Deviation factors

A.Yu. Konobeyev

Forschungszentrum Karlsruhe
in der Helmholtz-Gemeinschaft
Universität Karlsruhe (TH)
Research University · founded 1825

How to compare correctly results of calculations obtained using different nuclear models ?

Distribution of experimental points $\sigma_{exp}(i)$ (Z,A,E)

Distribution of calculated values $\sigma_{calc}(i)$ (Z,A,E)

Is the difference between distributions statistically significant?

Null hypothesis H_0 : distribution functions are identical

Alternative hypothesis H_1: H_0 does not hold

Normal distribution: t-test (Student's), Fisher test etc

$$\bar{x} = \frac{1}{m}\sum_{1\le i\le m} x_i, \qquad y = \frac{1}{n}\sum_{1\le i\le n} y_i \qquad s_x^2 = \frac{1}{m-1}\sum_{1\le i\le m}(x_i - \bar{x})^2$$

$$t = \frac{\bar{x} - \bar{y}}{\sqrt{(m-1)s_x^2 + (n-1)s_y^2}}\sqrt{\frac{mn(m+n-2)}{m+n}}$$

α (0.05), (n-m+2) degrees of freedom degrees,

tables of t-distribution : t_{crit}

$|t| < t_{crit}$: H_0

Deviation of results of calculations from measured data.
The type of the distribution.

Examples

Measured data: cross-sections

reactions: (p,x)

