Combined evaluation of prompt fission neutron spectra for $^{235}U(n_{th},f)$, $^{239}Pu(n_{th},f)$, $^{233}U(n_{th},f)$ and $^{252}Cf(sf)$

V.G. Pronyaev
pronyaev@ippe.ru

Institute of Physics and Power Engineering
249033 Obninsk, Russia

GMA approach to the evaluation of the standards

- GMA: generalized least-squares fit of experimental data
- Developed by Wolfgang Poenitz for standard neutron reaction cross sections evaluation
- Non-model fit: no physical or mathematical model used in the fit
- Parameters of the fit are cross sections in the energy nodes (or groups) and normalization constants

GMA approach to the evaluation of the standards

- Type of data used in the fit: absolute cross sections, cross section shapes, ratios of absolute cross sections, shapes of the ratios of absolute cross sections, cross section combinations, constraints
- Reactions included in the fit: standard reactions (^{6}Li(n,t), ^{10}B(n,α_0), ^{10}B(n,α_1), ^{197}Au(n,γ), ^{235}U(n,f), ^{238}U(n,f)) and other reactions (^{6}Li(n,n), ^{6}Li(n,tot), ^{10}B(n,n), ^{10}B(n,tot), ^{238}U(n,γ), ^{239}Pu(n,f)) which can reduce the uncertainty of the standards evaluation

GMA approach to the evaluation of the standards

- GMA approach is based on adjustment of a prior vector of evaluated data: iteration procedure is needed
- Chiba-Smith technical fix of Peelle's Pertinent Puzzle, where absolute uncertainties of experimental data are obtained from their relative uncertainties and “true” value, requires the iteration procedure
- 2 – 3 iterations are enough for convergence when experimental data are consistent

GMA approach to the evaluation of the standards

- Covariance matrix of uncertainties of evaluated data is calculated with the use of different components of the uncertainties: LERC – large energy range correlation; MERC – medium energy range correlation and SERC – short energy range correlation components
- Correlations between different components of uncertainties of different data sets can be introduced and accounted
- Max length of the vector of evaluated data is 1200 and max dimension of covariance matrix is 1200×1200

GMA approach to prompt fission neutron spectra evaluation

- GMA approach can be used for evaluation of prompt fission neutron spectra (PFNS) for $^{235}U(n_{th},f)$ – reference spectra
- Data on $^{235}U(n_{th},f)$, $^{239}Pu(n_{th},f)$, $^{233}U(n_{th},f)$ and $^{252}Cf(sf)$ can be used in the combined fit because they are coupled by the ratio measurements and $^{239}Pu(n_{th},f)$, $^{233}U(n_{th},f)$ data can improve our knowledge of $^{235}U(n_{th},f)$ PFNS
- $^{239}Pu(n_{th},f)$, $^{233}U(n_{th},f)$ PFNS are important for reactor applications

GMA approach to prompt fission neutron spectra evaluation

- Data used in the fit: absolute spectra normalized at 1 prompt fission neutron, absolute ratio of such spectra, shape of spectra and ratio of the shape of the spectra
- To convert spectra normalized at prompt fission neutron yield to normalized at 1 neutron, the following values of prompt fission neutron yields were used: 3.7606 for ^{252}Cf(sf), 2.4196 for ^{235}U(n_{th},f), 2.8772 for ^{239}Pu(n_{th},f) and 2.4894 for ^{233}U(n_{th},f)

GMA approach to prompt fission neutron spectra evaluation

- To remove strong energy dependence of the spectra, the spectra used in the fit were divided at the Maxwellian spectrum with kT=1.32 MeV
- Mannhart's non-model point-wise evaluation (1987) of $^{252}Cf(sf)$ PFNS can be used in the combined fit as pseudo-experimental data set. No new data are available for energy range of fission neutron in the evaluation (0.01 – 13.05 MeV, about 99.85% of all integral of the spectra). The same energy nodes as for $^{252}Cf(sf)$ were used for all data

GMA evaluation of prompt fission neutron spectra evaluation

- Experimental data used in the fit include the results of measurements done by several groups. Most detailed data are obtained at NIIAR by Starostov, Nefedov and Bojko. Their primarily measured measured data were analized and selected for the evaluation
- Two new experimental data sets for $^{235}U(n_{th},f)$ PFNS were included in the evaluation prior to their publication: data by F.-J. Hambsch et al. given as absolute spectra, and data by A. Vorobyev et al. obtained as absolute ratio to $^{252}Cf(sf)$

Experimental data for evaluation

- Experimental data used in the fit include the results of measurements done by several groups. Most detailed data are obtained at NIIAR by Starostov, Nefedov and Bojko. Their primarily measured data were analysed and selected for the evaluation
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Results of evaluation

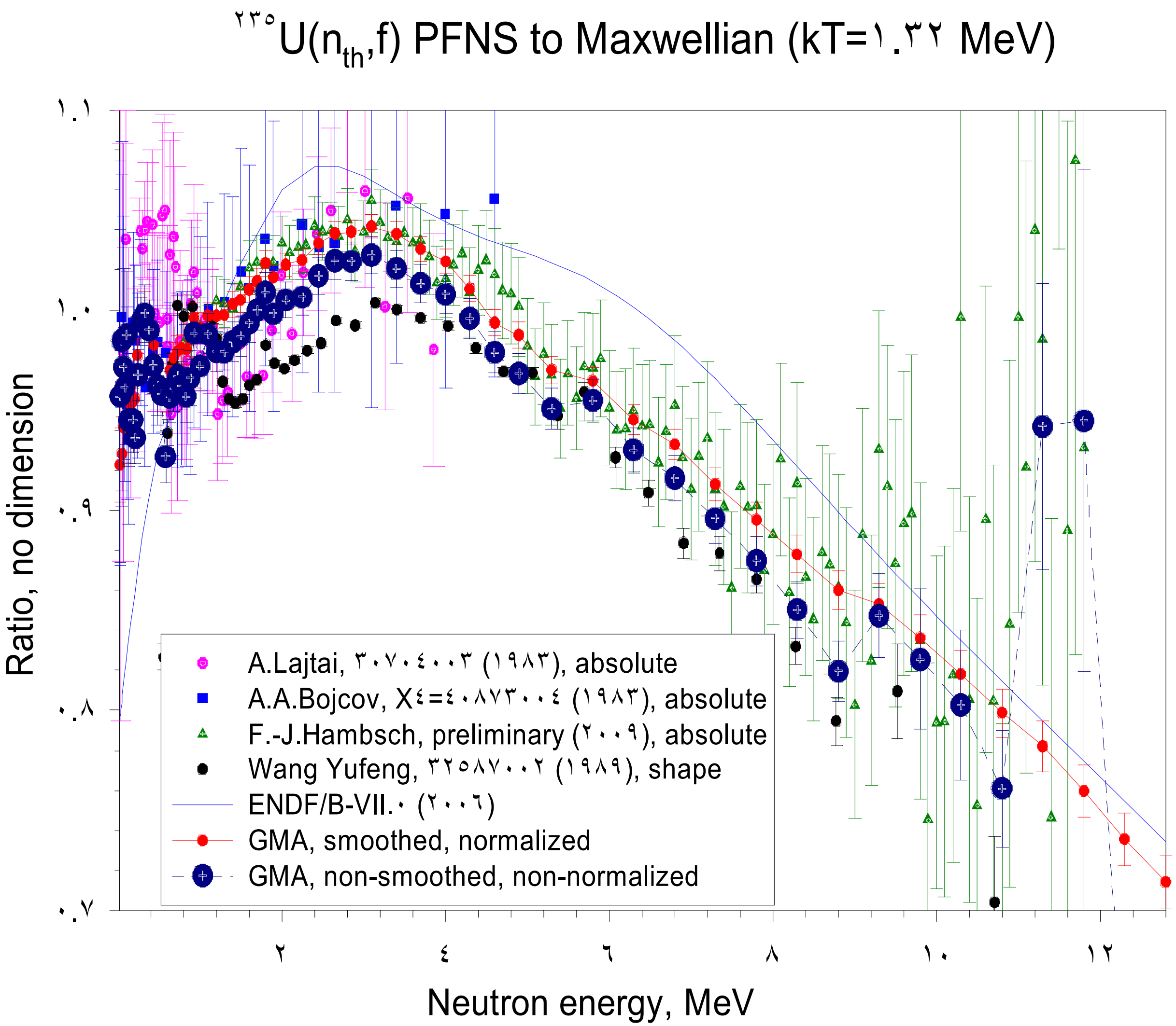
- Two different evaluations were obtained: a) result of non-smoothed and non-normalized evaluation which can be used further for least squares model fit with the adjustment of the model parameters

  b) result of smoothed and normalized evaluation which can be used further for adjustment of the model parameters without model least-squares fit.

Results of evaluation

- The smoothing was done using in the combined fit the results of model calculations close to the evaluated data (but not the model fit) and introduced as shape data with specific covariance matrix having strong correlations only between neighbouring points
- Such smoothing allows remove strong jumps in the shape of the spectra but it does not influence at the general energy behaviour
- Without the smoothing with a narrow error band, the normalization of the data is difficult to implement
- Detailed discussion of influence of such smoothing will be given later

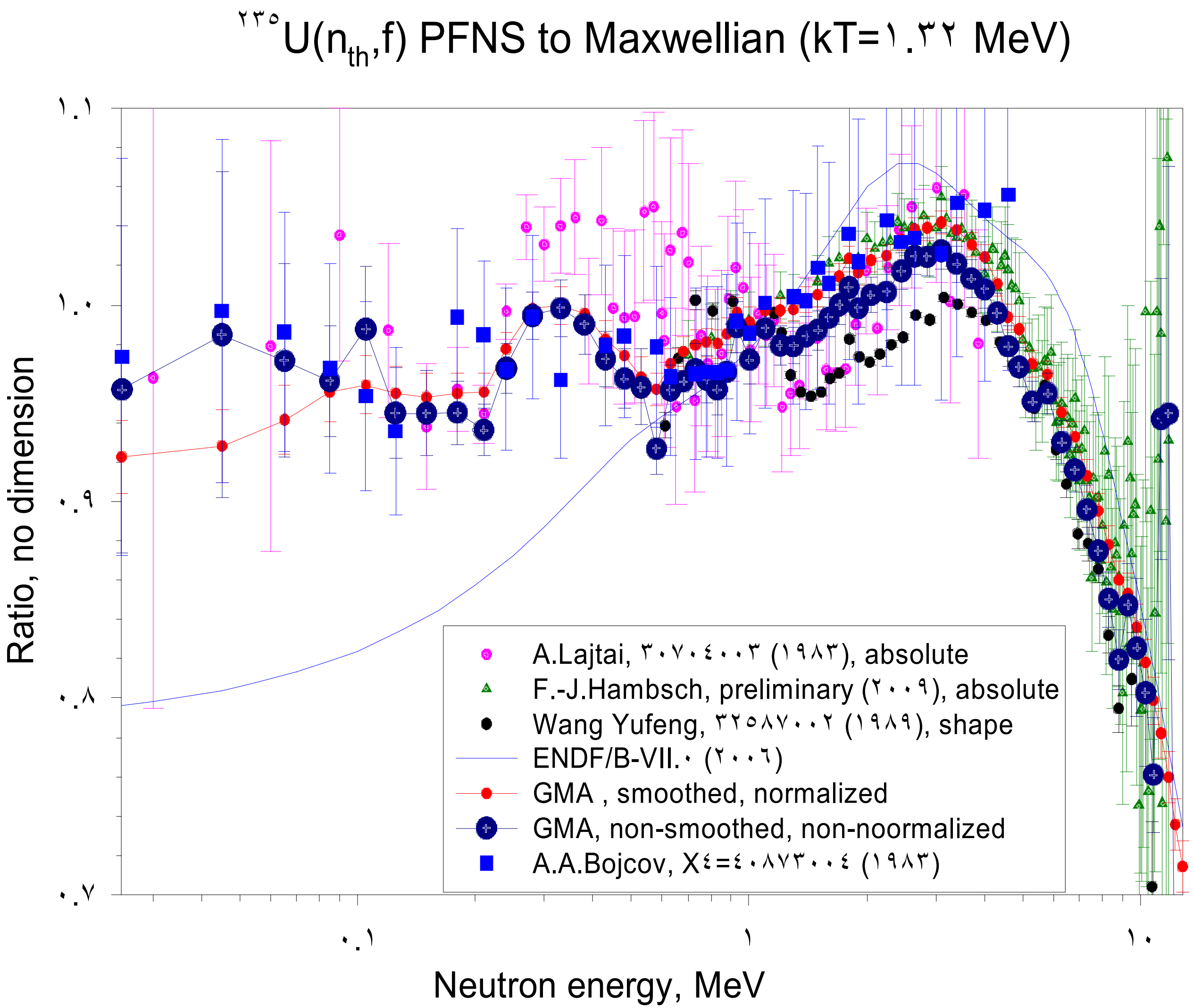
Results of the evaluation: $^{235}U(n_{th},f)$



