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Improved Full Bayesian Evaluation of Neutron-induced Reactions on ^{55}Mn

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EFNUDAT 2010, CERN ID29

Work supported by EURATOM via the F4E grant F4E-GRT-014 NUDATA_FILES.
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Content

Motivation

Mn-55 is an important component of structural materials used for a future fusion facility as well as for fission reactors and currently discussed accelerator driven systems (ADS).

There are two demands to the nuclear data community
- Extension of the energy range up to about 150 MeV
- Inclusion of uncertainty information in form of cross section uncertainties

PROBLEM
The generation of reliable covariance matrices is still an open Question and therefore a topic of research regarding
- Development of methods
- Validation of reliability

Concept of Nuclear Data Evaluation

Concept:

Nuclear Data Evaluation should provide a consistent set of cross section and spectral data and associated uncertainty information. At present it is well accepted that consistency can be best achieved via application of Bayesian statistics.

Development of
FULL BAYESIAN EVALUATION TECHNIQE

Characteristics:

- Evaluation fully based on Bayesian statistics
- Consistent inclusion of apriori knowledge associated with nuclear model
- Inclusion of Model defects in the prior
- Inclusion of proper covariance matrices of experiments
- Proper treatment of systematic errors

The Full Bayesian Evaluation Technique

Bayesian statistics:

sum rule: $p(\underline{x}|M) + p(\overline{\underline{x}}|M) = 1$

product rule: $p(\underline{x}|\underline{\sigma}\, M)\, p(\underline{\sigma}|M) = p(\underline{\sigma}|\underline{x}\, M)\, p(\underline{x}|M)$

Bayes Theorem (1763):

$$p(\underline{x}|\underline{\sigma}\, M) = \frac{1}{p(\underline{\sigma}|M)}\, p(\underline{\sigma}|\underline{x}\, M)\, p(\underline{x}|M)$$

updated probability distribution of the set of parameters

likelihood function, from experiment

PRIOR

$p(\underline{x}|\underline{\sigma}\, M)$

.... probability distribution of parameters $\underline{x}$ for a given model M and data $\underline{\sigma}$

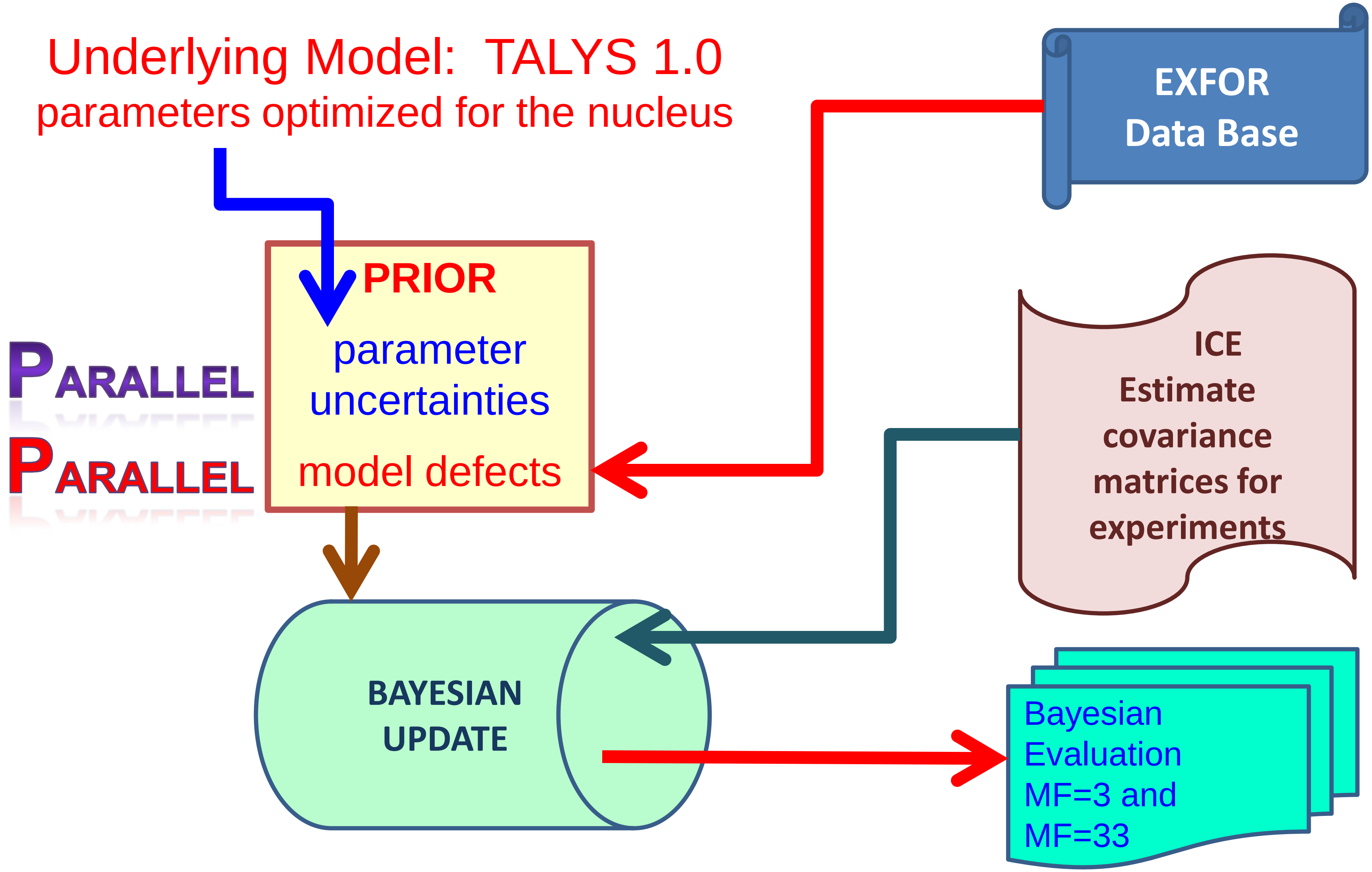
$p(\underline{\sigma}|\underline{x}\, M)$

.... probability distribution of data $\underline{\sigma}$ for a model M with parameters $\underline{x}$

$p(\underline{x}|M)$

.... probability for the ocurence of $\underline{x}$ when M is true

Evaluation Tool - GENEUS



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Objective of the present work

Application of the Full Bayesian Evaluation Technique to neutron-induced cross sections of ^{55}Mn

Status reported at the ND2010 Conference

At the ND2010 in Jeju (April 2010) a first application of the Full Bayesian Evaluation Technique (GENEUS 0.0) on neutron-induced cross sections of Mn-55 was presented. It differed from previous evaluations by following features

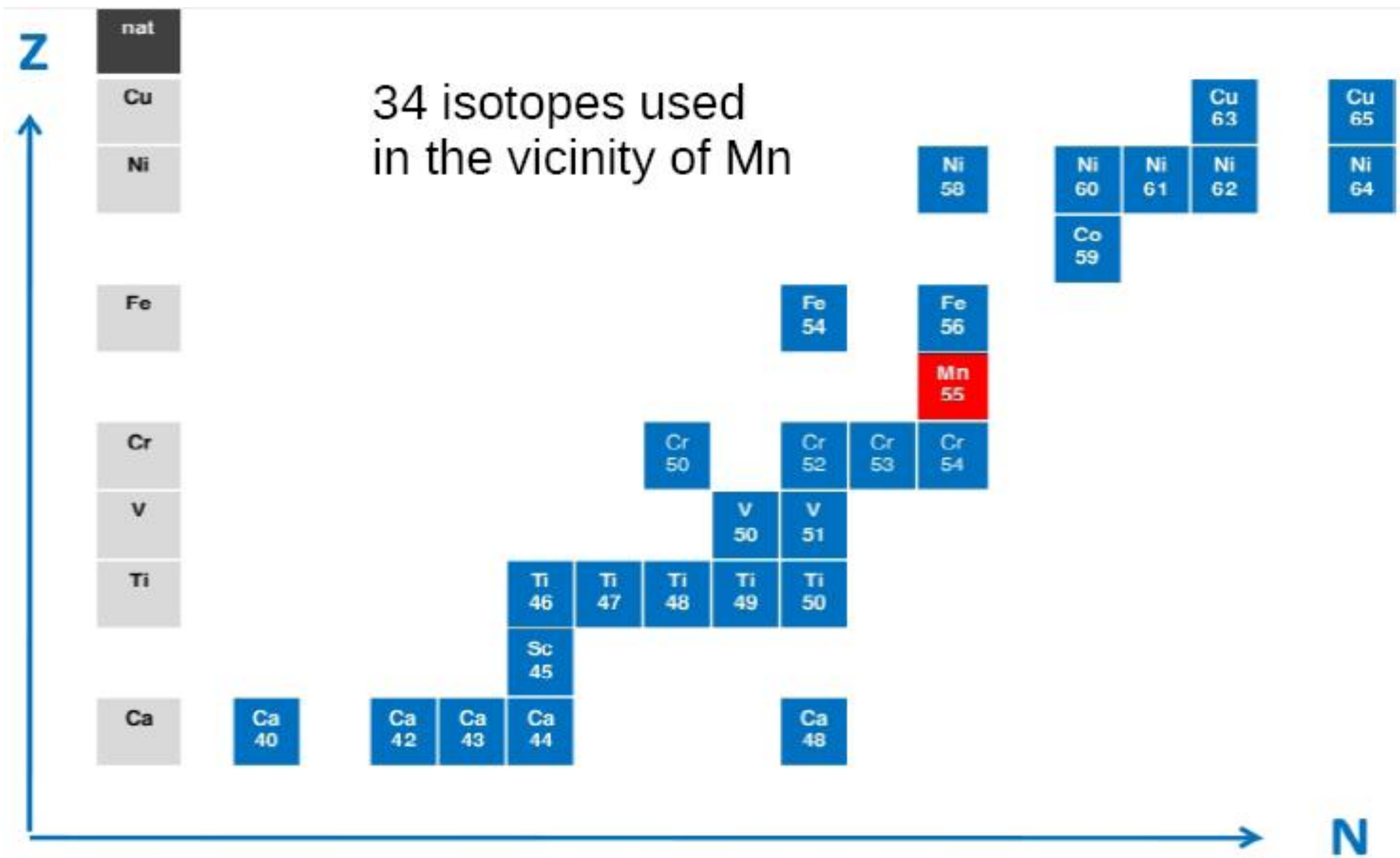
- Model Defects included,
- Estimate of experimental covariance matrices included,
- Cross experiment correlations included.

Advances in the meantime

- Uncertainties of p-, d- and α-nucleus optical potential parameters included
- Uncertainties in the level densities included
- Improved extrapolations of model defects in energy regions without experimental cross section data

Choice of Nuclear Model

The code TALYS with slightly different optical model and level density parameters was used. To optimize the parameters the cross section data of neighboring nuclei (not ^{55}Mn) were used.