targets : Z from 12 to 83

proton incident energy : from 20 to 150 MeV

Total number of (Z,A,Ep) points : 9452

Calculations: Bertini / MPM / Dresner

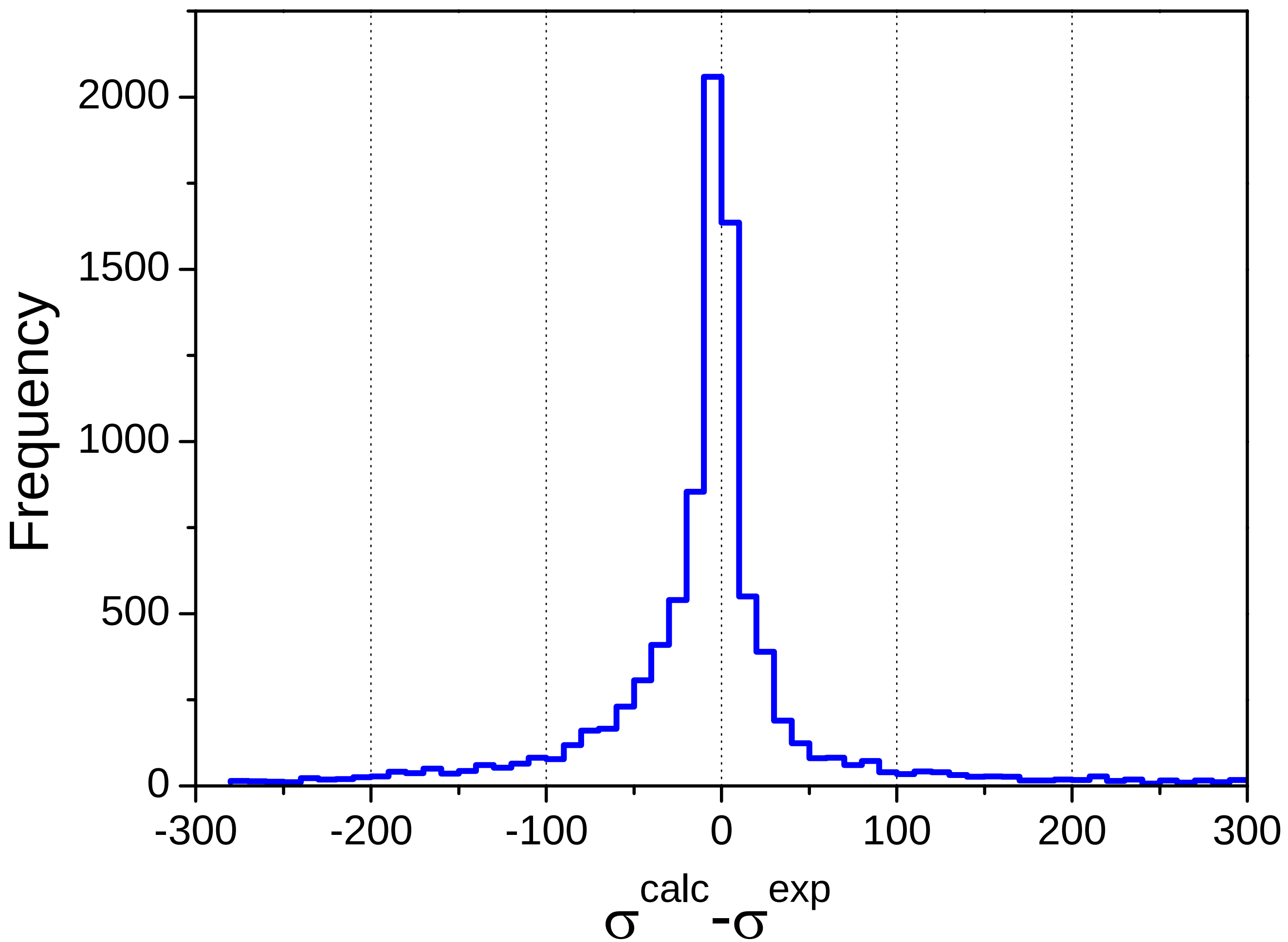
Tests of goodness of fit

Chi-squared goodness-of-fit test

Shapiro-Wilk test for normality

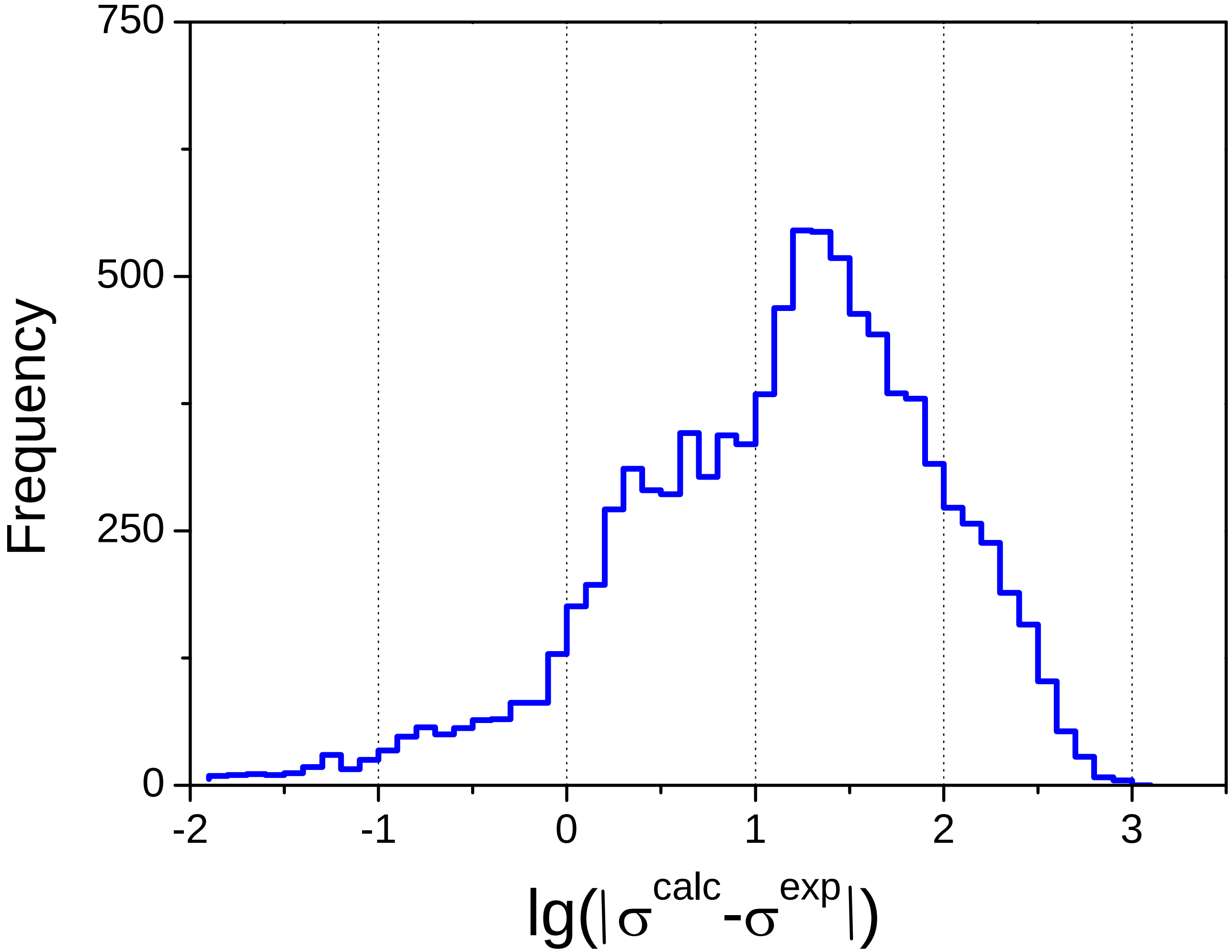
Search for normal or lognormal distribution