Linear scale on neutron energy

- 3 absolute and 1 shape (with free normalization) data sets
- Integral under non-normalized spectrum is about 1.5% below integral under smoothed and normalized spectrum
- Model (Madland-Nix) calculated spectrum (ENDF/B-VII.0) is rather different for neutrons below 1 MeV

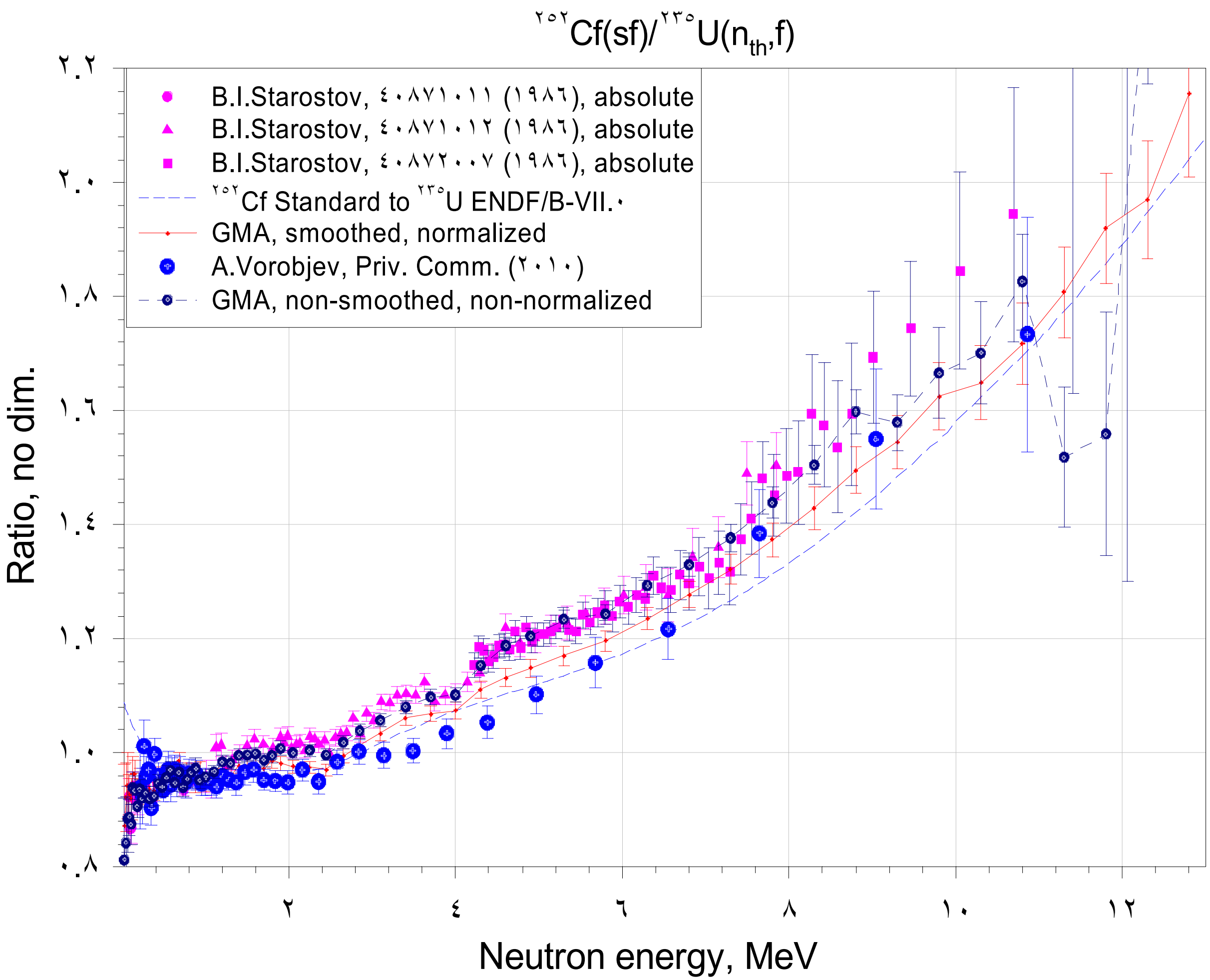
Results of the evaluation: $^{235}U(n_{th},f)$



Logarithmic scale on neutron energy

- Lajtai measurements were done with $^{6}Li(n,t)$ neutron detector (standard) which has broad resonance at 0.235 MeV. Structures observed in Lajtai (and evaluated) data near 0.3 MeV may appear if standard was not reduced to the experimental resolution

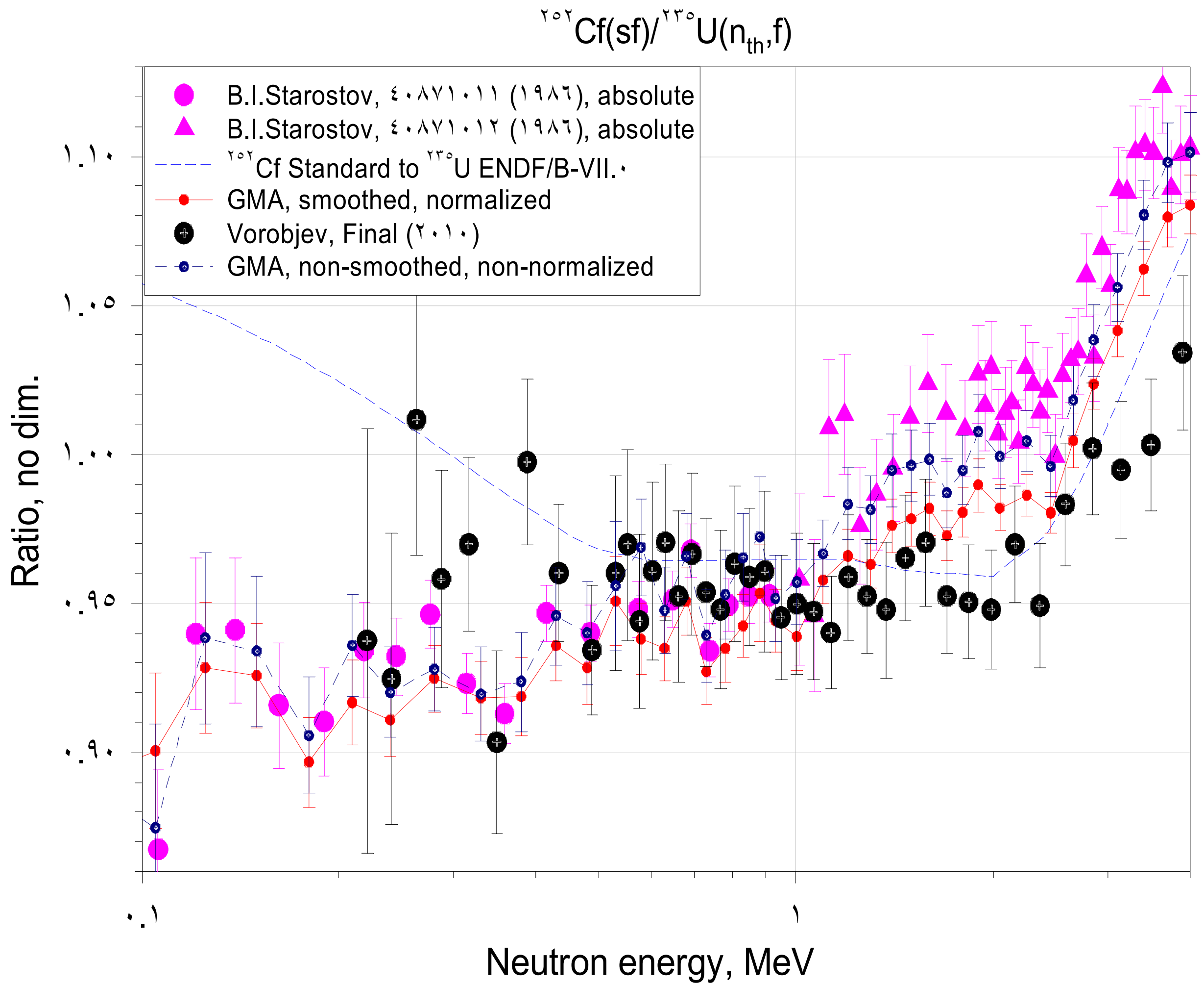
Results of the evaluation: $^{235}U(n_{th},f)$



Linear scale on neutron energy

- Data by Vorobyev have been added to the fit as absolute ratios after obtaining few versions of the evaluation
- At the first stage of evaluation, it was observed that the normalization of 2 data sets of ratios by Starostov for En > 1 MeV (X4=40871012 and X4=40872007) may be overestimated at 5 – 6%
- These data were renormalized and evaluation was done
- But because there were no direct experimental indications at this overestimation the data were used as are given by the authors

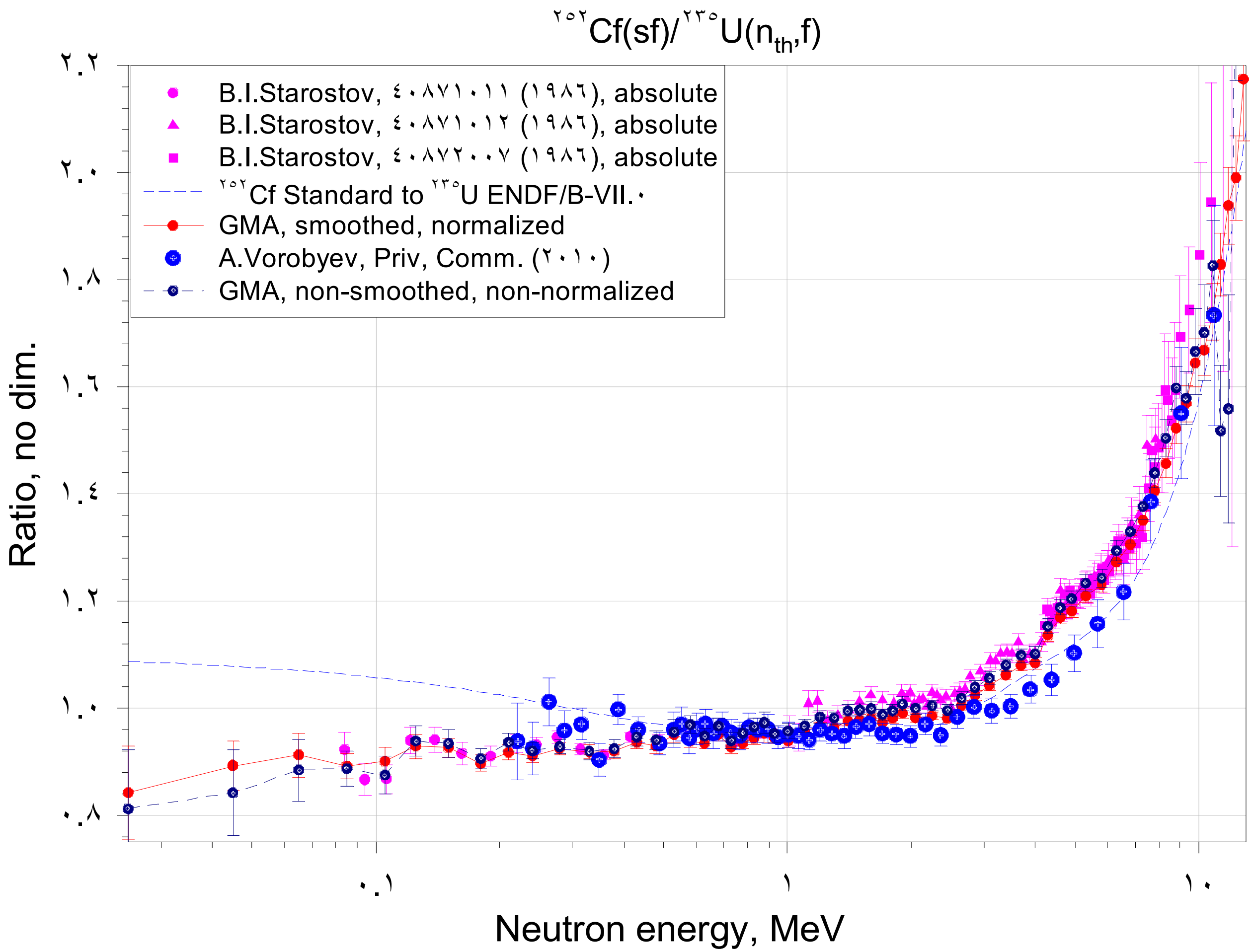
Results of the evaluation: $^{235}U(n_{th},f)$