Model Parameters

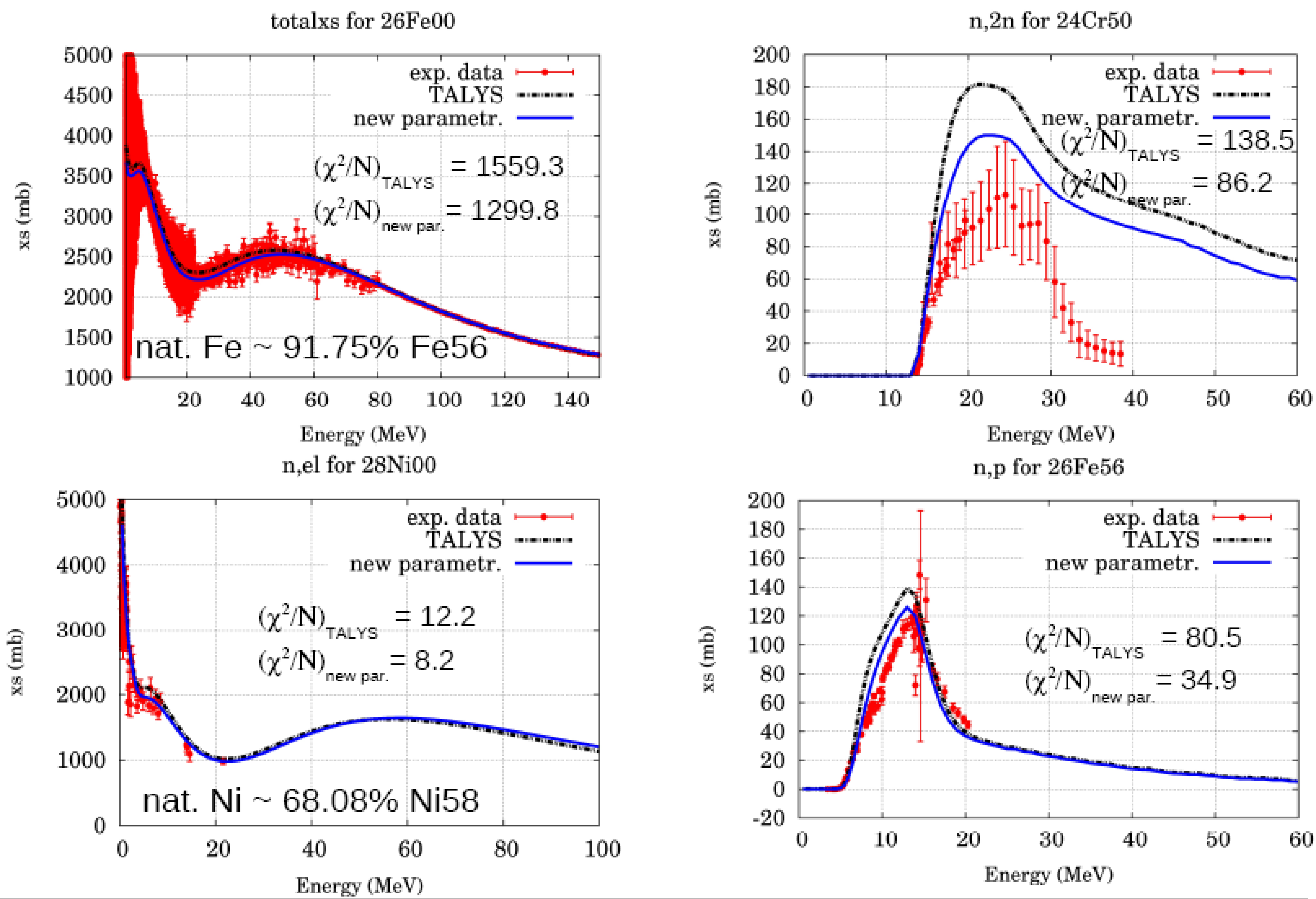
Parametrisation form of optical potential of Koning and Delaroche and level Densities (CTM – TALYS) have been used.

Optimisation on the cross sections of neighboring nuclei (40<A<60)

lane term in neutron opt. model:		level density parameters for CTM model:
$d_1 = 19.59 - 64.95\,\frac{N-Z}{A}$		$\alpha = 0.026220$ $\beta = 0.270416$ $\gamma_1 = 0.456296$
$d_1 = 16.0 - 16.0\,\frac{N-Z}{A}$	TALYS	$\alpha = 0.0207305$ $\beta = 0.229537$ $\gamma_1 = 0.473625$

channel:	n,tot	n,non	n,el	n,inl	n,2n	n,p	n,α
Nr. of isotopes	23	8	21	15	14	24	15
Nr. of data points	200162	173	2151	1666	1259	2498	772

Descriptive power of the model



Determination of Prior

Nuclear model calculations are used to determine the PRIOR:

The contributions to the covariance matrix of the model are:

$$M^{(mod)} = M^{(par)} + M^{(num)} + M^{(def)}$$

Parameter uncertainties

Numerical implementation errors

neglected

Deficiencies of the model, is of non-statistical nature

Method and code based on complete ignorance and transformation group invariance developed by Pigni and Leeb

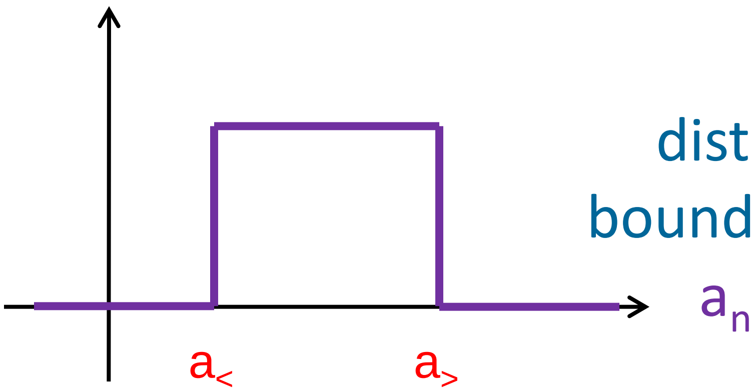
Improved method developed and first application to ^{55}Mn

Parameter uncertainties

In comparison to the evaluation presented at ND2010 we considered a wider class of nuclear models

- neutron optical potential
- proton-, deuteron- and alpha-optical potential
- level density

Probability density distribution

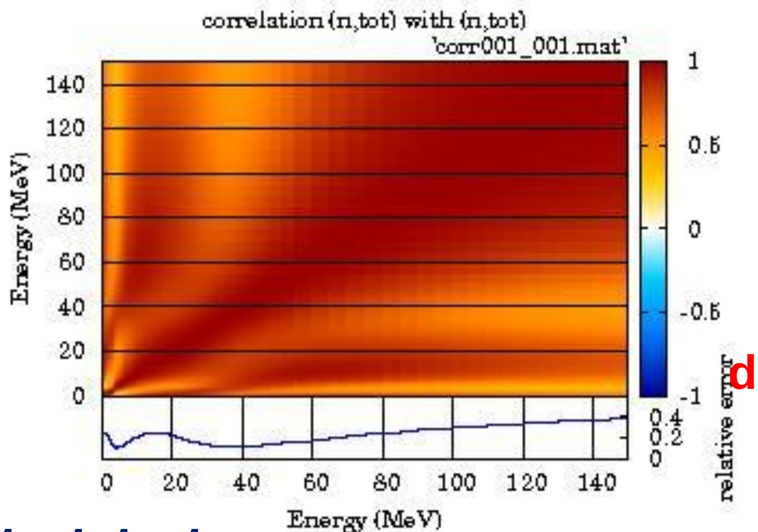


Assumption of equally distributed parameter values
boundaries are more important

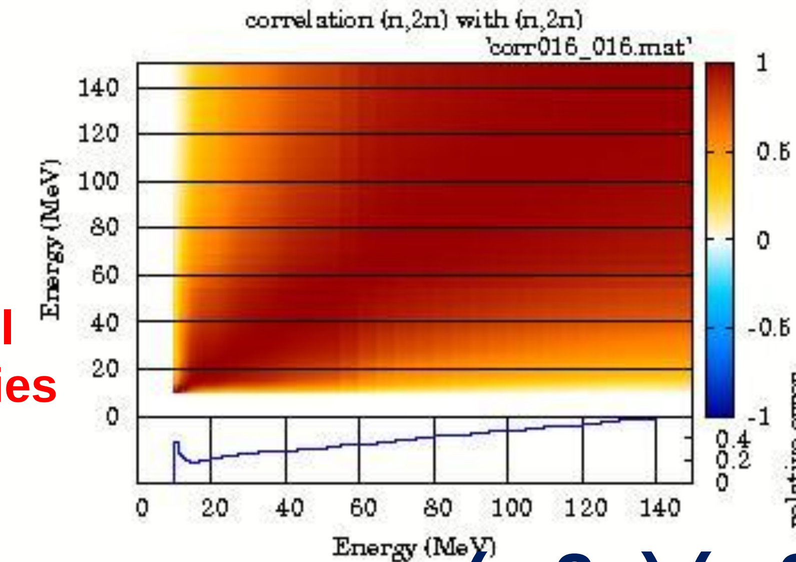
Simple probability sufficient for prior determination

Important: choice of physical and mathematical boundaries

Effect of increased parameter space

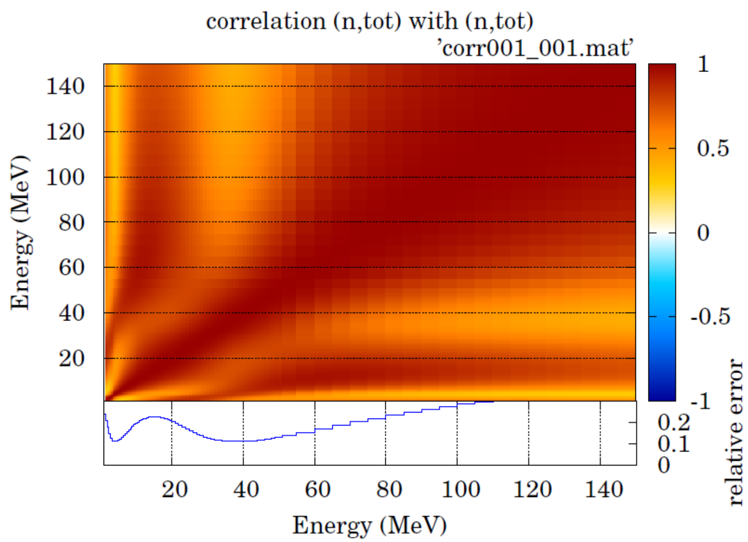


n,p,
d,α
+
Level
densities

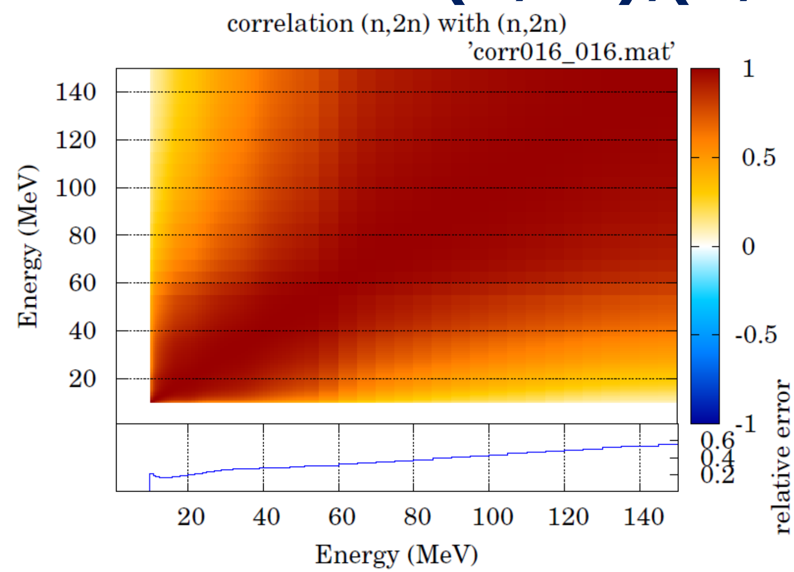


tot,tot

(n,2n),(n,2n)