Bertini/MPM/Dresner



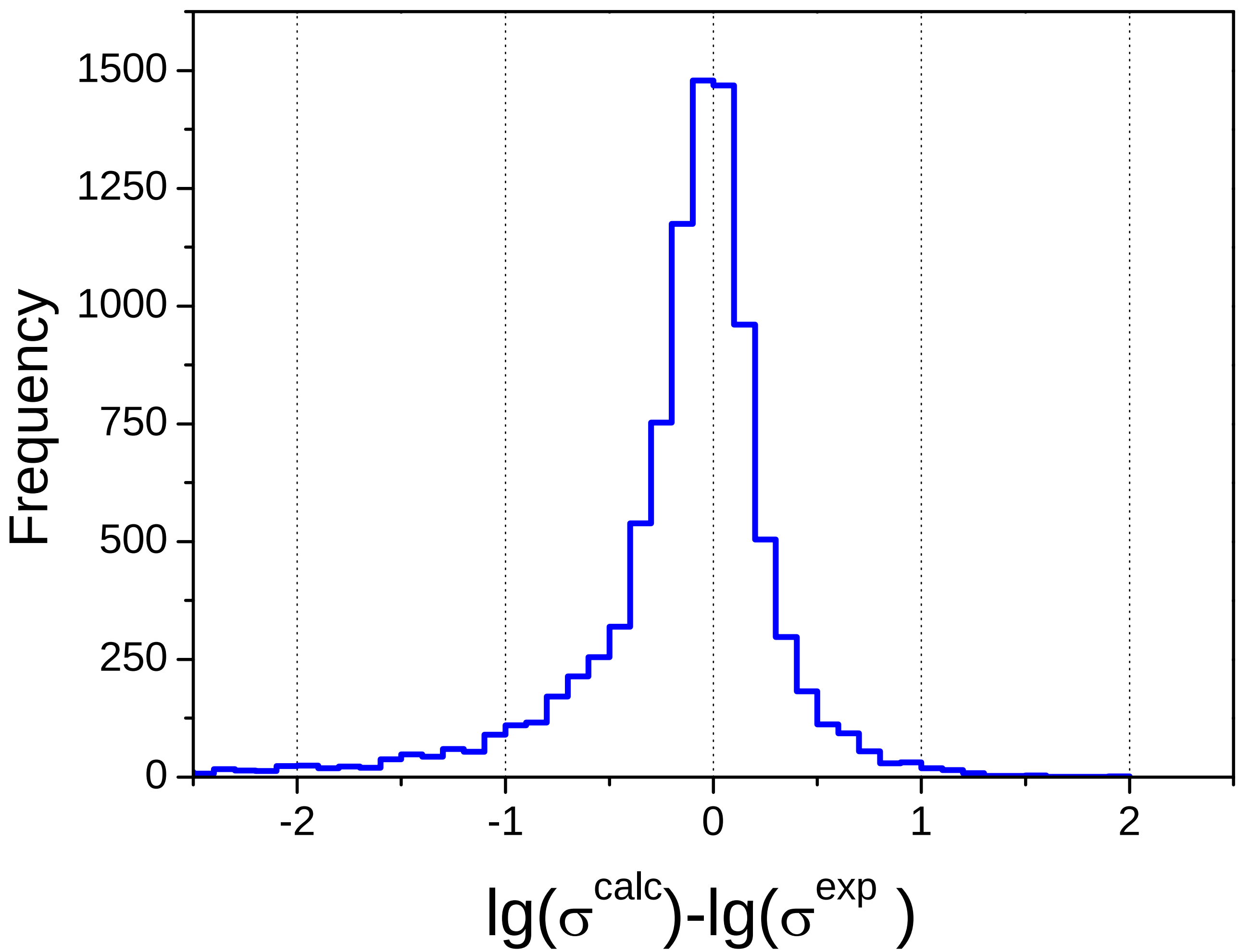
Normality rejected

Bertini/MPM/Dresner



Normality rejected

Bertini/MPM/Dresner



Normality rejected

Solution: use of nonparametric tests

No certain assumptions about distributions

Wilcoxon Mann-Whitney test for comparing two populations

Null hypothesis: two populations have identical distribution functions

Use of Wilcoxon Mann-Whitney or Mann–Whitney test

I. The comparison of measured data and results of calculations using a certain code

II. The comparison of difference between measured data and results of calculations using various codes

Answer the question: is the difference between two codes statistically significant ?

Deviation factors

I. $$H = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \right)^{1/2}$$

Model “deficiency”

$$C_H = \frac{H}{H'} = \frac{H}{H(0.1 < \sigma_i^{calc} / \sigma_i^{exp} < 10)}$$

Example

(p,x) reaction cross-sections from EXFOR
targets Z from 12 to 83
proton incident energy : from 20 to 150 MeV
total number of (Z,A,E_p) points ~ 9500

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
H	49.8	28.0	14.2
H'	15.7	17.7	10.4
C_H	3.2	1.6	1.4

II. $$R^{CE} = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{calc}}{\sigma_i^{exp}}$$

and

$$R^{EC} = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{exp}}{\sigma_i^{calc}}$$

Example

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
R^{CE}	1.3	1.3	1.1
R^{EC}	5.2	82.	3.8

III.

$$D^{CE} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\sigma_i^{exp}}\right|$$

and

$$D^{EC} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\sigma_i^{exp} - \sigma_i^{calc}}{\sigma_i^{calc}}\right|$$

IV. Deviation factors proposed by R.Michel