Logarithmic scale on neutron energy

- Data by Vorobyev show that if Starostov's data for low energy (X4= 40871011) are consistent data for higher energy (X4= 40871012) are really above the results of last measurements
- Probably the best approach will be the use of Starostov's data (X4= 40871012 and X4=40872007) as shape type of data (data with free normalization)

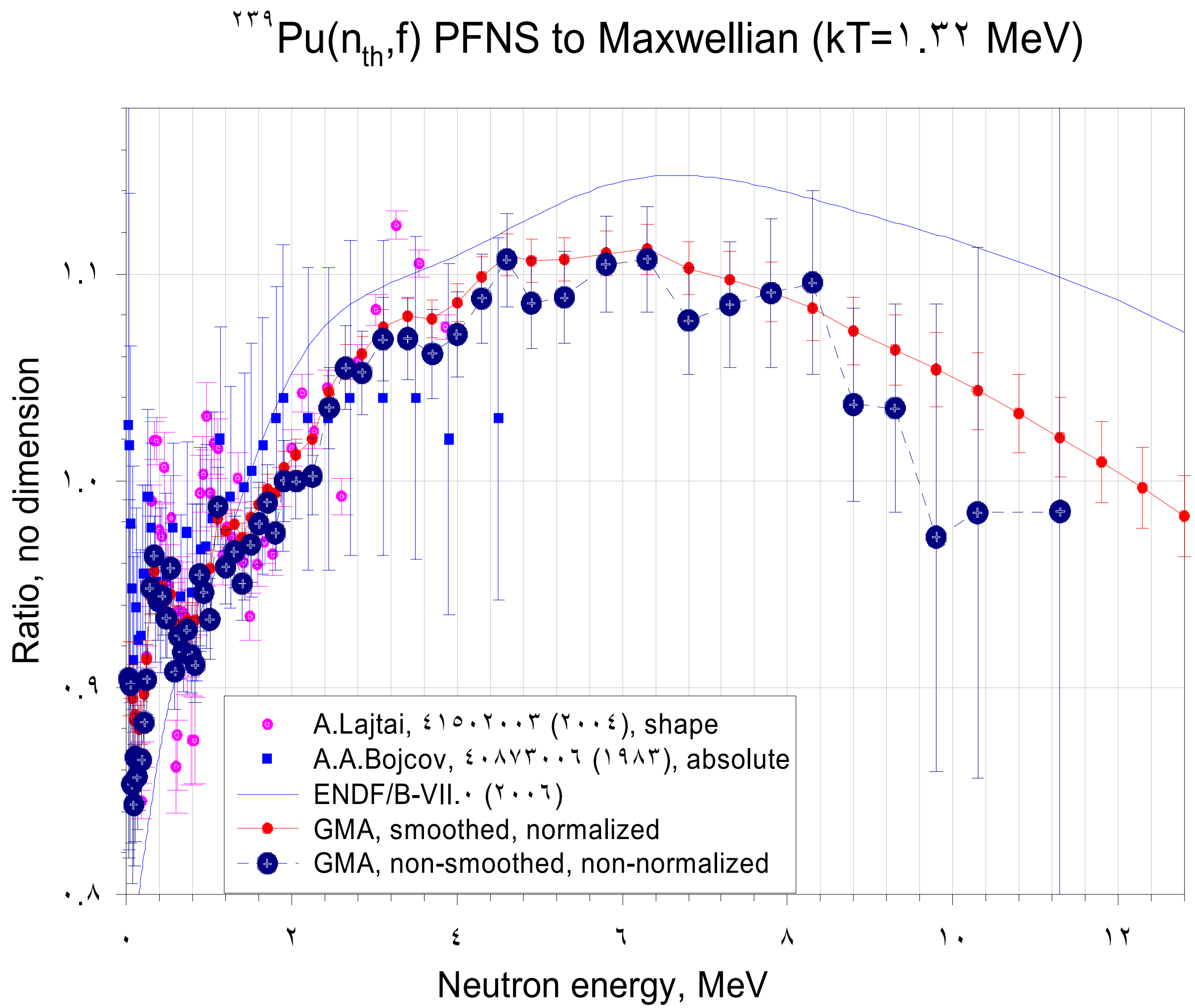
Results of the evaluation: $^{235}U(n_{th},f)$



- Data by Starostov (X4=40871012 and X4=40872007) can be included in the fit as shape type of data because the problem with their normalization

Logarithmic scale on neutron energy

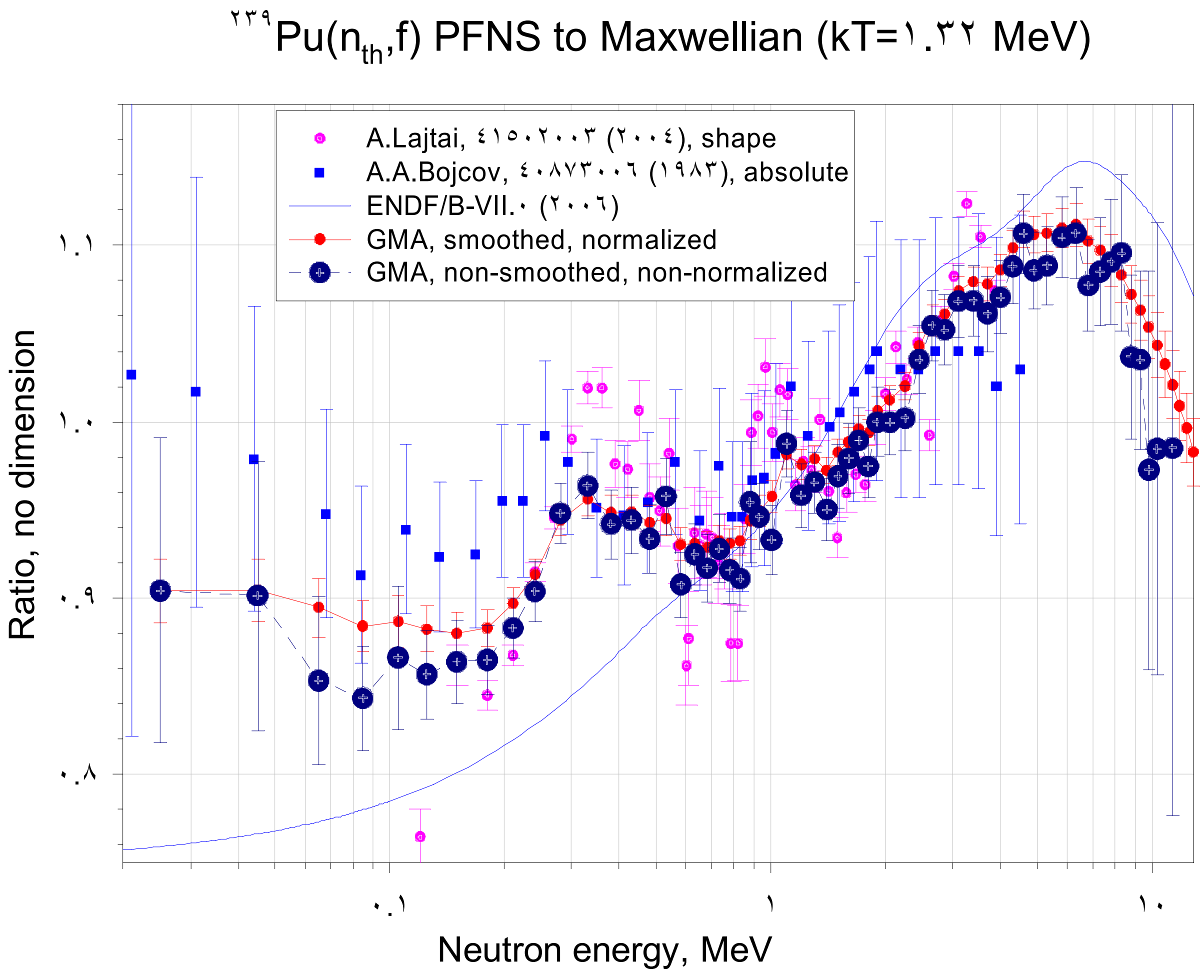
Results of the evaluation: $^{239}Pu(n_{th},f)$



Linear scale on neutron energy

- There is no absolute or or shape spectrum measurements for neutron energy above 4.5 MeV
- There is difference between ENDF/B-VII.0 and present evaluation in high energy region of spectrum

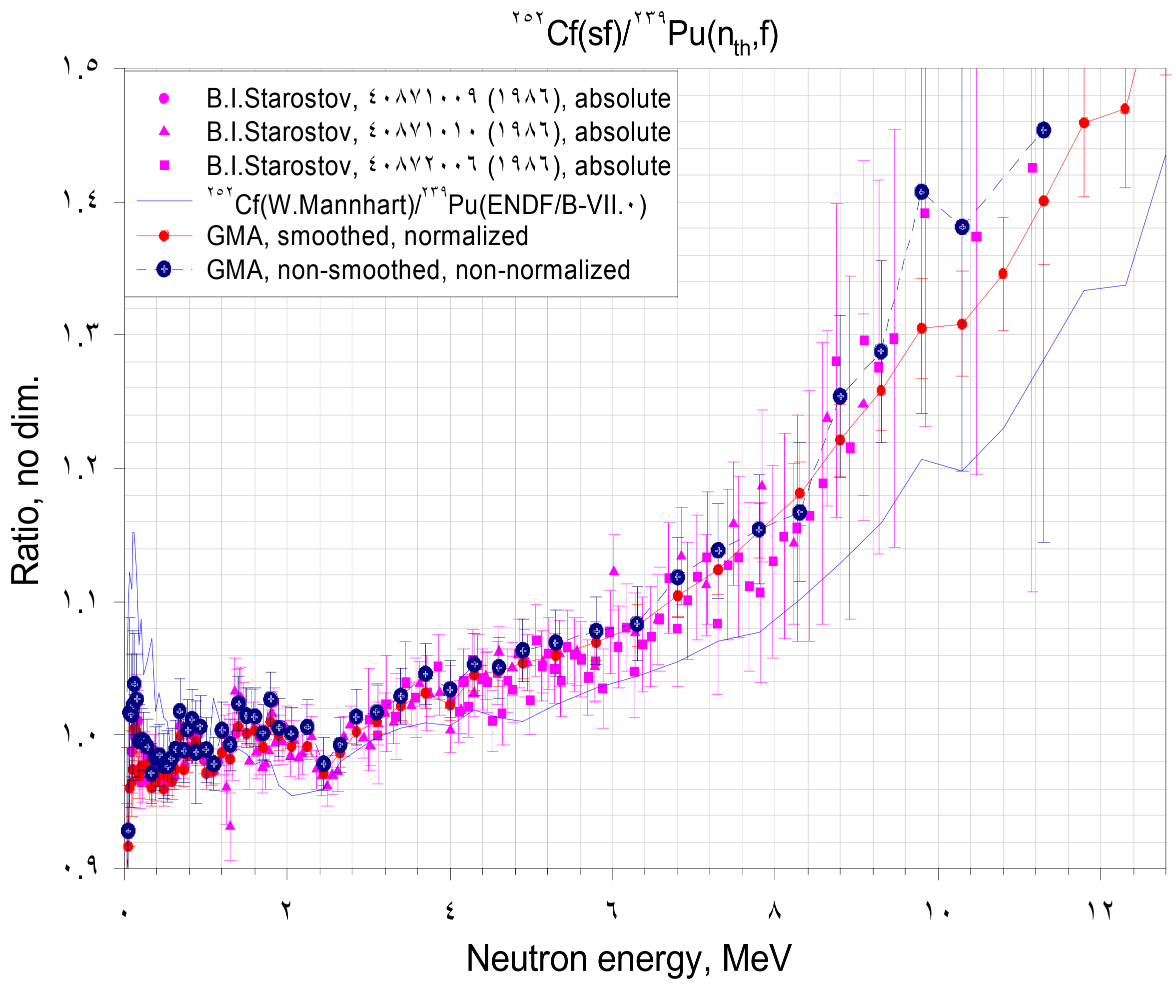
Results of the evaluation: $^{239}Pu(n_{th},f)$