only
n



Formulation of Model Defects

Basic idea: introduction of scaling factor for each channel *c* with a scaling factor per isotope *(n)*

$$D^{(c)} = \frac{1}{N}\sum_{n=1}^{N}\left\langle D_n^{(c)}\right\rangle$$

$$\left\langle D_n^{(c)}\right\rangle = \sum_{m=1}^{M} w_m^{(c,n)}\left\langle D_n^{(c)}(E_m)\right\rangle$$

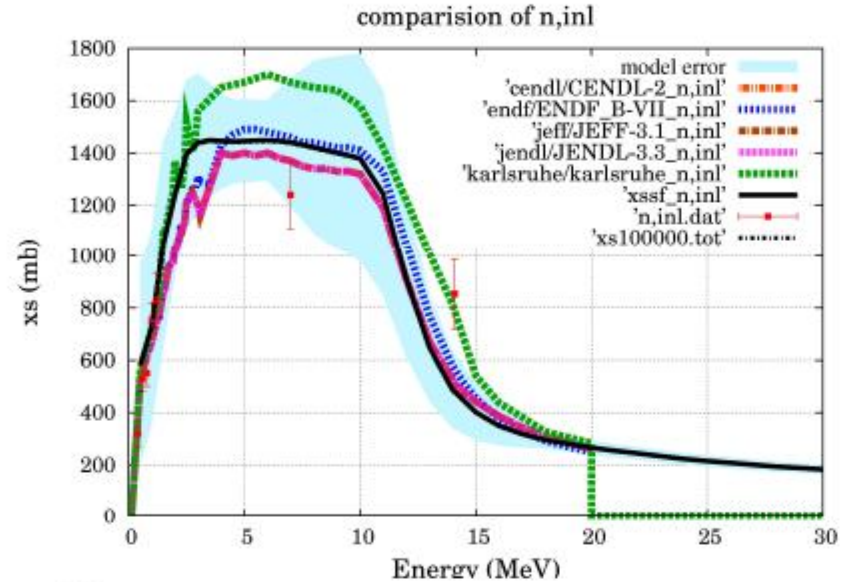
Scaling factor in the energy bin *M*

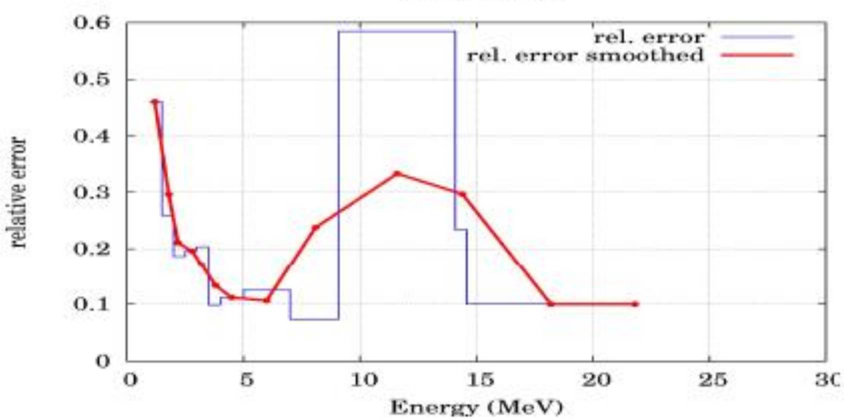
$$\left\langle D_n^{(c)}(E_m)\right\rangle = \sum_{j\in E_{bin}(m,n)} w_j^{(c,m,n)}\frac{\sigma_{ex}^{(c)}(E_j)}{\sigma_{th}^{(c)}(E_j)}$$

$$\begin{aligned}\left\langle \Delta^{(c)}(E_m)\Delta^{(c')}(E_{m'})\right\rangle &= \sigma_{th}^{(c)}(E_m)\sigma_{th}^{(c')}(E_{m'}) \\ &\cdot \frac{1}{\sqrt{N^{(c)}(E_m)}\sqrt{N^{(c')}(E_m')}}\sum_{n=1}^{N}\left\{\left[\left(\left\langle D_n^{(c)}(E_m)\right\rangle - D^{(c)}\right)\left(\left\langle D_n^{(c')}(E_{m'})\right\rangle - D^{(c')}\right)\right]\right. \\ &\left. +\delta_{cc'}\delta_{mm'}\left[\left\langle\left(D_n^{(c)}(E_m)\right)^2\right\rangle - \left(\left\langle D_n^{(c)}(E_m)\right\rangle\right)^2\right]\right\}\end{aligned}$$