Variants

R.Michel et al, NIMB129 (1997) 153

$$\langle F \rangle = 10^{\frac{1}{n_s}\sqrt{\sum_{i=1}^{n_s}[\log(\sigma_{\exp,i}) - \log(\sigma_{\mathrm{theo},i})]^2}}$$

International Codes and Model Intercomparison for Intermediate Energy Activation Yields," NSC/DOC(97)-1 (Jan. 1997)

$$<F> = 10.\ **\ \mathrm{SQRT}(<(\log\sigma_{\exp} - \log\sigma_{\mathrm{theo}})^2>)$$

$$<(\log\sigma_{\exp} - \log\sigma_{\mathrm{theo}})^2> = \sum_i (\log\sigma_{\exp,i} - \log\sigma_{\mathrm{theo},i})^2 / NS$$

$$\overline{F} = 10^{\frac{1}{N}\sum_{i=1}^{N}\left[\log(\sigma_i^{exp})-\log(\sigma_i^{calc})\right]}$$

and

$$< F > = 10^{\left(\frac{1}{N}\sum_{i=1}^{N}\left[\log(\sigma_i^{exp})-\log(\sigma_i^{calc})\right]^2\right)^{1/2}}$$

(symbols from NIMB129 (1997) 153)

Example

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
$\overline{F}$	0.72	0.83	0.87
<F>	3.17	3.15	2.21

Model "deficiency"

$$C_F = \frac{<F>}{<F>'} = \frac{<F>}{<F>(0.1 < \sigma_i^{calc} / \sigma_i^{exp} < 10)}$$

Example

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
<F>	3.17	3.15	2.21
<F>'	2.11	1.96	1.78
C_F	1.5	1.6	1.2

V. Modified F factor including experimental errors

D.Smith, private communication, 2007

$$\exp\left(\frac{1}{N}\sum_{i=1}^{N}\left[\frac{\ln(\sigma_i^{exp})-\ln(\sigma_i^{calc})}{\left(\frac{\Delta\sigma_i^{exp}}{\sigma_i^{exp}}\right)}\right]^2\right)^{1/2}$$

$$S = 10^{\left(\sum_{i=1}^{N} \left[\frac{\lg(\sigma_i^{exp}) - \lg(\sigma_i^{calc})}{\left(\Delta\sigma_i^{exp} / \sigma_i^{exp}\right)} \right]^2 \sum_{i=1}^{N} \left[\frac{\sigma_i^{exp}}{\left(\Delta\sigma_i^{exp}\right)} \right]^{-2} \right)^{1/2}}$$

$$C_F = \frac{S}{S'} = \frac{S}{S(0.1 < \sigma_i^{calc} / \sigma_i^{exp} < 10)}$$