Logarithm scale on neutron energy

- The same type of structure is observed in hundreds keV region as for $^{235}U(n_{th},f)$
- Mean energy of the evaluated spectrum is low comparing with the ENDF/B-VII.0 evaluation

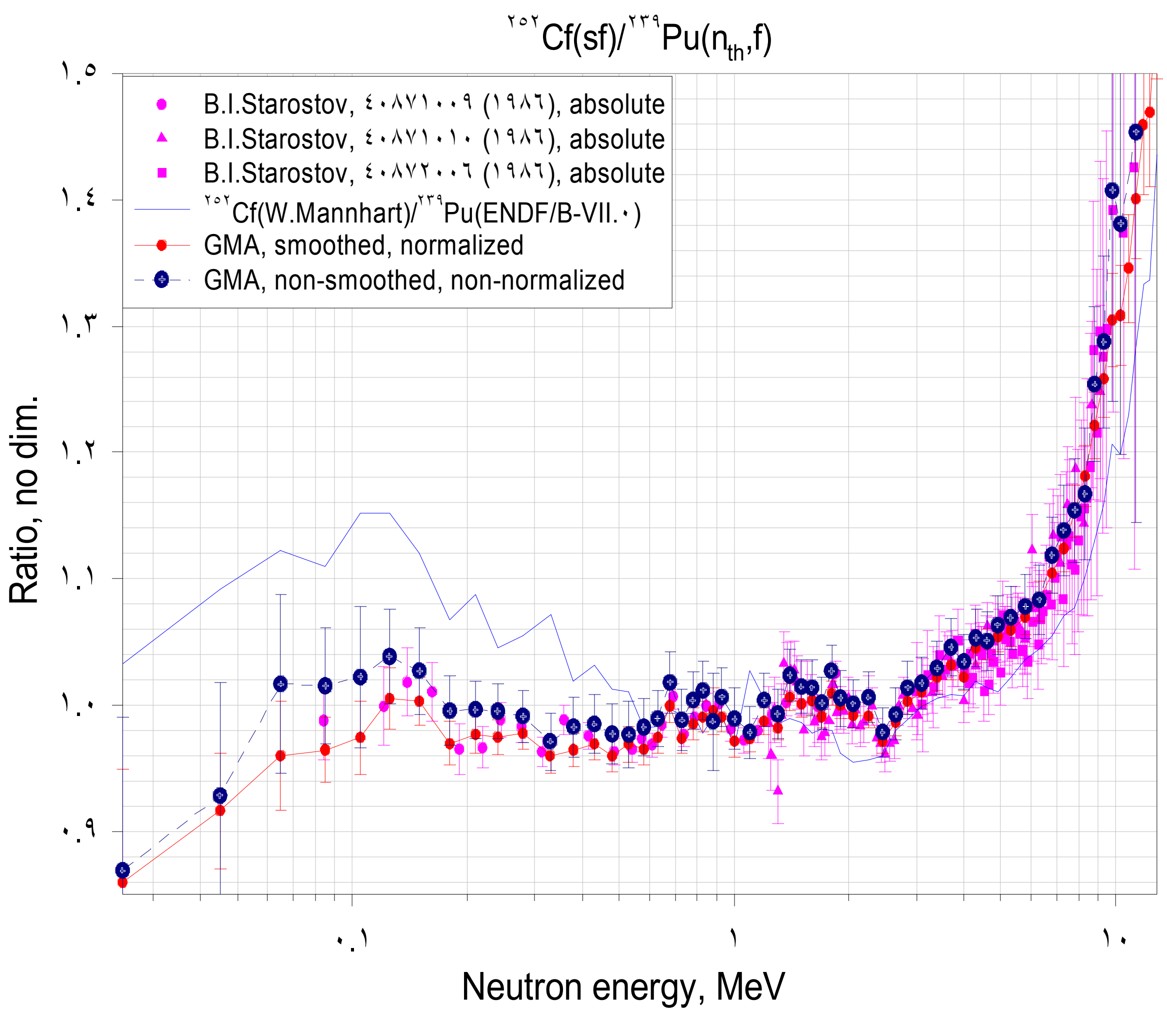
Results of the evaluation: $^{239}Pu(n_{th},f)$



Linear scale on neutron energy

- The evaluated data are determined mostly by the results of Starostov's measurements
- There are only small differences between normalized and non-normalized spectra

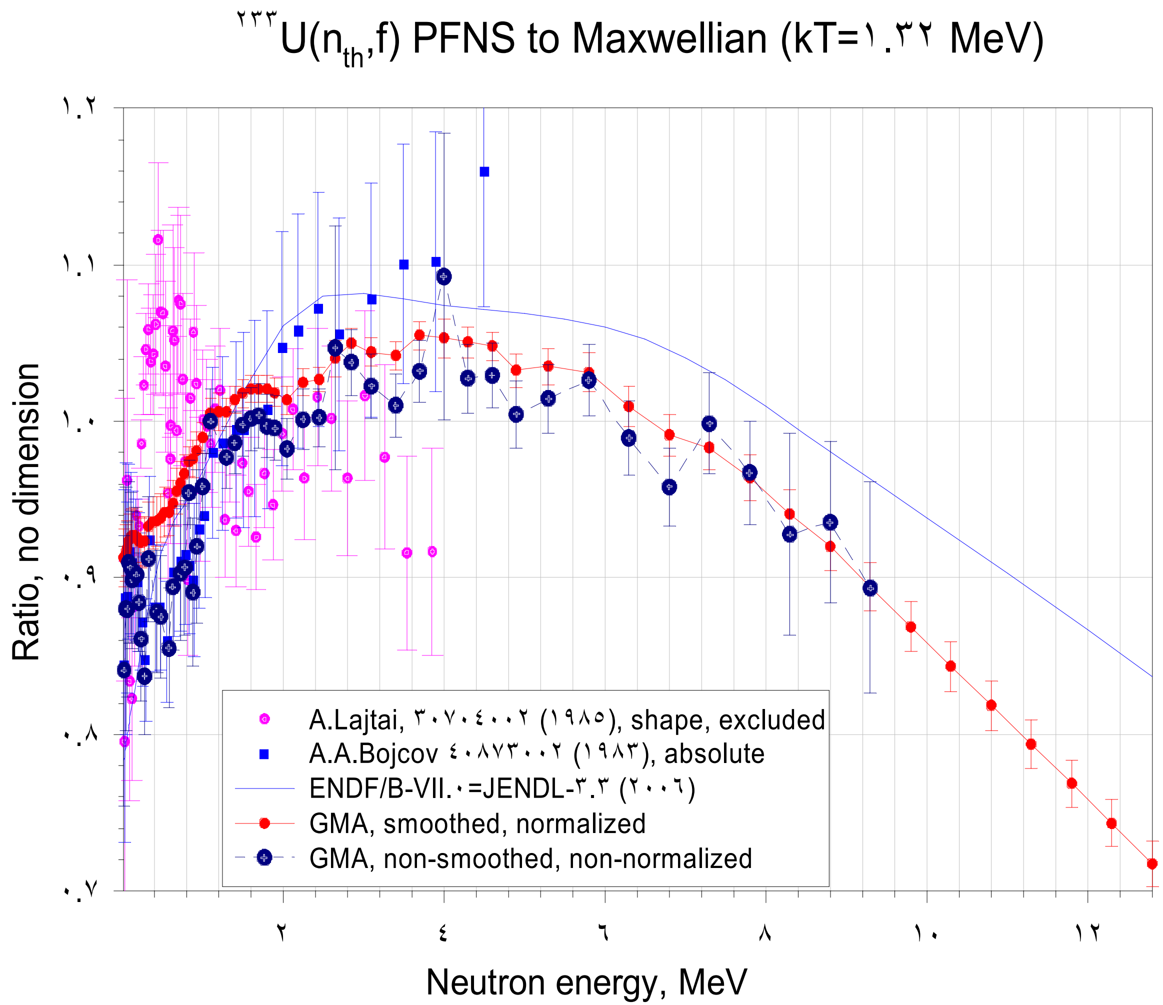
Results of the evaluation: $^{239}Pu(n_{th},f)$



Logarithmic scale on neutron energy

- Ratio of spectra evaluated with GMA shows that $^{239}Pu(n_{th},f)$ PFNS in neutron energy range below 1 MeV is underestimated

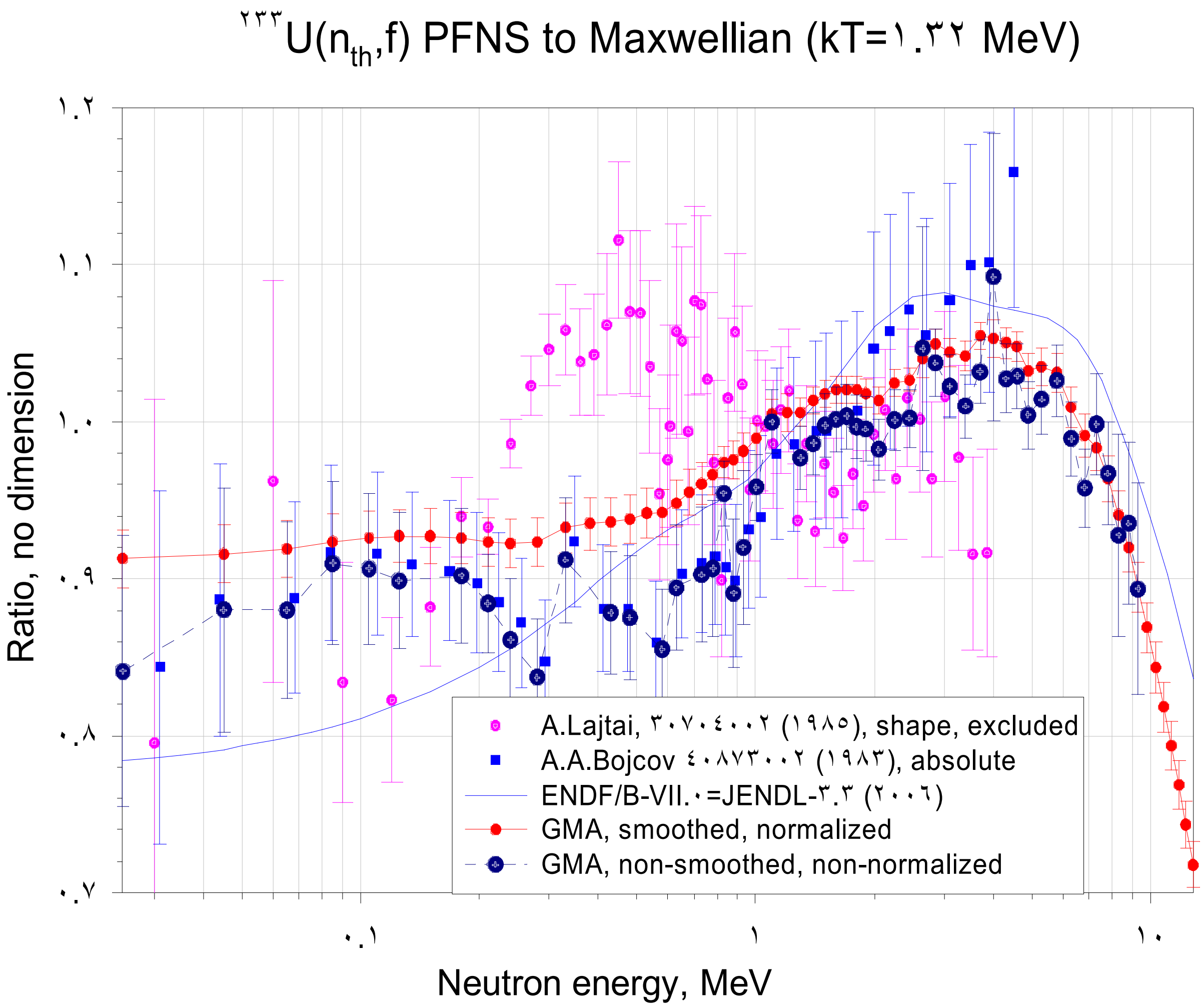
Results of the evaluation: $^{233}U(n_{th},f)$



Linear scale on neutron energy

- Data by Lajtai were excluded from the fit because their discrepancy with all other data
- Hard part of the evaluated spectrum is lower than calculated (ENDF/B-VII.0)