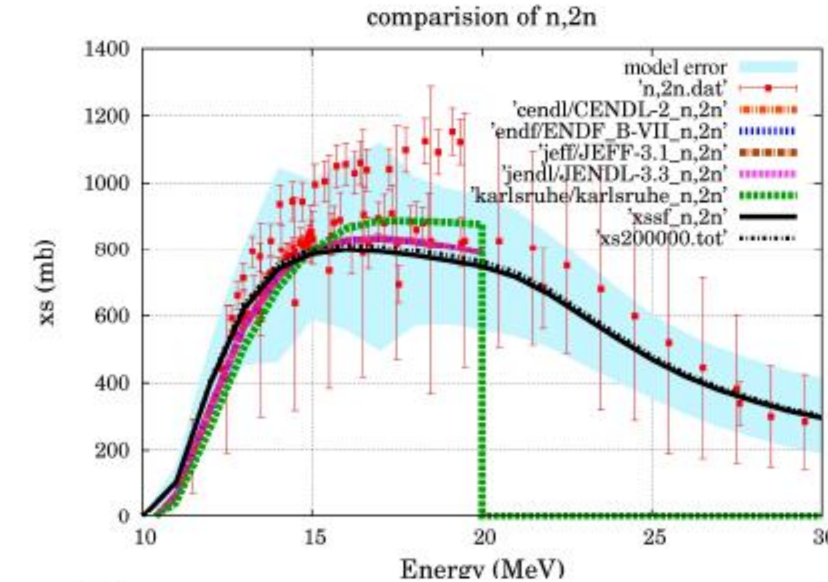
Scaling factors and uncertainties

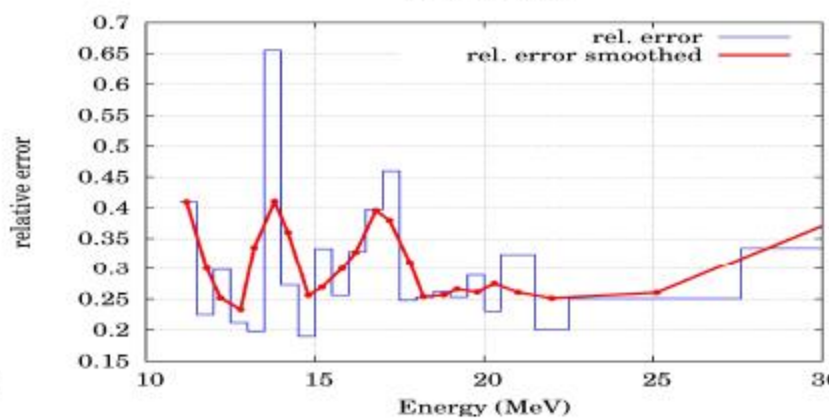
overall scaling factor (n,inl): 1.002





overall scaling factor (n,2n): 0.980





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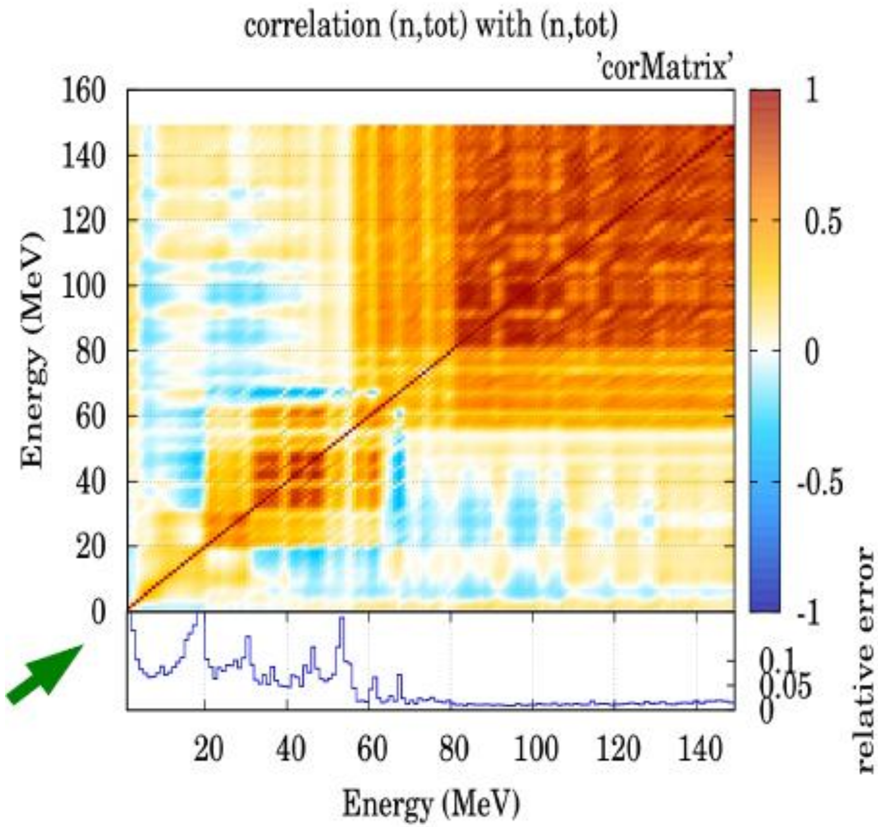
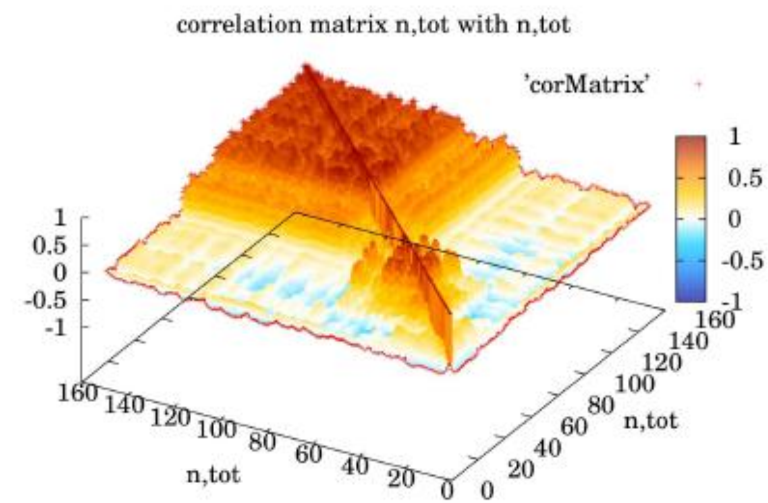
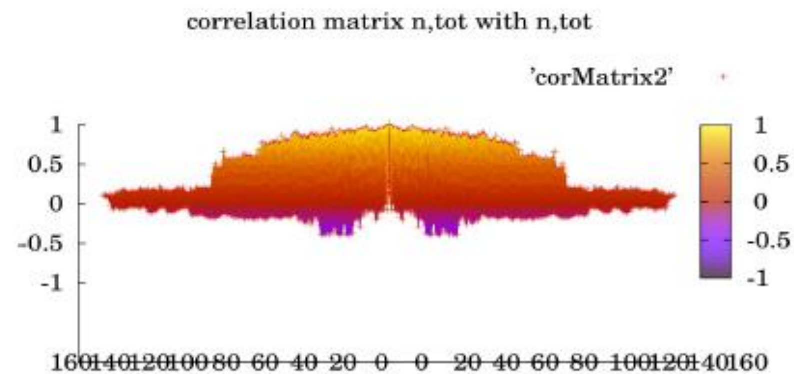
Correlation matrix $<\sigma_{tot}(E)\sigma_{tot}(E')>$



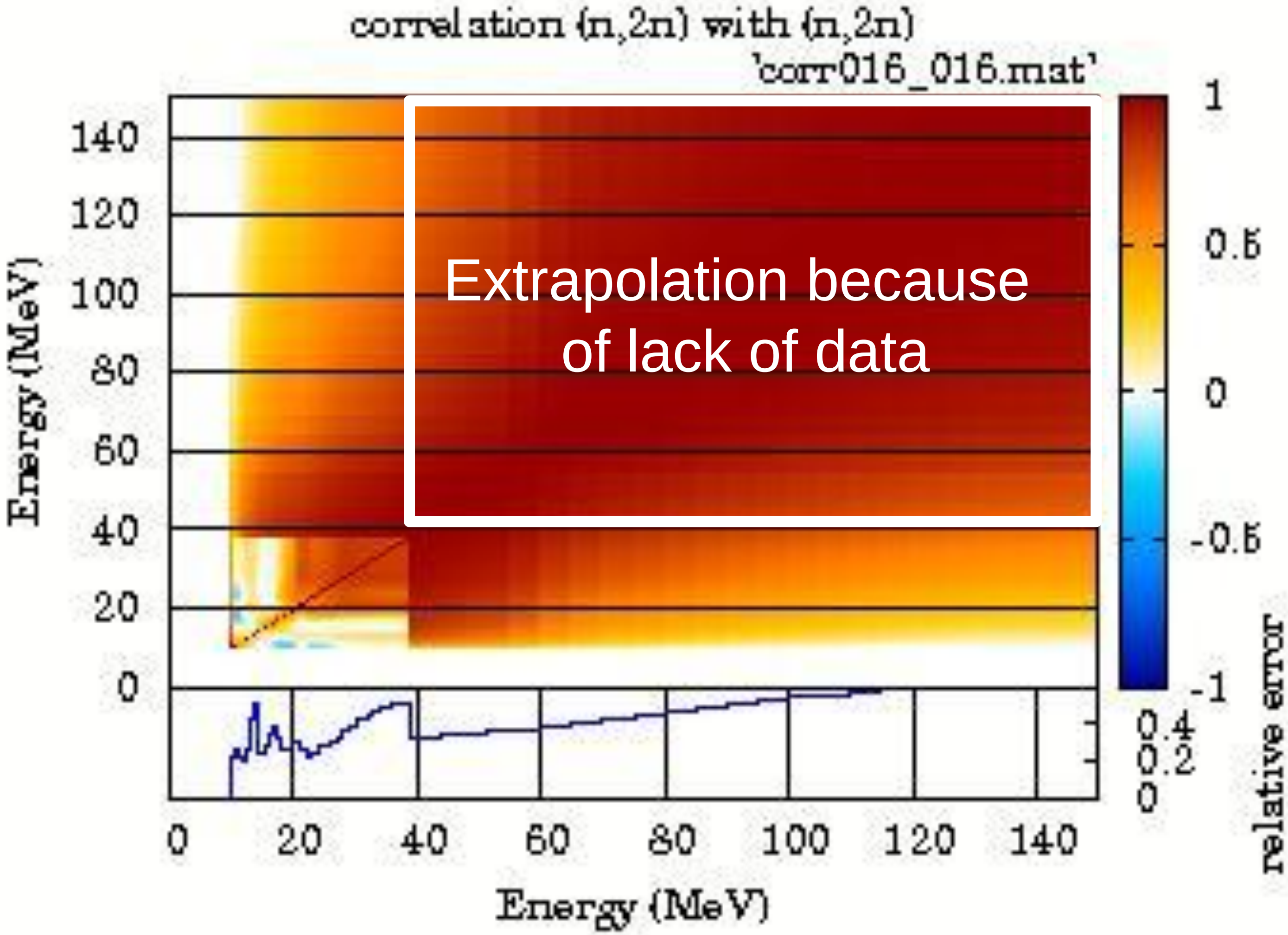




$E_m + E_{m'} = \text{const.}$

Problems with limited data

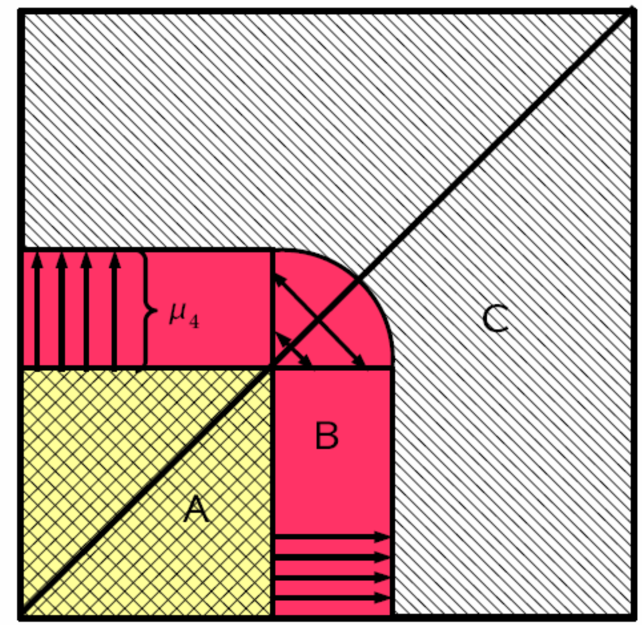
(n,2n) – (n,2n) correlation matrix



Extrapolation of Model Defects

C correlations

Phenomenological extrapolation in area *C*



$$C^{(c)}\left(E_m, E_{m'}\right) = 1 - \mu_1 + \mu_1 \exp\left(\mu_2\left(\frac{E_> - E_<}{E_>}\right)^{\mu_3}\right)$$

with
$$E_< = \min\left(E_m, E_{m'}\right)$$
$$E_> = \max\left(E_m, E_{m'}\right)$$

$$\mu_4 = E^{C,\min} - E^{A,\max}$$

Interpolation

$$C\left(E_m^B, E_{m'}^B\right) = C^C\left(E_m^B, E_{m'}^B\right)\frac{r}{r_{\max}} + C^{li}\left(E_m^B, E_{m'}^B\right)\left(1 - \frac{r}{r_{\max}}\right)$$

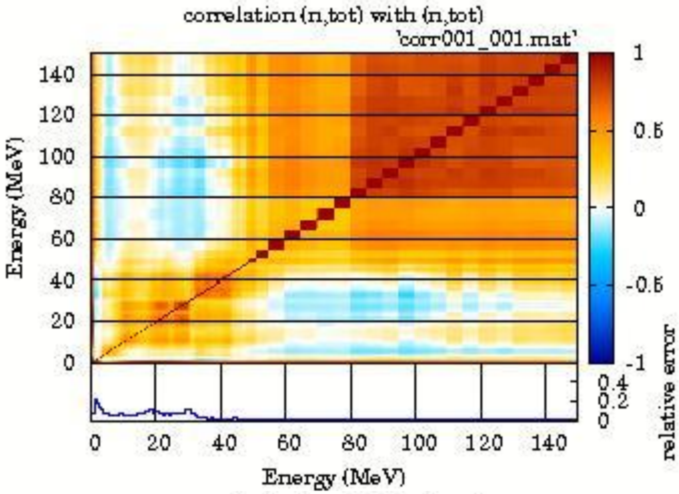
with $r_{\max} = \sqrt{2}\mu_4$ and $r = \sqrt{\left(E_m - E^{A,\max}\right)^2 + \left(E_{m'} - E^{A,\max}\right)^2}$