Example

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
S	1.83	1.63	1.31
S’	1.76	1.52	1.288
C_S	1.04	1.07	1.02

VI. H.Leeb et al. Santa Fe (2004)

$$L = \left[\sum_{i=1}^{N} \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \left(\frac{\sigma_i^{calc} - \sigma_i^{exp}}{\sigma_i^{calc}} \right)^2 \Bigg/ \sum_{i=1}^{N} \left(\frac{\sigma_i^{calc}}{\Delta\sigma_i^{exp}} \right)^2 \right]^{1/2}$$

Example

Factor	Bertini/MPM/ Dresner	CEM03	TALYS
L	0.875	0.534	0.343

VII.

$$P_{1.3} = N_{1.3}/N, \quad N_{1.3} : \; 0.77 < \sigma_i^{calc} / \sigma_i^{exp} < 1.3$$

$$P_{2.0} = N_{2.0}/N, \quad N_{2.0} : \; 0.50 < \sigma_i^{calc} / \sigma_i^{exp} < 2.0$$

$$P_{10.0} = N_{10.0}/N, \quad N_{10.0} : \; 0.1 < \sigma_i^{calc} / \sigma_i^{exp} < 10.0$$

N can be total number of experimental points or points available for each set of the calculation

Example

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
$P_{1.3}$	0.35	0.35	0.44
$P_{2.0}$	0.68	0.70	0.82
$P_{10.0}$	0.94	0.95	0.98

KIT
Karlsruhe Institute of Technology

Number of points available in one set of model calculations

$N_{calc}(m) \le N_{exp}$

Factors:

H, R^{CE}, D^{CE}, L: $\sigma_i^{calc} = 0$ can be included

R^{EC}, D^{EC}, <F>, S: not

It is reasonable to exclude zeroes from the consideration and calculate values for all factors with the same number of points $N_{calc}(m)$

Relative number of available points as an additional characteristics of calculations

Example

(p,x) reaction cross-sections from EXFOR
targets Z from 12 to 83
proton incident energy : from 0 to 150 MeV

	Bertini/MPM/ Dresner	CEM03	TALYS
N_{calc}	16139	15162	19021
N_{calc}/N_{exp}	0.85	0.80	1.00

Number of points N_{calc}(m) and deviation factors

The difference in N_{calc}(m) can be important for the comparison of models of different “quality”

Example

Individual N_{calc}(m)

Factors	Bertini/ Dresner	CEM03	TALYS
H	70.0	35.3	14.0
R	1.53	1.54	1.16
<F>	2.76	2.60	2.59
N_{calc}	4006	4008	3975

Points available in all calculations

Factors	Bertini/ Dresner	CEM03	TALYS
H	11.9	14.6	7.1
R	1.11	1.34	1.06
<F>	2.41	2.23	2.21
N_{calc}	3869	3869	3869

(p,x) reactions, Z=12-83, E_p=50-150 MeV

Deviation factors

H, R^{CE}, R^{EC}, D^{CE}, D^{EC}, $\bar{F}$, $\langle F \rangle$, S, L

P_x, $N_{calc}/_{Nexp}$, C_H, C_F, C_S

Two types of the comparison:

a) with individual $N_{calc}(m)$

b) with reduced number of points available in all sets of calculations

"Badness" of the model

The conclusion about the predictive power

$$B_m = \frac{H_m < F >_m}{H_{ref} < F >_{ref}}$$

or

$$B_m = \frac{H_m S_m}{H_{ref} S_{ref}}$$

In the case of small N_{calc}/N_{exp} values: $B_m (N_{calc}/N_{exp})^{-1}$

Choice of "reference values": best result or averaged value

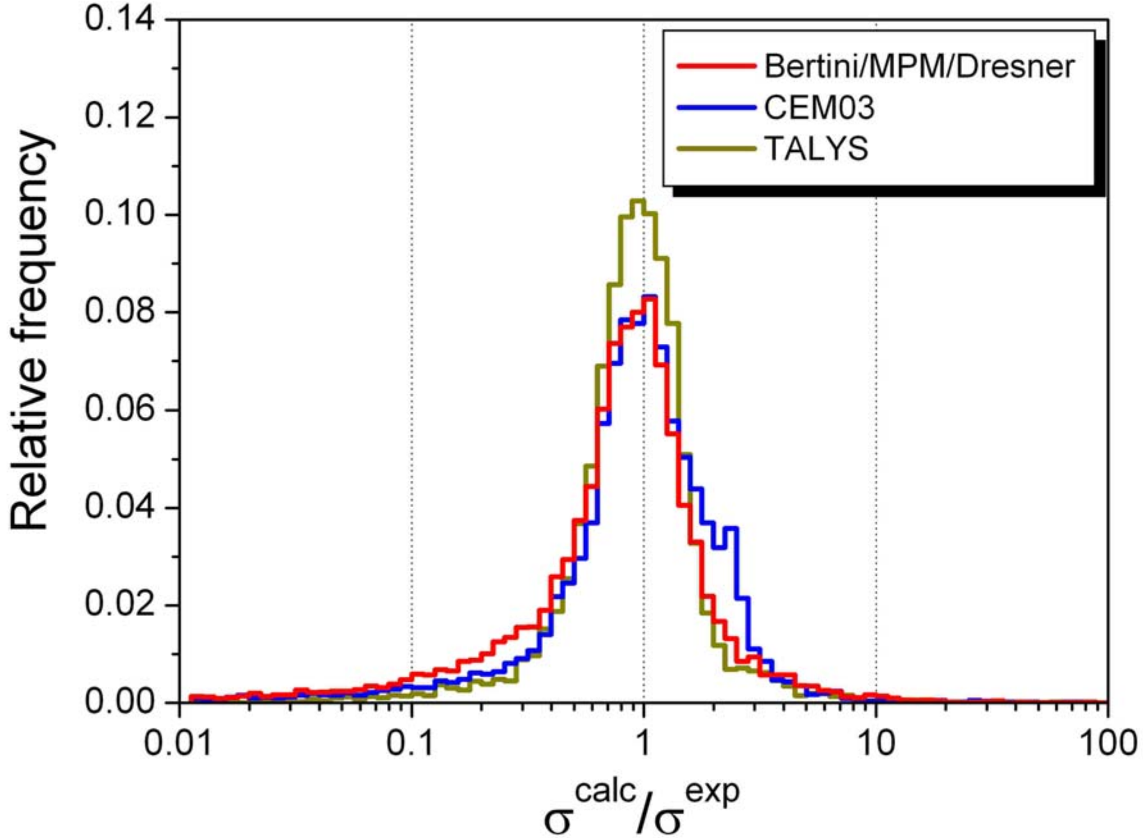
Example

Factors	Bertini/MPM/ Dresner	CEM03	TALYS
H	49.8	28.0	14.2
D	0.85	0.73	0.53
R^{CE}	1.32	1.31	1.15
<F>	3.17	3.15	2.21
N_{calc}/N_{exp}	1.00	0.98	1.00
B	5.0	2.8	1.0

(p,x) reactions, Z=12-83, E_p=20-150 MeV

Visualization

Example



Conclusion

For the comparison of various sets of calculations with measured data can be used deviation factors:

$H, R^{CE}, R^{EC}, D^{CE}, D^{EC}, F, \langle F \rangle, S, L,$

values

$P_x, N_{calc}/_{Nexp}, C_H, C_F, C_S$

product of factors

$B = H\langle F\rangle/(H_{ref}\langle F\rangle_{ref})$ or $H\ S\ /(H_{ref}\ S_{ref})$

The promising ones: S –factor, B

Karlsruhe Institute of Technology

Mann-Whitney test

Is the difference between two set of calculations statistically significant ?

Factors	ISABEL/MPM/ Dresner	ISABEL/MPM/ ABLA
H	43.4	47.1
D	0.89	1.19
R	1.36	1.80
F	3.56	3.15
L	0.72	0.73
$P_{1.3}$	0.30	0.29
$P_{2.0}$	0.63	0.59
$P_{10.0}$	0.93	0.95
N_{calc}/N_{exp}	0.99	0.99

(p,x) reactions, Z=12-83, E_p=20-150 MeV