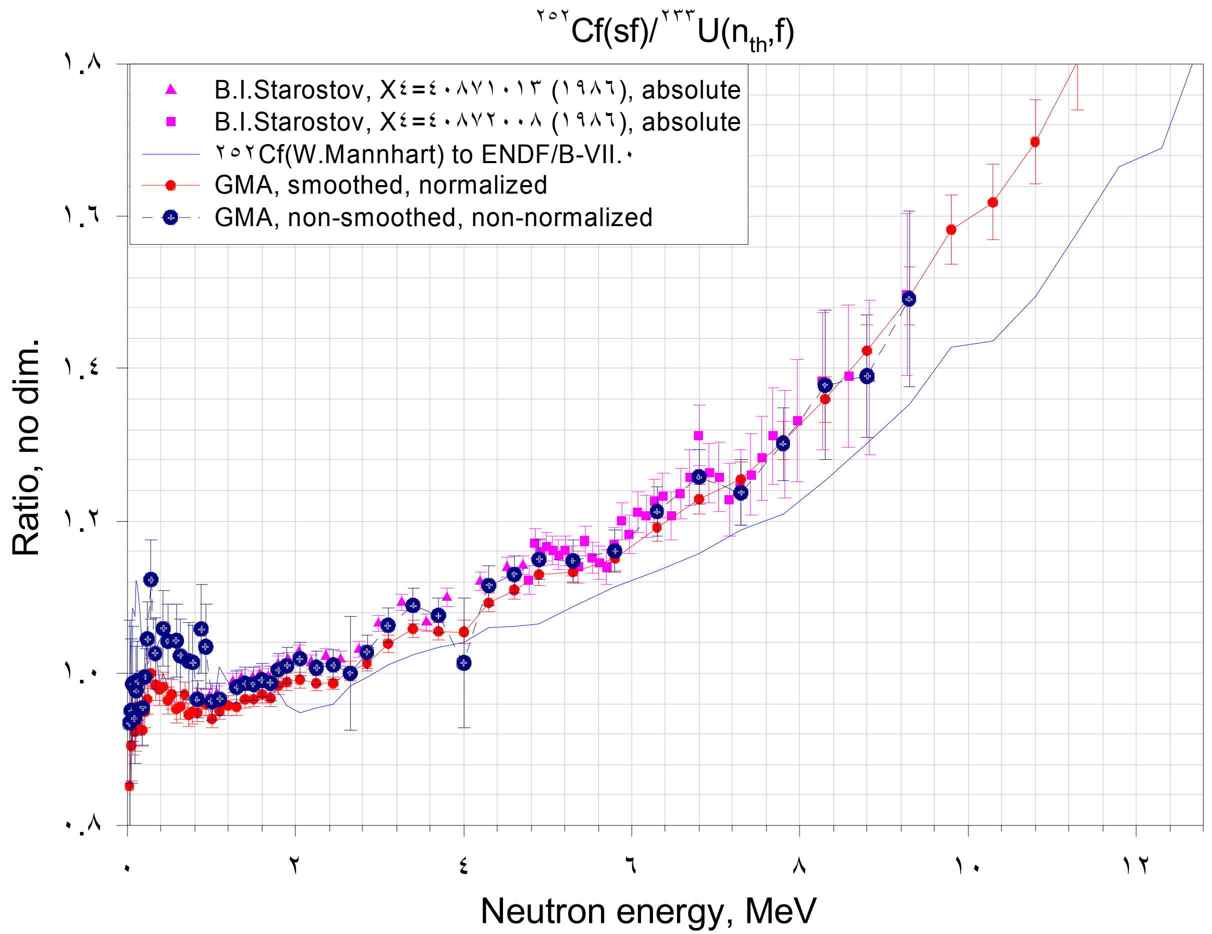
Results of the evaluation: $^{233}U(n_{th},f)$



Logarithmic scale on neutron energy

- Normalized evaluation is above of non-normalized evaluation
- Low-energy part of the evaluated spectrum is higher than the calculated spectrum (ENDF/B-VII.0)

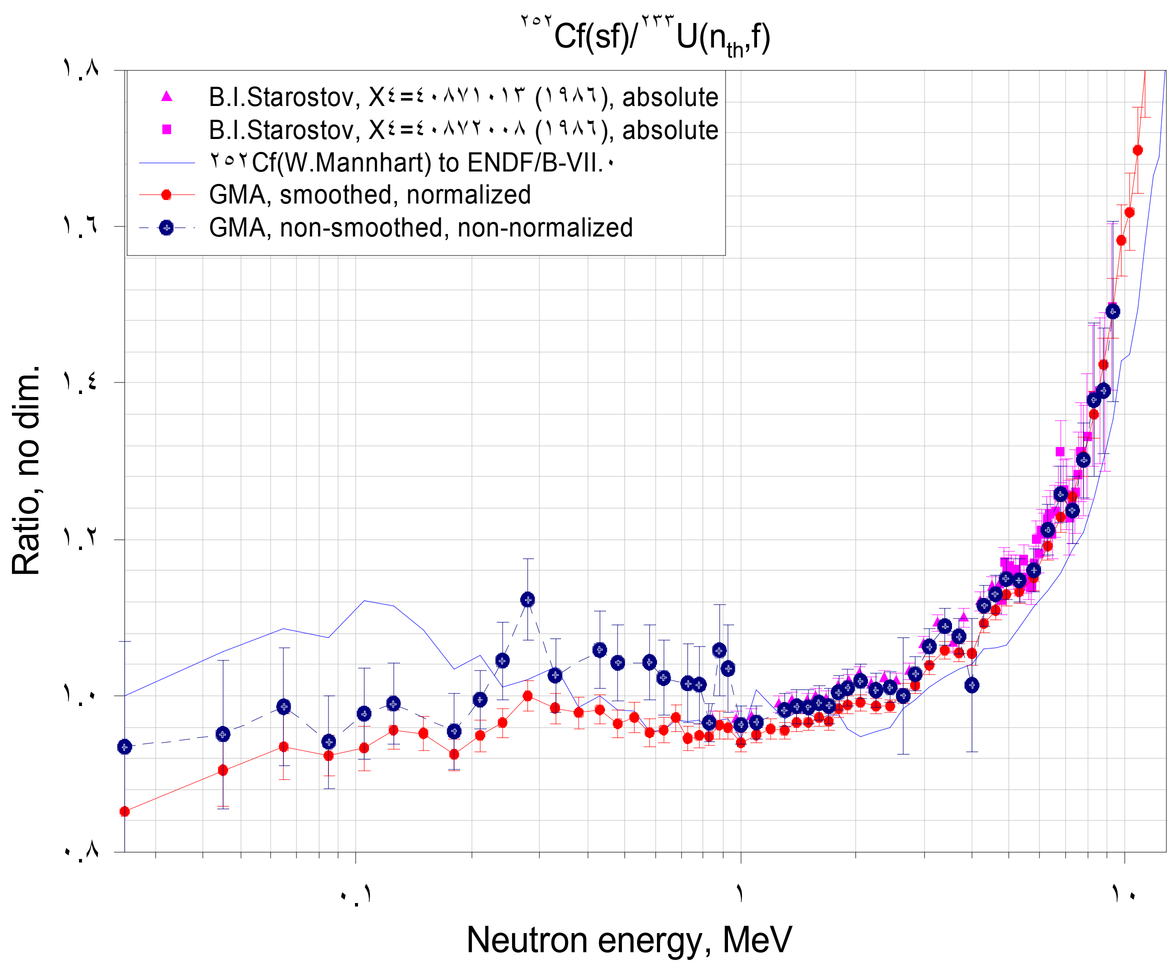
Results of the evaluation: $^{233}U(n_{th},f)$



Linear scale on neutron energy

- The evaluated data are determined mostly by the results of Starostov's measurements

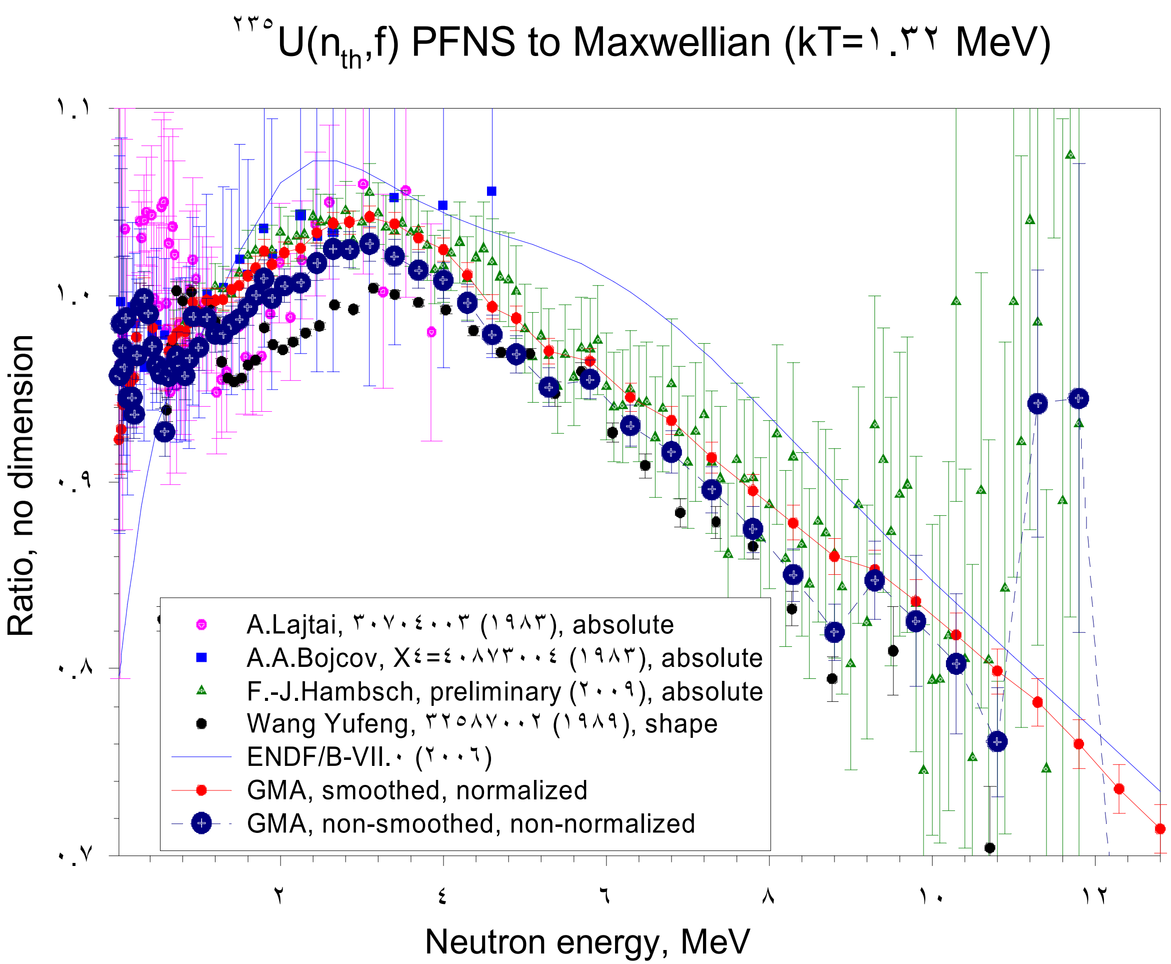
Results of the evaluation: $^{233}U(n_{th},f)$



Logarithmic scale on neutron energy

- There is no data on ratio measurements below 1 MeV of neutron energy. Absolute data by Bojko determine the ratio of spectra in this energy range

$^{235}U(n_{th},f)$: smoothing procedure



Linear scale on neutron energy

- Smoothing done with using of the results of model calculations and specially designed covariance matrix does not change the global shape of the evaluated spectra
- It reduces substantially the percent uncertainties because narrow (2%) error band was used for model curve for smoothing
- Evaluated uncertainties for the curve are determined not the percent errors, but covariance matrix which is changed substantially due to smoothing

$^{235}U(n_{th},f)$: smoothing procedure

Non-smoothed evaluation for ^{235}U PFNS

RESULT 5U(nth,f)