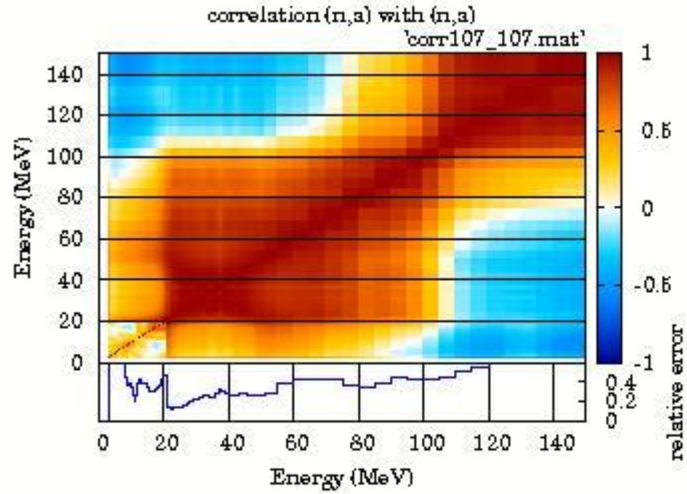
Impact of improved extrapolation

total cross section

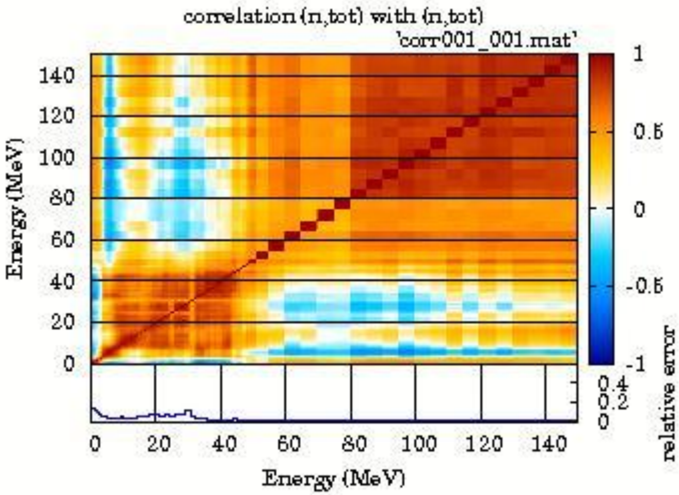
(n,α) cross section

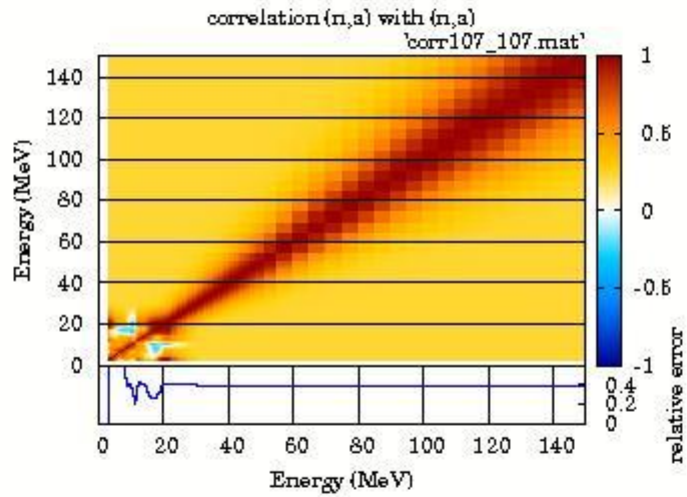
OLD





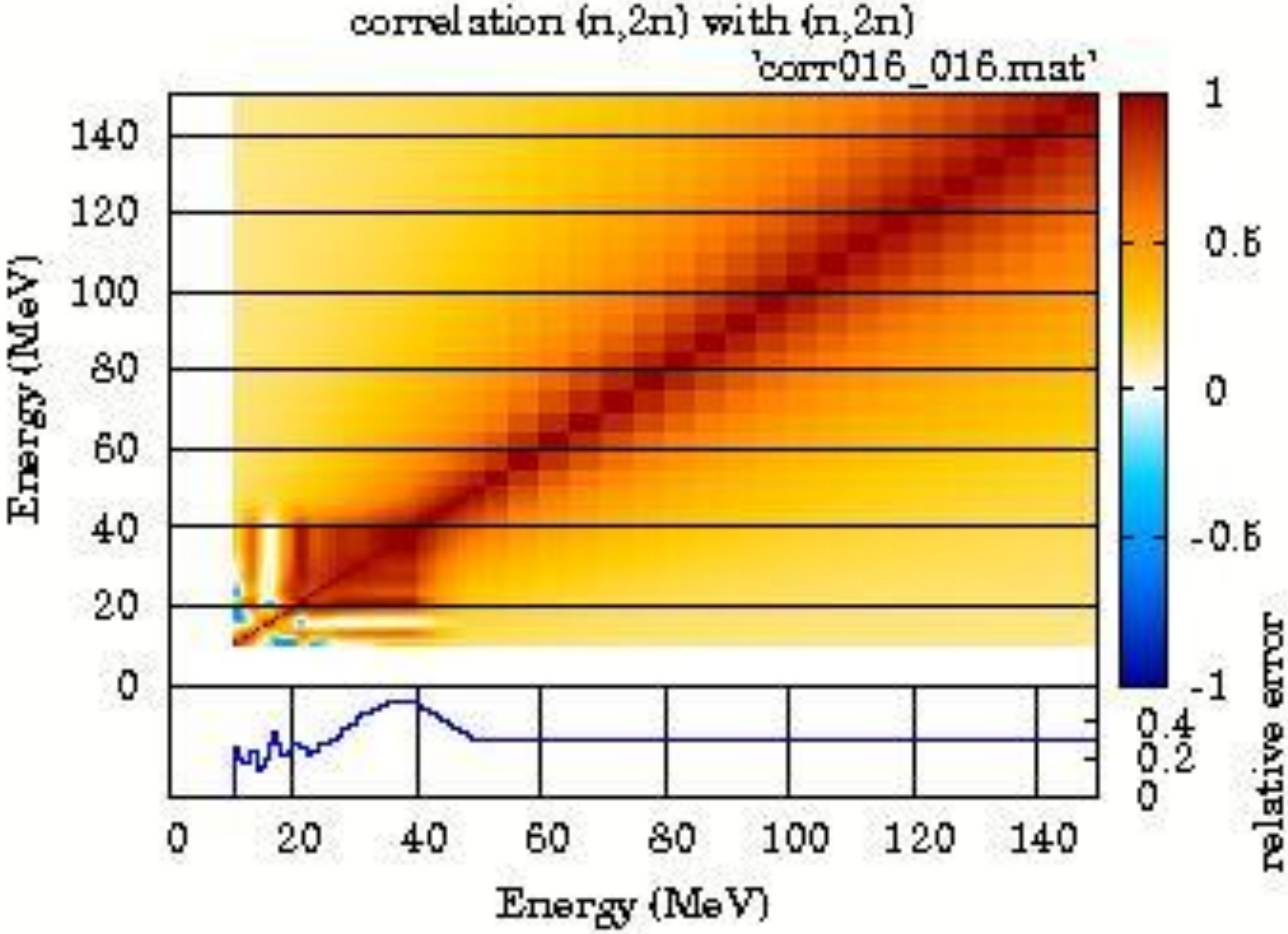
NEW





Model defects: (n,2n) reaction

edge because of lack of data



Combination to complete prior

$$\text{Rescaling - ansatz } \sigma_0^c = D^{(c)} \sigma_{th}^c$$

$$M_0^{(cc')}(E_m, E_{m'}) = D^{(c)} \underbrace{\left\langle \Delta\sigma_{th}^{(c)}(E_m)\, \Delta\sigma_{th}^{(c')}(E_{m'}) \right\rangle D^{(c')}}_{\text{Parameter Uncertainties}}$$

$$+ \underbrace{\sigma_{th}^{c}(E_m) \left\langle \Delta D^{(c)}(E_m)\, \Delta D_{th}^{(c')}(E_{m'}) \right\rangle \sigma_{th}^{c}(E_{m'})}_{\text{Model Defects}}$$

$$M^{(prior)} = M^{par} + M^{def}$$

Analysis of experiments

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	EXFOR number	reaction channel	number of data points	source of information	quantity of information	block assignment
Block 1	13753.018	total	467	[1]	high	1
	10047.031	total	248	[21]	high	1
	11308.008	total	30	[46]	high	1
	20169.002	total	62	[39]	medium/scarce	1
	30463.042	elastic	1	[50]	high	1
	20019.081	elastic	8	[27]	high	1
Block 3	31458.005	$(n,2n)$	1	[38], [30]	scarce	3
	30400.005	$(n,2n)$	1	[14]	medium	3
	20109.003	$(n,2n)$	1	[52]	high	3
	12936.006	$(n,2n)$	7	[4]	medium	3
	11421.005	$(n,2n)$	10	[40]	high	3
	22292.006	$(n,2n)$	3	[11]	high	3
	22703.011	$(n,2n)$	28	[58]	high	3
	41298.011	$(n,2n)$	1	[18]	scarce	3
	41240.010	$(n,2n)$	7	[18]	scarce	3
Block 2	30473.003	(n,t)	2	[53]	medium	2
	22335.007	$(n,4n)$	1	[51]	medium	2
	22703.010	$(n,4n)$	6	[58]	high	2

Analysis of each experiment

Each experiment has been considered with regard to uncertainties and reliabilities on the basis of the available literature.

↓

The information was fed into the programme ICE (Interactive Covariance Estimator) to estimate covariance matrices of cross section uncertainties for each experiment

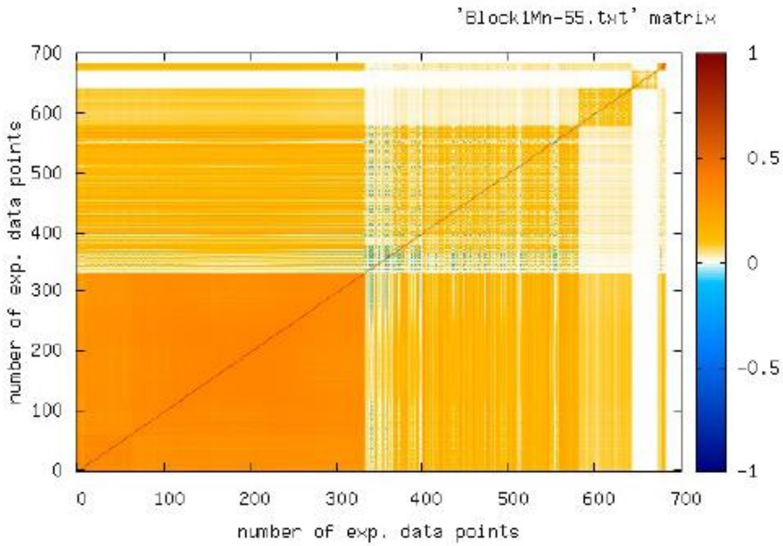
↓

Generate a full covariance matrix for each block in order to include correlations of data and to avoid statistical treatment of systematic errors.

