	0.00265	0.00581	0.00636
HEU-COMP-THERM-009-005		8.62	11	U235	elastic	-0.00154	0.00082	0.00311	0.00238
HEU-COMP-MIXED-003-006		15.5	18.5	U235	elastic	-0.00144	0.00136	0.00334	0.00326
HEU-SOL-THERM-026-001	1a			U235	elastic	-0.00142	0.00135	-0.00095	-0.00102
HEU-SOL-THERM-048-018	22	0.655	1.03	U235	elastic	-0.00138	0.00244	0.00017	0.00123
HEU-COMP-MIXED-004-004		12.8	15.7	U235	elastic	-0.00138	0.00252	0.00407	0.00521
HEU-COMP-THERM-016-004				U235	elastic	0.00150	0.00035	0.00105	0.0029
HEU-SOL-THERM-032-001		0.0313	0.0374	U235	fission	0.55011	0.00924	0.00076	0.5601
HEU-SOL-THERM-042-004	15	0.0312	0.037	U235	fission	0.55799	0.00916	0.00074	0.56789
HEU-SOL-THERM-042-006	21	0.0311	0.0368	U235	fission	0.56257	0.00912	0.00073	0.57241
HEU-SOL-THERM-042-005	16	0.031	0.0367	U235	fission	0.56456	0.00905	0.00072	0.57433
HEU-SOL-THERM-042-007	22	0.031	0.0366	U235	fission	0.56662	0.00902	0.00071	0.57636
HEU-SOL-THERM-042-008	23	0.0309	0.0364	U235	fission	0.56923	0.00895	0.00071	0.57889
HEU-SOL-THERM-009-001	ORNL_S1								
HEU-SOL-THERM-009-002	ORNL_S2								
HEU-SOL-THERM-009-003	ORNL_S3								
HEU-SOL-THERM-009-004	ORNL_S4								
HEU-SOL-THERM-013-001	ORNL_T1								
HEU-SOL-THERM-013-002	ORNL_T2								
HEU-SOL-THERM-013-003	ORNL_T3								
HEU-SOL-THERM-013-004	ORNL_T4								

Epithermal benchmarks

HEU-COMP-INTER-003-003		2460	4100	U235	capture	-0.00669	-0.16895	-0.01326	-0.1889
HEU-MET-INTER-006-001	Configuration 1	4440	3960	U235	capture	-0.00167	-0.1689	-0.01426	-0.18483
HEU-COMP-INTER-003-002		2450	4070	U235	capture	-0.00665	-0.16756	-0.01327	-0.18748
HEU-COMP-INTER-003-005		3240	3300	U235	capture	-0.00619	-0.16652	-0.01402	-0.18673
HEU-COMP-INTER-003-004		3080	4980	U235	capture	-0.00613	-0.16437	-0.01396	-0.18446
HEU-COMP-INTER-004-001		132	138	U235	capture	-0.00246	-0.1601	-0.00308	-0.16564
HEU-MET-FAST-058-002		220000	209000	U235	elastic	-0.00003	-0.00865	0.03531	0.02663
HEU-MET-FAST-058-001		34800	34800	U235	elastic	-0.00009	-0.00862	0.02245	0.01374
HEU-MET-FAST-041-002		149000	117000	U235	elastic	-0.00003	-0.00848	0.0301	0.02159
HEU-MET-FAST-066-001		226000	190000	U235	elastic	-0.00003	-0.00604	0.03026	0.02419
HEU-MET-FAST-076-012	Exp No 17	7280	6670	U235	elastic	-0.00017	-0.00583	0.01681	0.01081
HEU-MET-FAST-076-018	Exp No 23	6290	5810	U235	elastic	-0.00016	-0.00555	0.01805	0.01234
HEU-MET-FAST-007-028		275000	233000	U235	elastic	0	0.02272	0.05842	0.08114
HEU-MET-FAST-007-008		204000	165000	U235	elastic	0	0.0229	0.05869	0.08159
HEU-MET-FAST-007-007		196000	157000	U235	elastic	0	0.02305	0.05606	0.07911
HEU-MET-FAST-007-009		179000	142000	U235	elastic	0	0.02327	0.05822	0.0815
HEU-MET-FAST-007-029		161000	126000	U235	elastic	0	0.02339	0.05397	0.07736
HEU-MET-FAST-007-010		27300	22000	U235	elastic	0.00002	0.02377	0.04263	0.06642
HEU-MET-INTER-001-001	ZPR-9/34	29400	26100	U235	fission	-0.00006	0.27412	0.28318	0.55724
IEU-MET-INTER-001-003	6A-S	14300	12000	U235	fission	0.00342	0.27932	0.16558	0.44831
HEU-MET-INTER-006-002	Configuration 2	9450	8300	U235	fission	0.00047	0.28616	0.18439	0.47102
HEU-MET-INTER-006-001	Configuration 1	4440	3960	U235	fission	0.00196	0.29657	0.15982	0.45836
IEU-COMP-INTER-005-001	ZPR-6/6A	81600	68000	U235	fission	0	0.31112	0.22565	0.53676
HEU-COMP-INTER-004-001		132	138	U235	fission	0.02615	0.59065	0.03544	0.65224
HEU-MET-FAST-075-001	ZPPR-20/C	226000	198000	U235	inelastic	0	0.00042	0.03602	0.03646
HEU-MET-FAST-007-032		773000	762000	U235	inelastic	0	0.00045	0.07077	0.07122
HEU-MET-FAST-007-034		642000	627000	U235	inelastic	0	0.00045	0.06538	0.06584
IEU-MET-FAST-015-001	ZPR-3/6F	537000	519000	U235	inelastic	0	0.00048	0.00682	0.00729
MIX-MISC-FAST-001-009	BFS-31-4	175000	146000	U235	inelastic	0	0.00065	-0.00662	-0.00597