E/MEV	CS/B	Uncert/B	Uncert/%
0.2500E-01	0.95692736	0.08312536	8.7
0.4500E-01	0.98479678	0.08269180	8.4
0.6500E-01	0.97167988	0.04923534	5.1
0.8500E-01	0.96131513	0.02836578	3.0
0.1050E+00	0.98768544	0.03196099	3.2
0.1250E+00	0.94504090	0.02298817	2.4
0.1500E+00	0.94488792	0.02152497	2.3
0.1800E+00	0.94522256	0.01617718	1.7
0.2100E+00	0.93629392	0.01316840	1.4
0.2400E+00	0.96774827	0.01267273	1.3
0.2800E+00	0.99466882	0.01191867	1.2
0.3300E+00	0.99835824	0.01417137	1.4
0.3800E+00	0.99022766	0.01500059	1.5
0.4300E+00	0.97247675	0.01419838	1.5
0.4800E+00	0.96242403	0.01512008	1.6
0.5300E+00	0.95823769	0.01935835	2.0

CORRELATION MATRIX OF THE RESULT 5U(nth,f) 5U(nth,f)

1.00															
0.01	1.00														
0.02	0.02	1.00													
0.02	0.03	0.04	1.00												
0.02	0.03	0.04	0.09	1.00											
0.03	0.03	0.05	0.09	0.10	1.00										
0.02	0.02	0.04	0.09	0.09	0.11	1.00									
0.04	0.04	0.06	0.12	0.11	0.14	0.16	1.00								
0.04	0.04	0.08	0.14	0.13	0.17	0.19	0.26	1.00							
0.05	0.04	0.08	0.14	0.12	0.17	0.20	0.26	0.32	1.00						
0.05	0.05	0.08	0.15	0.13	0.19	0.21	0.28	0.34	0.38	1.00					
0.04	0.04	0.07	0.13	0.12	0.16	0.17	0.23	0.28	0.31	0.34	1.00				
0.04	0.03	0.06	0.12	0.10	0.14	0.16	0.21	0.26	0.29	0.31	0.27	1.00			
0.04	0.04	0.07	0.12	0.11	0.15	0.16	0.22	0.26	0.29	0.31	0.28	0.26	1.00		
0.04	0.04	0.06	0.11	0.09	0.13	0.14	0.19	0.23	0.25	0.27	0.24	0.23	0.27	1.00	
0.02	0.02	0.04	0.07	0.06	0.09	0.10	0.14	0.17	0.19	0.21	0.18	0.17	0.18	0.17	1.00

- **Jumps in the spectra for neighbouring energy points**
- **Low level of correlations between neighbouring points**
- **Uncertainties in some points are large**

$^{235}U(n_{th},f)$: smoothing procedure

Model calculations used for smoothing of ^{235}U PFNS

DATA SET 912 CS-SHAPE 5U(nth,f)

YEAR 2010 TAG 1 AUTHOR: Kornilov's model Smoothing

ENERGY/MEV	VALUE	ABS. UNCERT.	PRIOR/EXP	Uncert./%
0.2500E-01	0.9118E+00	0.1824E-01	0.9938	2.0
0.4500E-01	0.9137E+00	0.1827E-01	0.9972	2.0
0.6500E-01	0.9156E+00	0.1831E-01	1.0062	2.0
0.8500E-01	0.9174E+00	0.1835E-01	1.0140	2.0
0.1050E+00	0.9193E+00	0.1839E-01	1.0179	2.0
0.1250E+00	0.9211E+00	0.1842E-01	1.0115	2.0
0.1500E+00	0.9233E+00	0.1847E-01	1.0063	2.0
0.1800E+00	0.9259E+00	0.1852E-01	1.0073	2.0
0.2100E+00	0.9286E+00	0.1857E-01	1.0076	2.0
0.2400E+00	0.9311E+00	0.1862E-01	1.0285	2.0
0.2800E+00	0.9345E+00	0.1869E-01	1.0493	2.0
0.3300E+00	0.9386E+00	0.1877E-01	1.0478	2.0
0.3800E+00	0.9426E+00	0.1885E-01	1.0361	2.0
0.4300E+00	0.9465E+00	0.1893E-01	1.0192	2.0
0.4800E+00	0.9503E+00	0.1901E-01	1.0053	2.0
0.5300E+00	0.9540E+00	0.1908E-01	0.9934	2.0

APRIORI NORM 232 0.9838 912 Smoothing

CORRELATION MATRIX OF DATA BLOCK

1.00															
0.06	1.00														
0.05	0.32	1.00													
0.05	0.05	0.46	1.00												
0.05	0.05	0.18	0.54	1.00											
0.05	0.05	0.05	0.29	0.60	1.00										
0.05	0.05	0.05	0.08	0.33	0.59	1.00									
0.05	0.05	0.05	0.05	0.11	0.32	0.59	1.00								
0.05	0.05	0.05	0.05	0.05	0.13	0.36	0.63	1.00							
0.05	0.05	0.05	0.05	0.05	0.05	0.19	0.43	0.67	1.00						
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.22	0.43	0.63	1.00					
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.21	0.38	0.61	1.00				
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.20	0.40	0.65	1.00			
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.06	0.24	0.46	0.68	1.00		
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.11	0.31	0.51	0.70	1.00	
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.19	0.36	0.54	0.72	1.00

- **Fit close to the results of non-model calculations**
- **Data are introduced in the fit as shape type of data**
- **Error band is taken in 2%, but can be variable**
- **Large level of correlations between neighbouring points**

$^{235}U(n_{th},f)$: smoothing procedure

Smoothed evaluation for ^{235}U PFNS

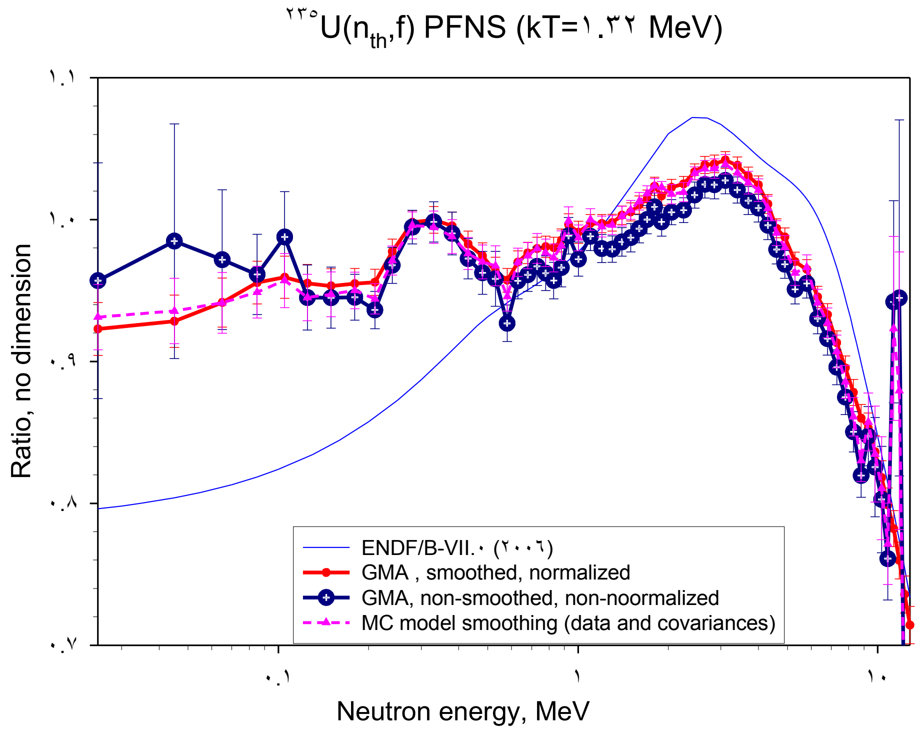
E/MEV	CS/B	Uncert./B	Uncert./%		
0.2500E-01	0.90618668	0.01886569	2.1	0.01	0.14328
0.4500E-01	0.91124672	0.01881637	2.1	0.01	0.19330
0.6500E-01	0.92162683	0.01778062	1.9	0.04	0.23497
0.8500E-01	0.93130801	0.01598866	1.7	0.11	0.27152
0.1050E+00	0.93701323	0.01576630	1.7	0.13	0.30363
0.1250E+00	0.93261931	0.01447349	1.6	0.10	0.32973
0.1500E+00	0.93005232	0.01377225	1.5	0.10	0.36021
0.1800E+00	0.93325759	0.01220016	1.3	0.07	0.39595
0.2100E+00	0.93606243	0.01097750	1.2	0.04	0.42896
0.2400E+00	0.95802119	0.01076189	1.1	0.04	0.46933
0.2800E+00	0.98075249	0.01051403	1.1	0.02	0.51897
0.3300E+00	0.98367612	0.01149592	1.2	0.02	0.56508
0.3800E+00	0.97674699	0.01167410	1.2	0.01	0.60211
0.4300E+00	0.96457697	0.01129881	1.2	-0.01	0.63252
0.4800E+00	0.95525068	0.01147233	1.2	-0.01	0.66182
0.5300E+00	0.94750594	0.01201156	1.3	-0.02	0.68979

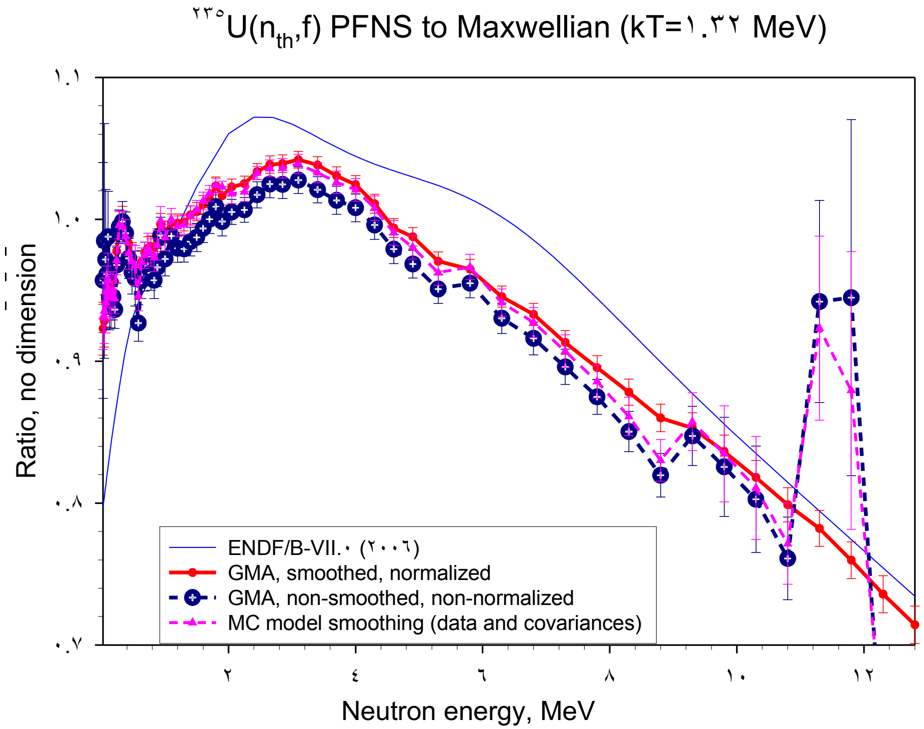
CORRELATION MATRIX OF THE RESULT 5U(nth,f) 5U(nth,f)

1.00															
0.18	1.00														
0.17	0.40	1.00													
0.18	0.17	0.47	1.00												
0.17	0.17	0.24	0.52	1.00											
0.18	0.18	0.16	0.33	0.54	1.00										
0.18	0.18	0.19	0.19	0.35	0.52	1.00									
0.19	0.19	0.21	0.22	0.23	0.35	0.50	1.00								
0.20	0.20	0.22	0.25	0.24	0.28	0.38	0.52	1.00							
0.20	0.20	0.22	0.26	0.26	0.27	0.32	0.42	0.55	1.00						
0.21	0.21	0.23	0.26	0.27	0.30	0.29	0.38	0.46	0.55	1.00					
0.19	0.19	0.21	0.24	0.25	0.28	0.30	0.29	0.39	0.44	0.53	1.00				
0.19	0.19	0.20	0.23	0.24	0.26	0.29	0.33	0.33	0.40	0.45	0.53	1.00			
0.19	0.19	0.21	0.24	0.24	0.26	0.29	0.33	0.37	0.35	0.42	0.44	0.54	1.00		
0.19	0.19	0.20	0.23	0.23	0.25	0.27	0.31	0.35	0.36	0.36	0.39	0.44	0.55	1.00	
0.17	0.17	0.19	0.21	0.21	0.23	0.24	0.28	0.33	0.35	0.33	0.34	0.37	0.44	0.55	1.00