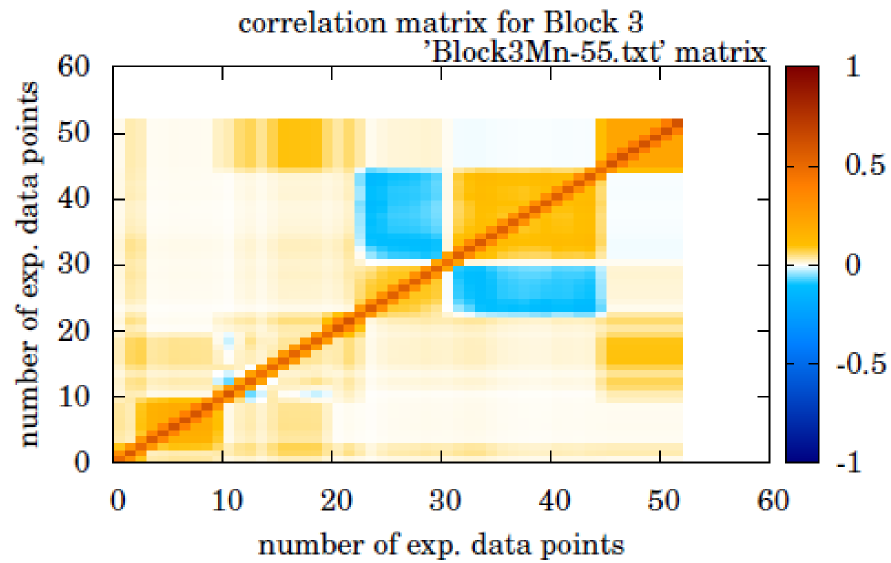
↓

Block Covariance Matrices

Covariance Matrix of Experiments



Block 1
correlation matrix



Block 3
correlation matrix

reference	[1]	[21]	[46]	[39]	[50] + [27]
[1]		0.05	0.05	0.12	0.1
[21]			0.15	0.05	0.05
[46]				0.05	0.01
[39]					0.05
[50] + [27]					

Ref.	[38]	[14]	[52]	[4]	[40]	[11]	[58]	[18]	[18]
[38]		0.5	0.45	0.05	0.3	0.3	0.15	0.23	0.23
[14]			0.2	0.15	0.2	0.25	0.15	0.23	0.23
[52]				0.05	0.2	0.05	0.05	0.05	0.05
[4]					0.1	0.05	0.1	0.15	0.15
[40]						0.2	0.05	0.2	0.2
[11]							0.17	0.33	0.33
[58]								0.2	0.2
[18]									1.0
[18]									

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Available covariance matrices

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Prior covariance matrix:

$$\langle \Delta\sigma_c(E)\,\Delta\sigma_{c'}(E') \rangle_{PRIOR} = \underbrace{\langle \Delta\sigma_c(E)\,\Delta\sigma_{c'}(E') \rangle_{ParUnc}}_{\text{cov.matrix + prob. distr.}} + \underbrace{\langle \Delta\sigma_c(E)\,\Delta\sigma_{c'}(E') \rangle_{ModDef}}_{\text{only cov. matrix}}$$

Covariance matrix of experiments:

$$\langle \Delta\sigma_c(E)\,\Delta\sigma_{c'}(E') \rangle = \underbrace{\sum_{i=1}^{M} \frac{\partial\sigma_c(E)}{\partial E_i} \langle \Delta E_i \Delta E_j \rangle \frac{\partial\sigma_{c'}(E')}{\partial E_j}}_{\text{energy calcibration error}} + \underbrace{\sum_{i=1}^{M} \sigma_c(E) \langle \delta\sigma_c(E_i)\,\delta\sigma_{c'}(E_j) \rangle \sigma_c(E')}_{\text{measurement uncertainties}}$$

Likelyhood function:

$$p(\sigma \mid xM) = \frac{1}{\sqrt{(2\pi)^d \det V}} \exp\left[(\sigma - S_M(x))^T V^{-1} (\sigma - S_M(x)) \right]$$

$V = \langle \Delta\sigma_c(E)\,\Delta\sigma_{c'}(E') \rangle_{Exp}$ experimental covariance matrix

$\sigma_{Model} = S_M(x)$ model value

Bayesian Update Procedure

At present normal probability distributions are assumed
→ linearized expression for Bayes theorem can be applied

$$x' = x + M(1+Q)^{-1}G^T V^{-1}(D-T)$$
$$= x + (M^{-1}+W)^{-1}G^T V^{-1}(D-T)$$

parameter vector

$$M' = M(1+Q)^{-1} = (M^{-1}+W)^{-1}$$

covariance matrix

with $Q = G^T V^{-1} G M = WM$

G sensitivity matrix

Difference to previous approaches:
$V = \langle \Delta\sigma_c(E)\, \Delta\sigma_{c'}(E')\rangle_{Exp}$ contains the covariance matrices of all available correlated experimental data for the system.

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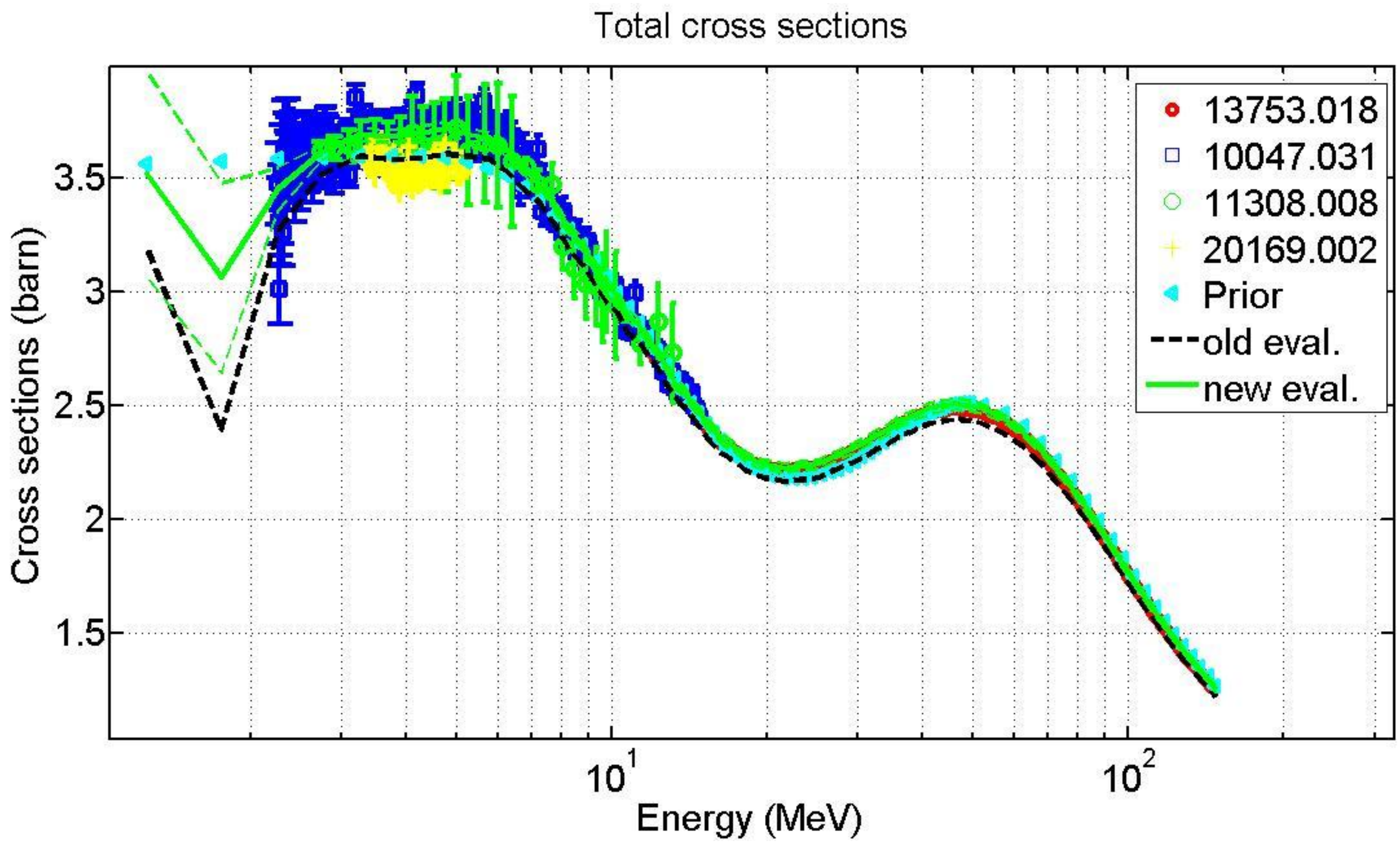
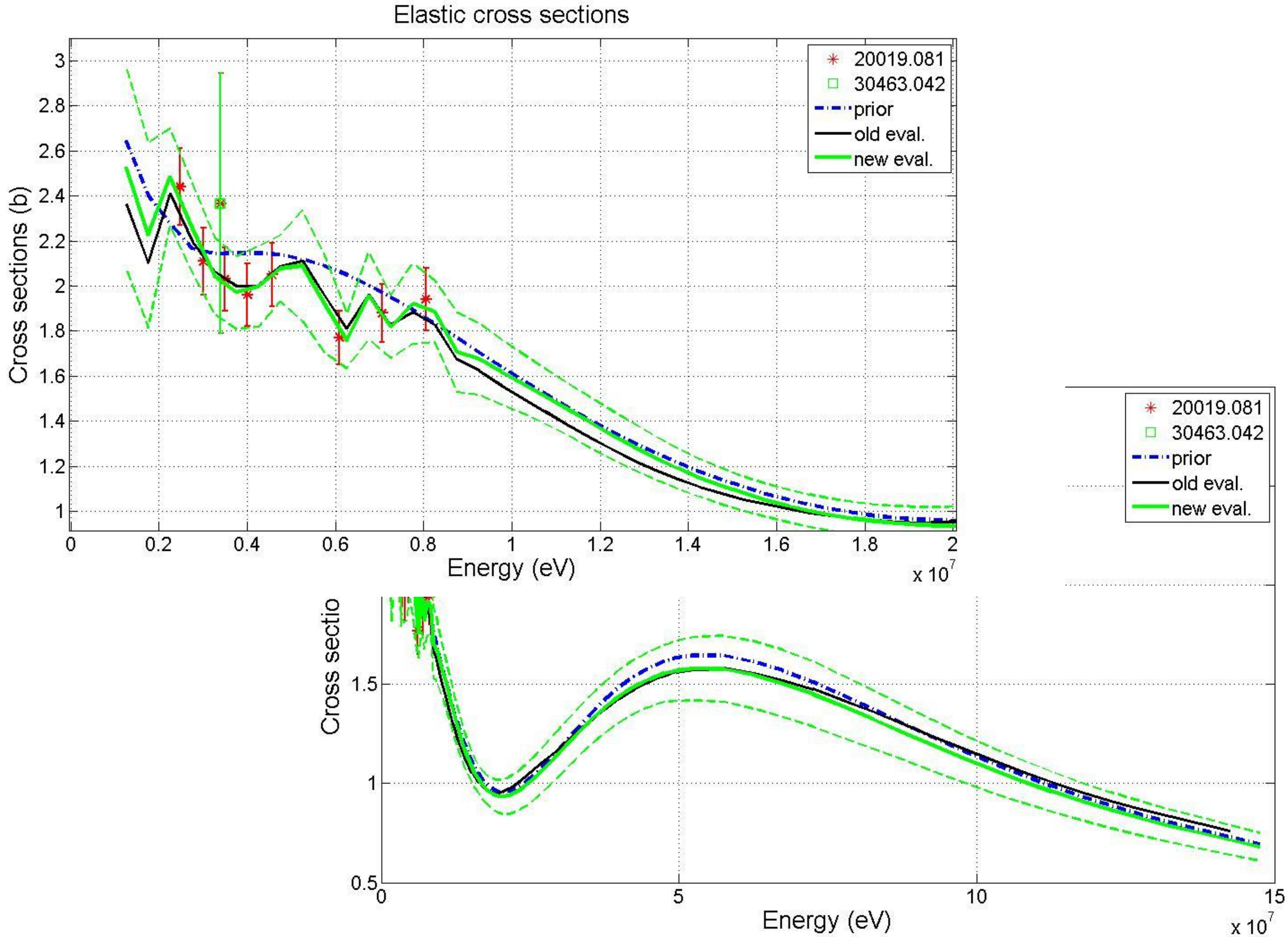
Evaluated σ_{tot}