Fast benchmarks

HEU-MET-FAST-060-001	ZPR-9/4	223000	217000	U235	capture	0	-0.03685	-0.04512	-0.08197
HEU-MET-FAST-067-002	ZPR-9/6	209000	201000	U235	capture	0	-0.03939	-0.045	-0.08438
HEU-MET-FAST-073-001		421000	400000	U235	capture	0	-0.02423	-0.04457	-0.06881
HEU-MET-FAST-072-002	Zeus-2/Fe	236000	215000	U235	capture	0	-0.04172	-0.04455	-0.08626
HEU-MET-FAST-072-001	Zeus-1/Fe	235000	213000	U235	capture	0	-0.04209	-0.0444	-0.08648
HEU-MET-FAST-005-001		640000	626000	U235	capture	0	-0.01244	-0.04211	-0.05456
HEU-MET-FAST-015-001		894000	878000	U235	elastic	0	0.00748	0.08709	0.09457
HEU-MET-FAST-051-014		884000	869000	U235	elastic	0	0.00766	0.08764	0.09531
HEU-MET-FAST-008-001	Russian Godiva	870000	855000	U235	elastic	0	0.00753	0.08817	0.0957
HEU-MET-FAST-065-001		893000	877000	U235	elastic	0	0.00775	0.08994	0.09769
HEU-MET-FAST-001-001	Godiva	881000	866000	U235	elastic	0	0.00877	0.09299	0.10175
HEU-MET-FAST-018-001		868000	853000	U235	elastic	0	0.00835	0.10035	0.1087
HEU-MET-FAST-079-001		884000	869000	U235	fission	0	0.02492	0.6262	0.65112
HEU-MET-FAST-079-002		879000	864000	U235	fission	0	0.0255	0.62717	0.65267
HEU-MET-FAST-043-001		886000	870000	U235	fission	0	0.02577	0.628	0.65377
HEU-MET-FAST-051-014		884000	869000	U235	fission	0	0.02623	0.62809	0.65432
HEU-MET-FAST-015-001		894000	878000	U235	fission	0	0.02589	0.62938	0.65527
HEU-MET-FAST-065-001		893000	877000	U235	fission	0	0.02574	0.62941	0.65515
HEU-MET-FAST-044-001		885000	870000	U235	inelastic	0	0.00015	0.07742	0.07757
HEU-MET-FAST-015-001		894000	878000	U235	inelastic	0	0.00027	0.07781	0.07808
HEU-MET-FAST-065-001		893000	877000	U235	inelastic	0	0.00026	0.07979	0.08005
HEU-MET-FAST-001-001	Godiva	881000	866000	U235	inelastic	0	0.00027	0.08517	0.08545
HEU-MET-FAST-018-001		868000	853000	U235	inelastic	0	0.00028	0.0863	0.08659
HEU-MET-FAST-051-005		894000	878000	U235	inelastic	0	0.00023	0.0974	0.09762
HEU-MET-FAST-028-001	Flattop-25								
IEU-MET-FAST-001-007	Big_Ten								
IEU-MET-FAST-001-001	Jemima-1								
IEU-MET-FAST-001-002	Jemima-2								
IEU-MET-FAST-001-003	Jemima-3								
IEU-MET-FAST-001-004	Jemima-4								
MIX-MET-INTER-004-001	ZPR-3/53								