- Data (and uncertainties) have been smoothed
- Per-cent uncertainties have been decreased
- Non-diagonal covariances have been increased and compensated decrease of the diagonal covariances (variances)
- Large level of correlations between neighbouring points
- Difference with smoothing using model least-squares fit – result is practically independent from the model used and practically has no limitations, which model can put on the result of evaluation

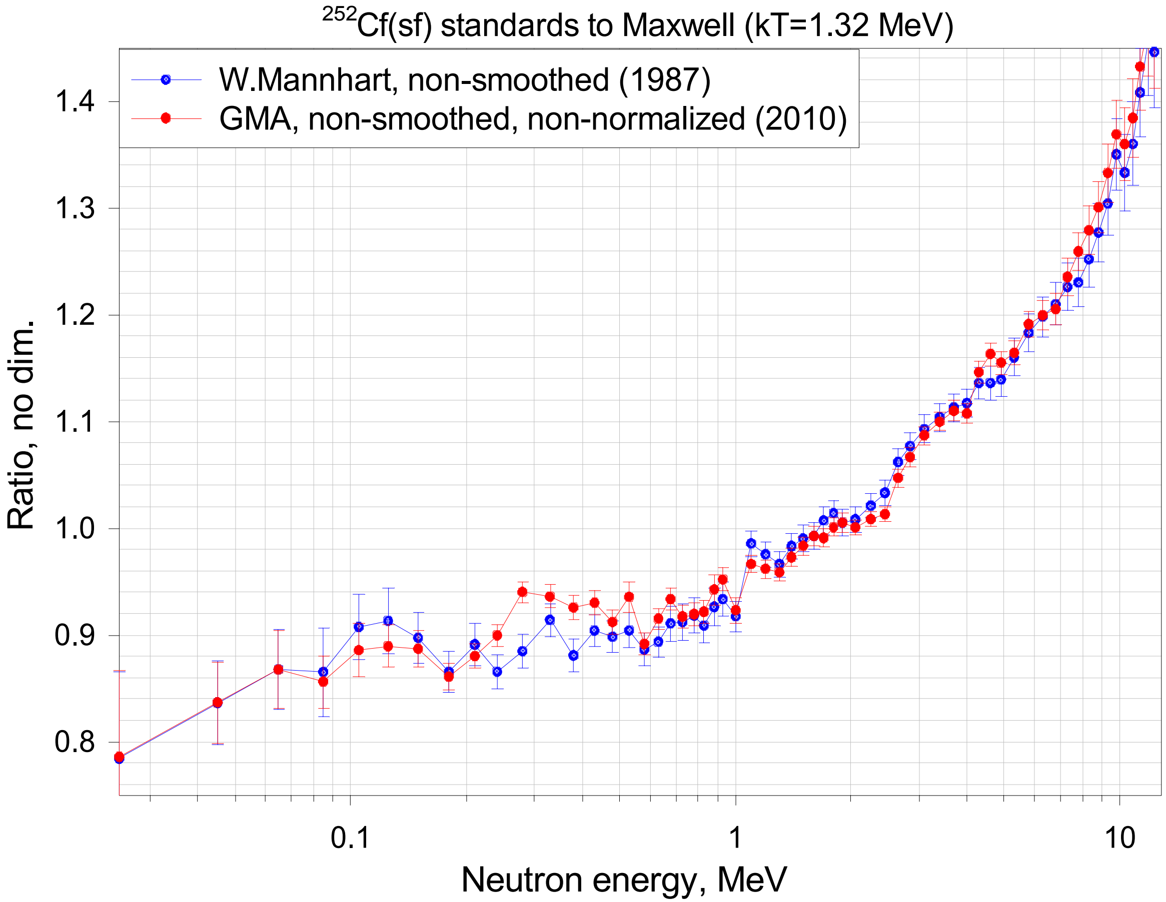
Use of model smoothing and combined fit with MC model calculations





GMA result:
Smoothed, normalized – smoothed with the results of the Kornilov's model calculations (V.M. Maslov, May 2010) used as shape data. Specially designed correlation matrix keeping strong positive correlations between neighboring points was used. Normalization constraint at the integral under the spectrum was used in the fit for spectrum normalization
MC model smoothing (data and covariances) – combined fit with the results of MC evaluation for Kornilov's model (R. Capote, October 2010). Model evaluated data and covariances were used. Covariance matrix of MC evaluation has strong anti-correlations because of the used model.
Model has high predictive force at low energies (below 1 MeV), but low at high energies (above 6 MeV)

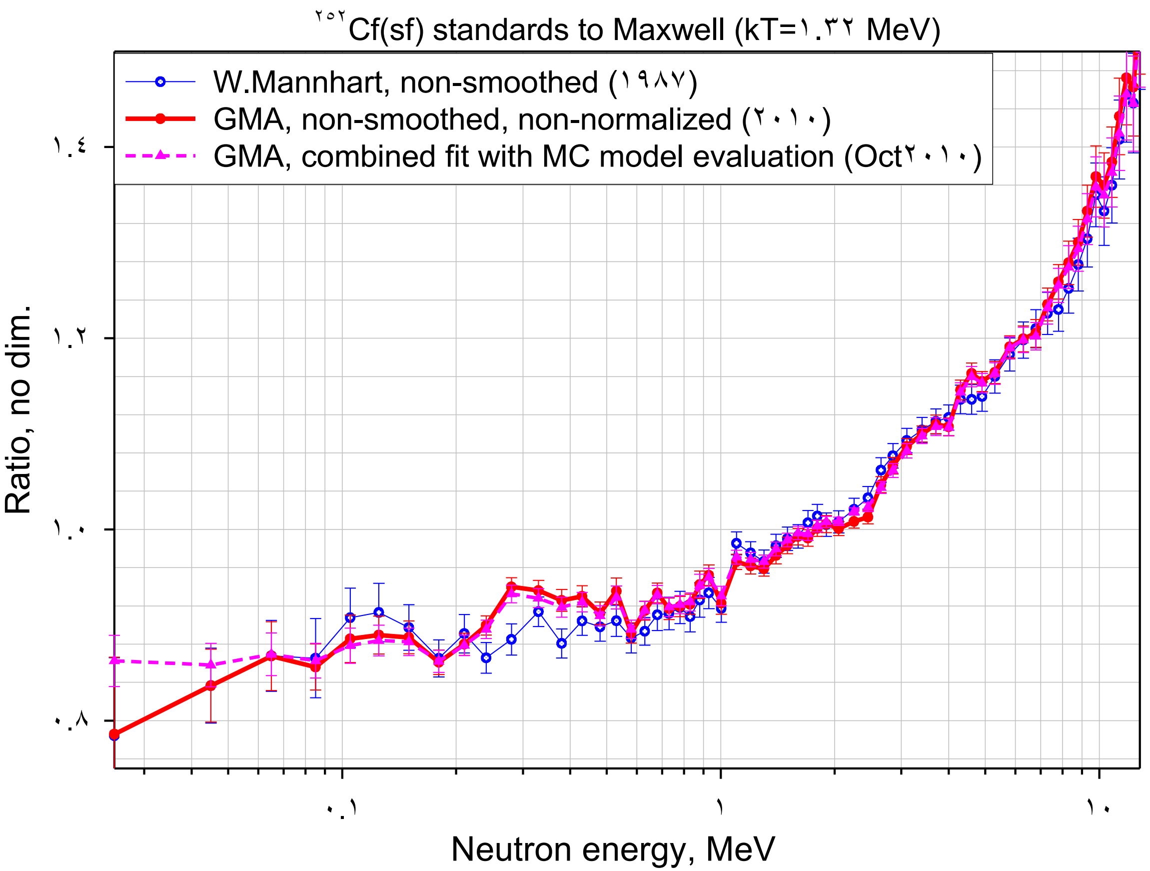
New evaluation of ^{252}Cf(sf)



Logarithmic scale on neutron energy

- Combined fit of ^{252}Cf(sf) prompt fission neutron spectra with ^{235}U(n_{th},f), ^{239}Pu(n_{th},f), ^{233}U(n_{th},f) and PFNS introduces small (in the limits of the uncertainties) changes in the central values
- The percent uncertainties of new ^{252}Cf(sf) PFNS evaluation are reduced for neutrons with energy above 0.5 MeV at about 1/3.
- Largest differences in the energy range 0.2 – 0.6 MeV are caused the corresponding structures in the ^{235}U(n_{th},f) PFNS

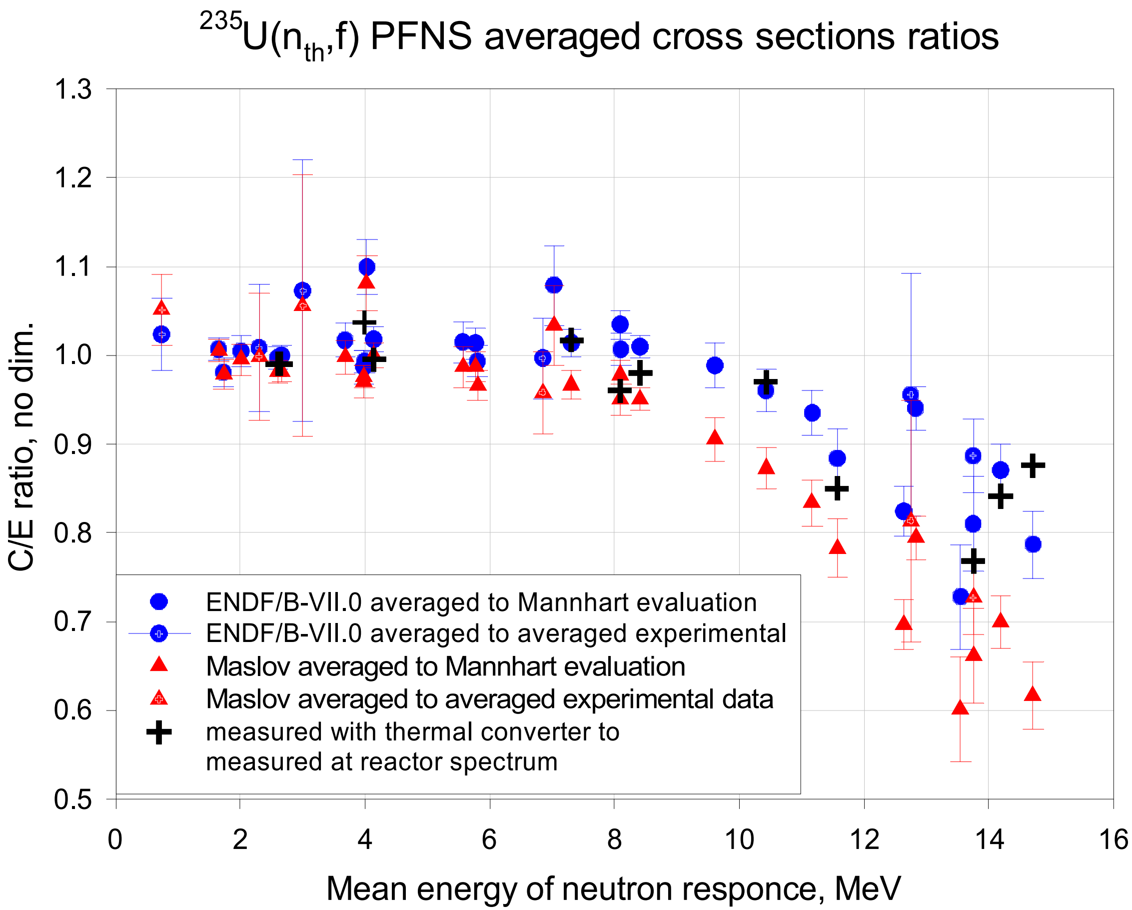
Combined fit with MC model evaluation



Logarithmic scale on neutron energy

- Combined fit of $^{252}Cf(sf)$ prompt fission neutron spectra with $^{235}U(n_{th},f)$, $^{239}Pu(n_{th},f)$, $^{233}U(n_{th},f)$.
- Results of MC evaluation (central values and covariances) based on Kornilov's model with physical parameters and their estimated uncertainties was added to the fit.
- Model smoothes and reduces uncertainties in low-energy part of the spectrum

Test of the $^{235}U(n_{th},f)$ PFNS in the integral experiments



Ratio of spectrum averaged cross sections: Madland-Nix or Maslov-GMA spectrum to Mannhart evaluation of cross sections or averaged experimental data