Evaluated $\sigma_{elastic}$



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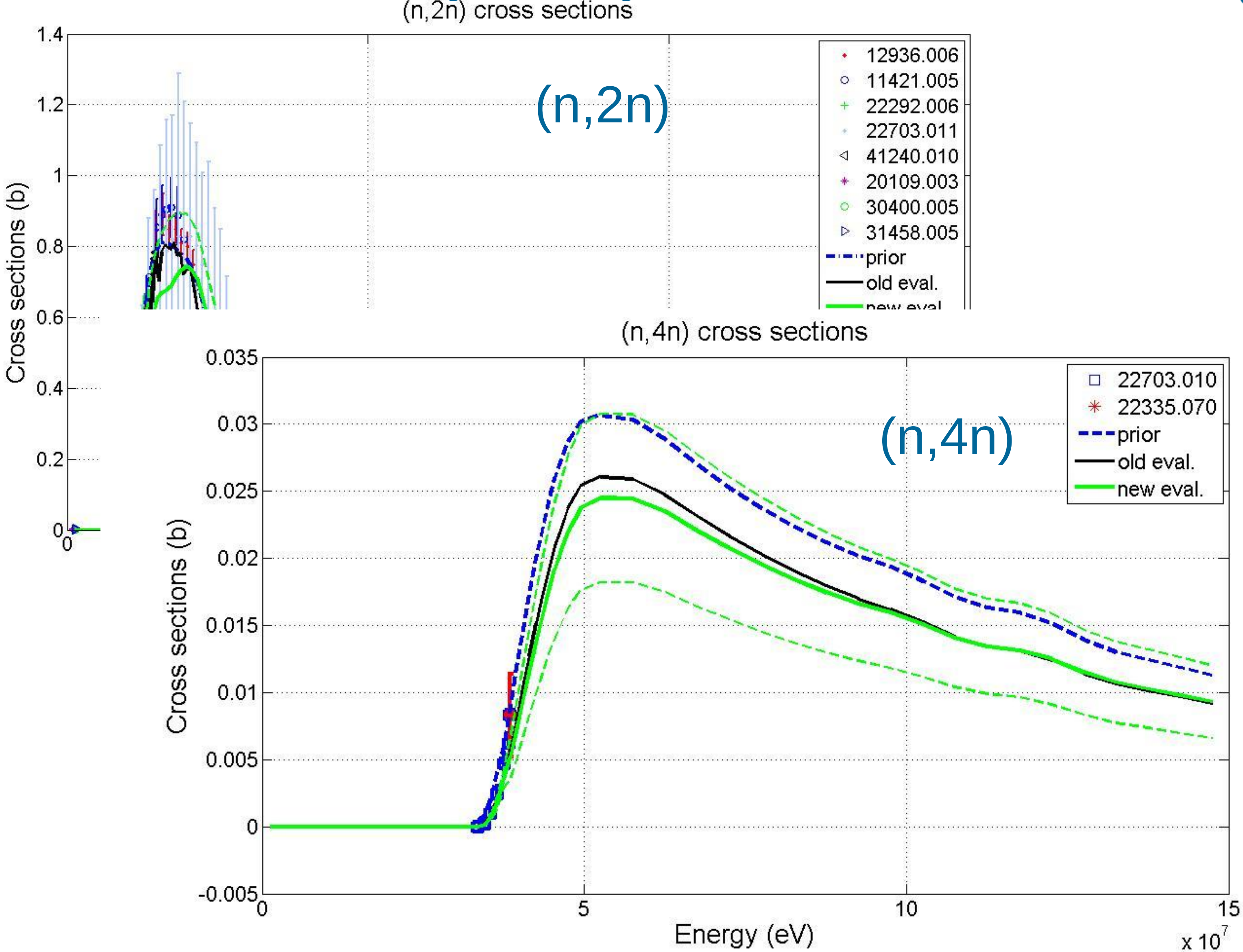
Evaluated (n,xn) cross sections



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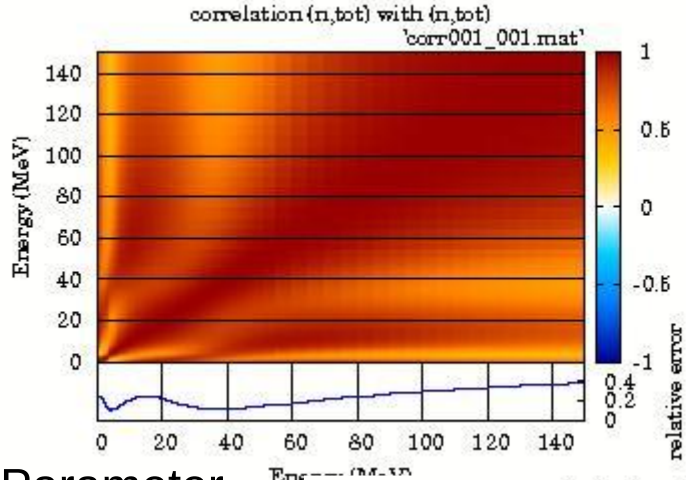
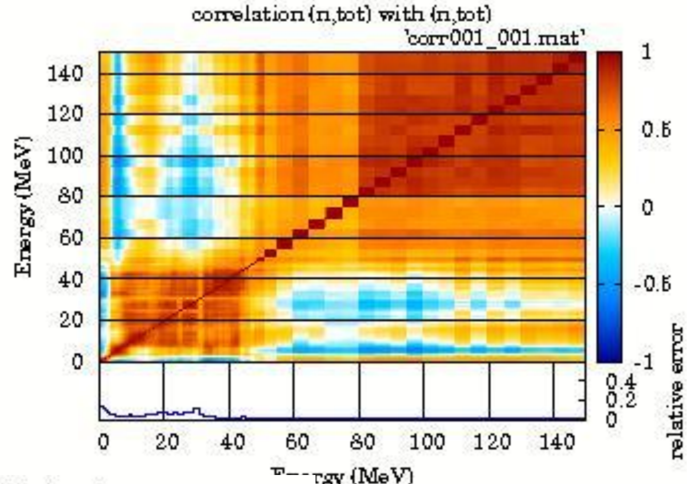
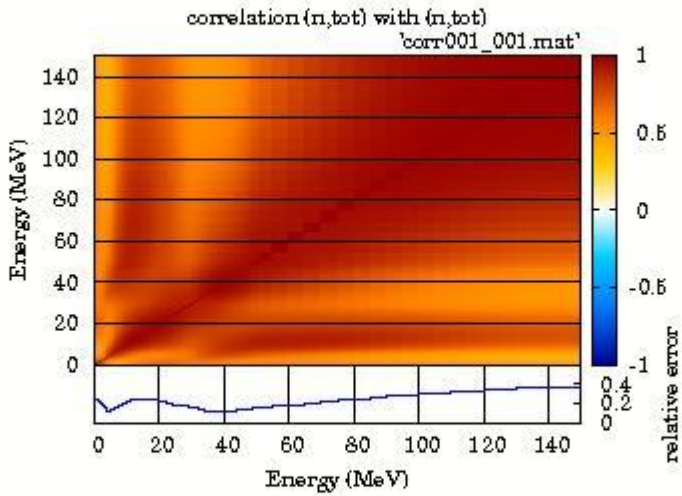
Correlations $<\sigma_{tot}(E),\sigma_{tot}(E')>$