- Below 8 MeV of mean neutron energies ENDF/B-VII.0 (Madland-Nix) and Maslov (GMA) PFNS give good agreement with evaluated and experimental spectrum averaged cross sections
- Ratios of averaged measurements with thermal converter to reactor measurements are show by pluses. As seems the reactor ^{235}U spectra are rather strongly disturbed in the high-energy part
- Spectrum obtained with thermal converter is most probably also effective and to some extent disturbed in the high energy part

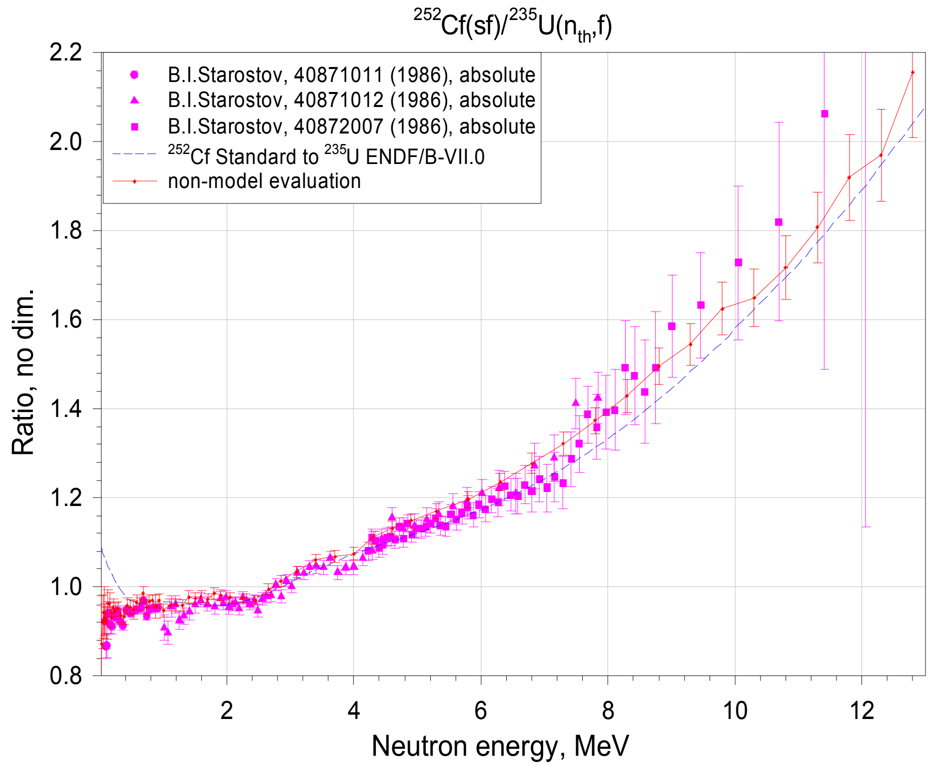
Conclusion

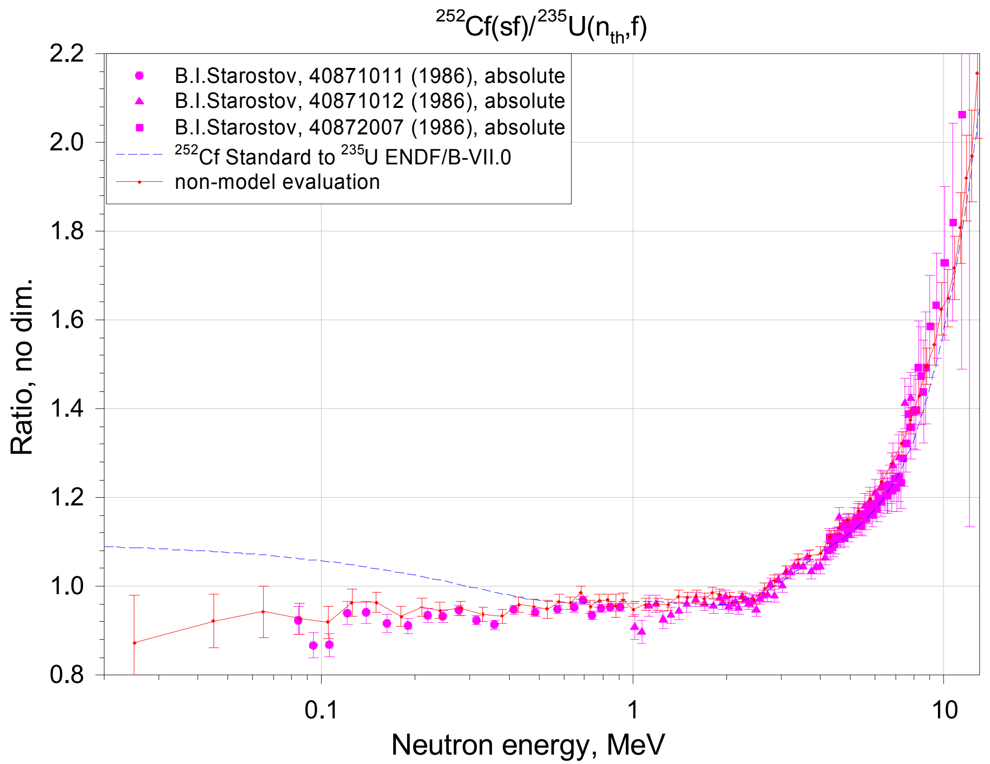
- $^{235}U(n_{th},f)$ reference prompt fission spectrum can be evaluated in the combined fit with $^{239}Pu(n_{th},f)$, $^{233}U(n_{th},f)$ and $^{252}Cf(sf)$ PFNS
- Results of new measurements of absolute ratio of $^{252}Cf(sf)/^{235}U(n_{th},f)$ PFNS by A. Vorobyev shows that Starostov's data for En > 1 MeV are 5 – 6% higher
- For adjustment of parameters in the model least-squares fit (Watt, Madland-Nix, Kornilov models) can be used non-model, non-smoothed, non-normalized evaluation including as central values as well as covariance matrix of uncertainties
- GMA non-model evaluated spectra differ from those presently used in the evaluated data libraries by higher number of neutrons in the soft part of the spectra ($E_n < 1$ MeV)

Conclusion

- Comparison of experimental and calculated data on spectrum averaged cross sections for $^{235}U(n_{th},f)$ and on $^{239}Pu(n_{th},f)$ criticality benchmarks for system with thermal neutron spectrum shows for new evaluations the same level of agreement between experimental and calculated values as for spectra for evaluated data libraries. But new evaluated spectra are in good agreement with the experimental data
- This demonstrate the sensitivity in the criticality benchmarks not only to the mean energy of the spectra but also to he shape of the spectra

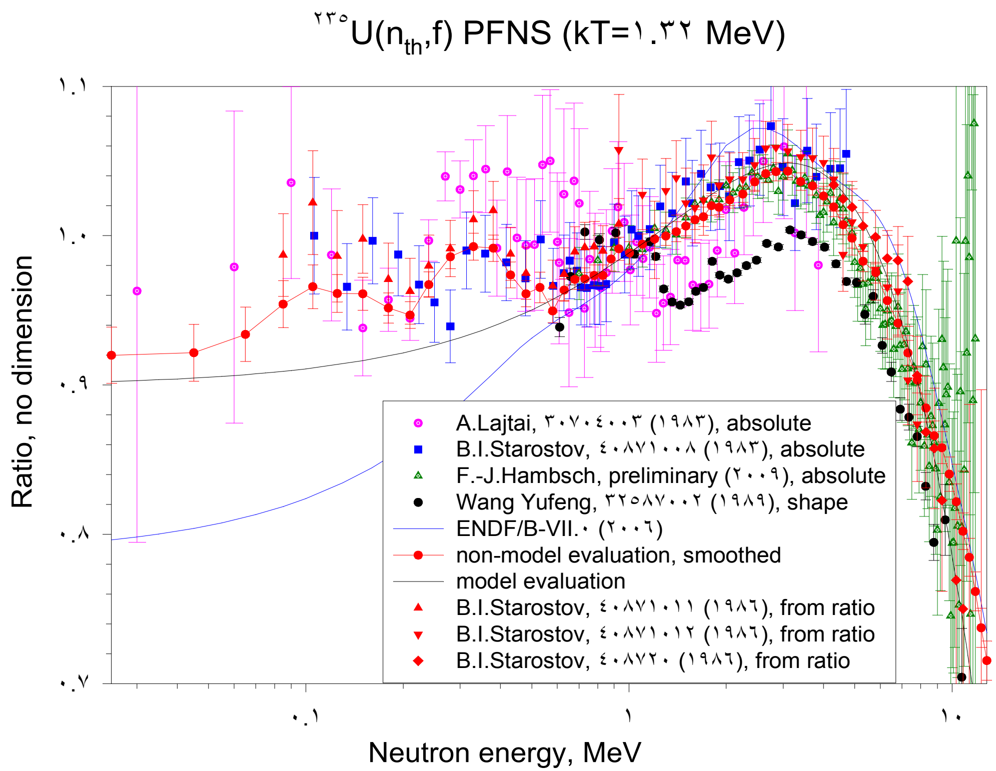
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results (May2010)

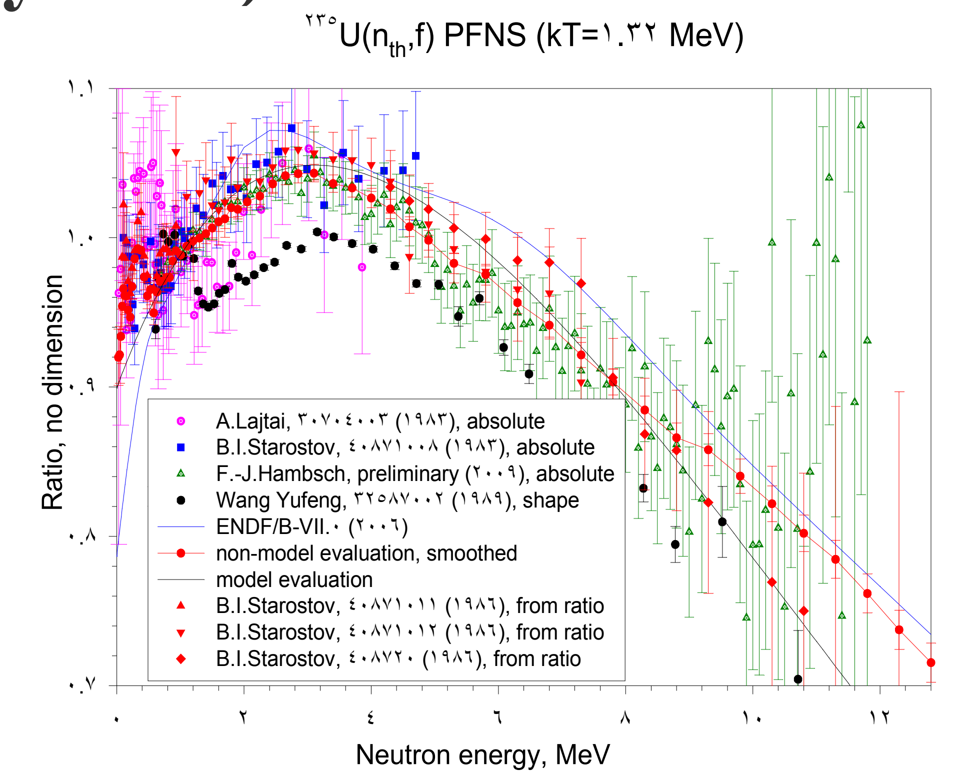




Comparison of the results of measurements of absolute ratio of the PFNS spectra ^{252}Cf(sf)/^{235}U(n_{th},f) in linear and logarithmic scales on neutron energy.

GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results (May 2010)





Comparison of the $^{235}U(n_{th},f)$ PFNS in linear and logarithmic scale on the neutron energy. Starostov's (NIIAR) data of absolute measurements of ratios were reduced to absolute spectra using new ^{252}Cf simultaneous evaluation. Results of the non-model and model evaluations are shown.

Questions to be answered

- Can be this approach appropriate for $^{235}U(n_{th},f)$ reference PFNS evaluation?
- Should be 2 Starostov's data sets, with absolute ratio of $^{252}Cf(sf)/^{235}U(n_{th},f)$ PFNS for En > 1 MeV, used as they are given by the authors, renormalized to be more close to the normalization at 1, or used as shape data?
- Which reactions with mean neutron energy response in the range 0.1 MeV – 0.8 MeV can be used in the integral experiments for verification of soft part of the evaluated spectra?
- Can be present $^{235}U(n_{th},f)$ PFNS evaluation after some needed data adjustment and model fits used as reference evaluation?