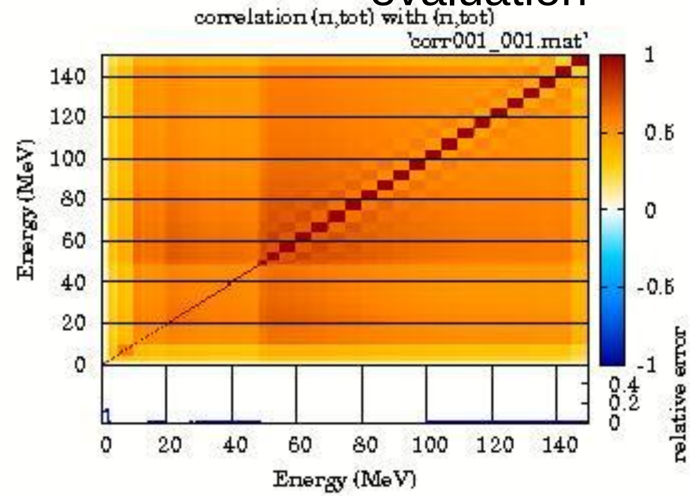
Model defects

Parameter uncertainties

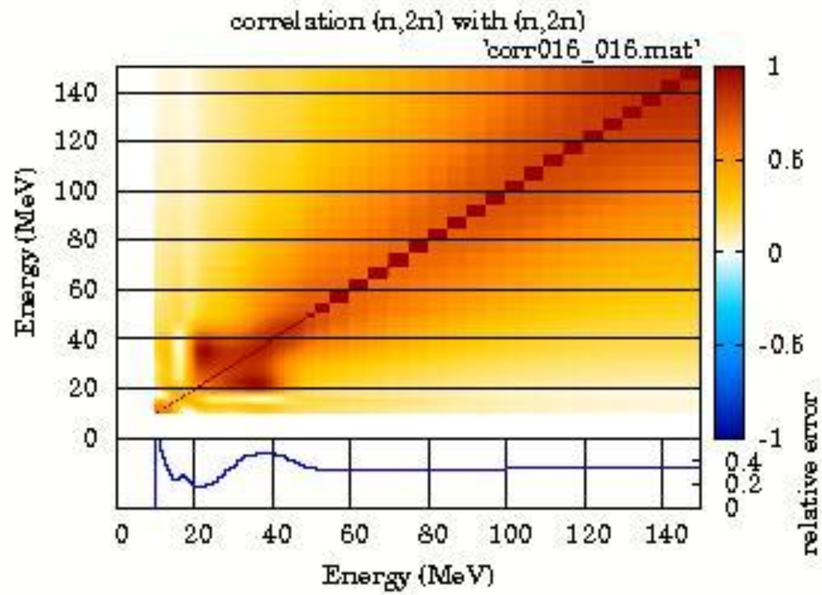


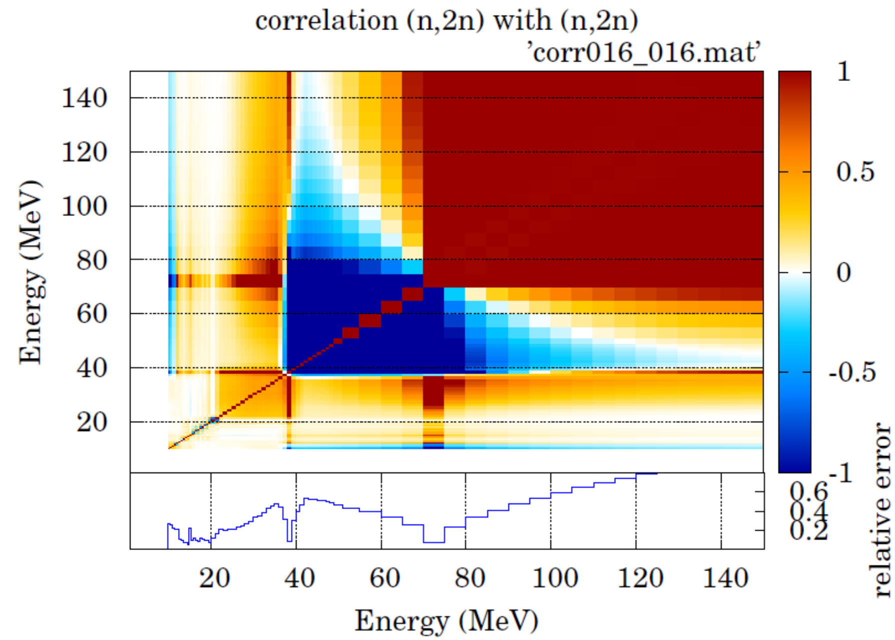
prior

evaluation



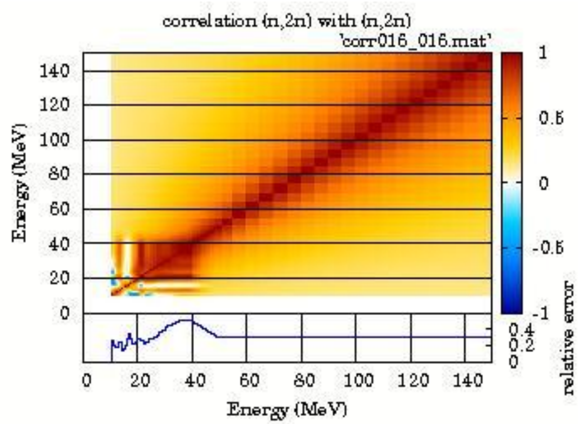
Correlations $<\sigma_{(n,2n)}(E),\sigma_{(n,2n)}(E')>$



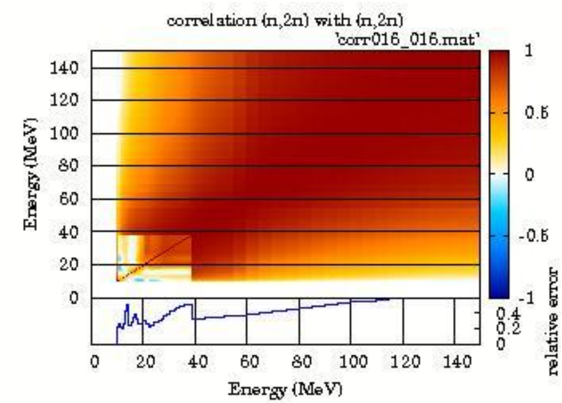


NEW EVALUATION

OLD EVALUATION



model defects



Cross channel correlations

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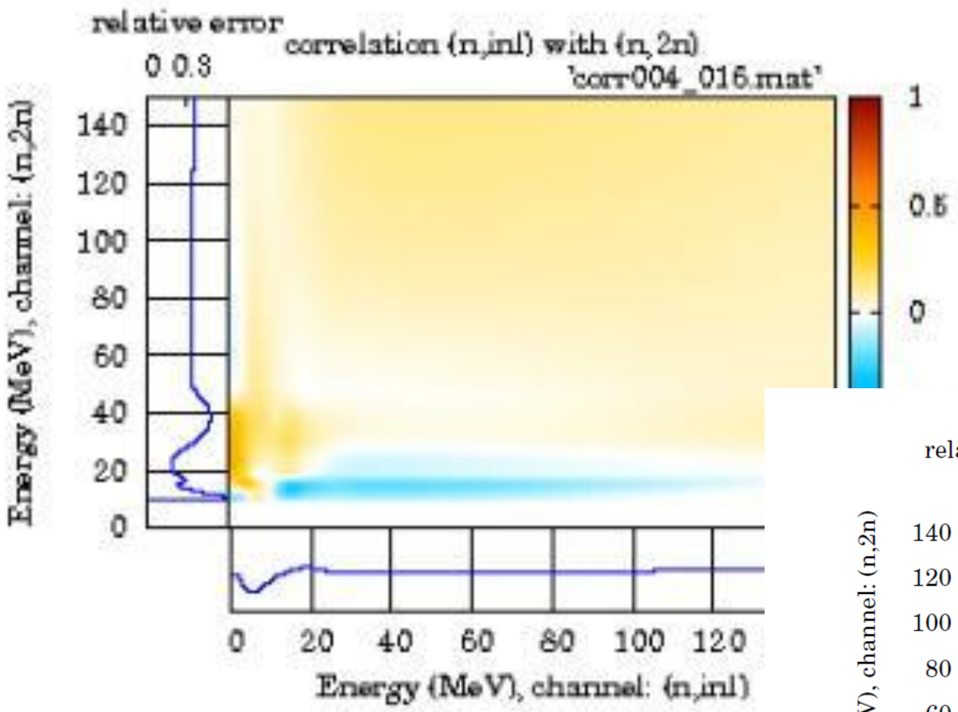
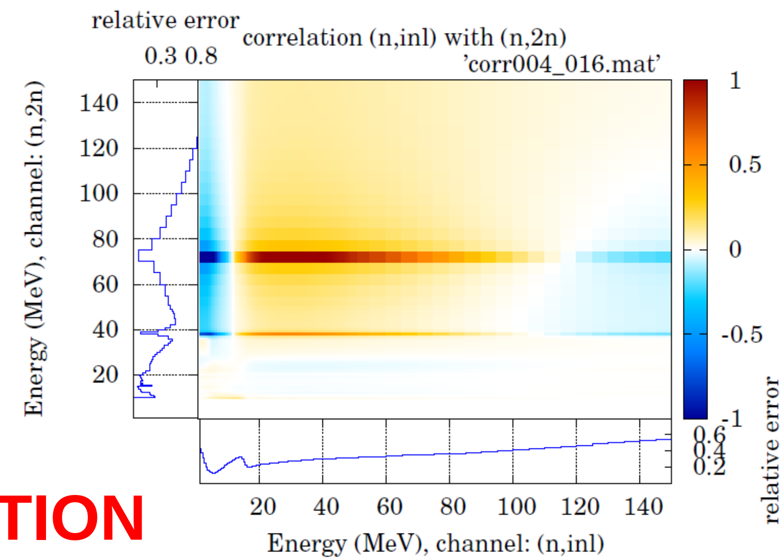
All cross channel correlations have been determined

n,inl – n,2n
NEW EVALUATION





n,inl – n,2n
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Cross channel correlations

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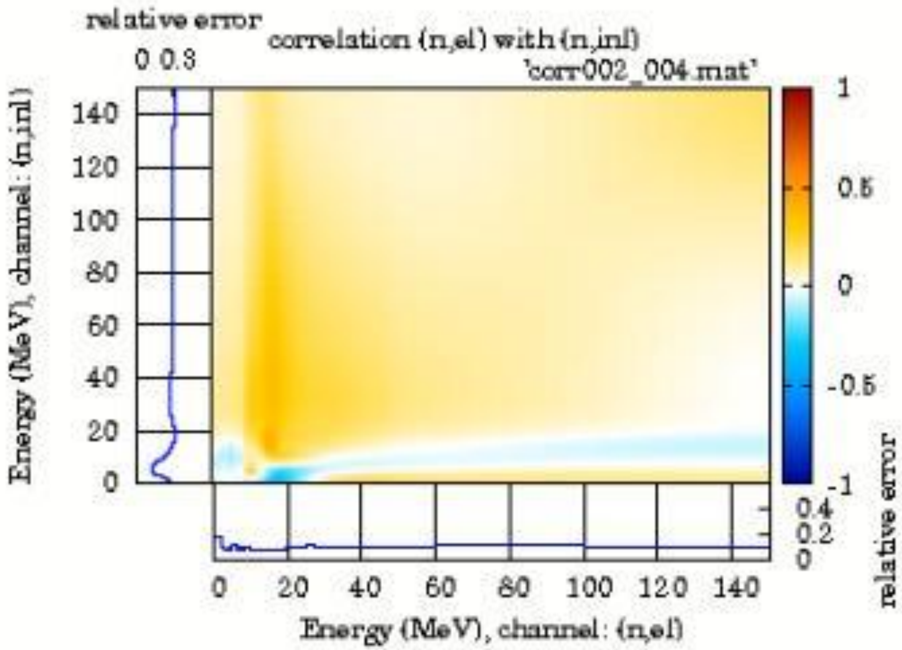
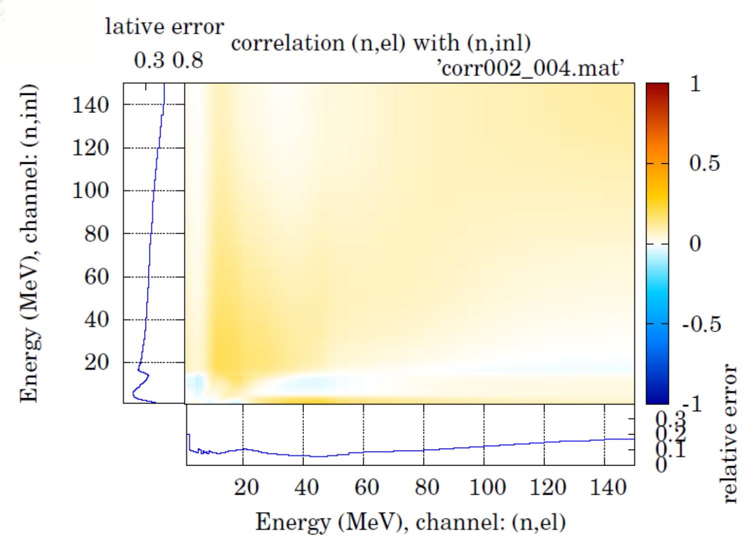


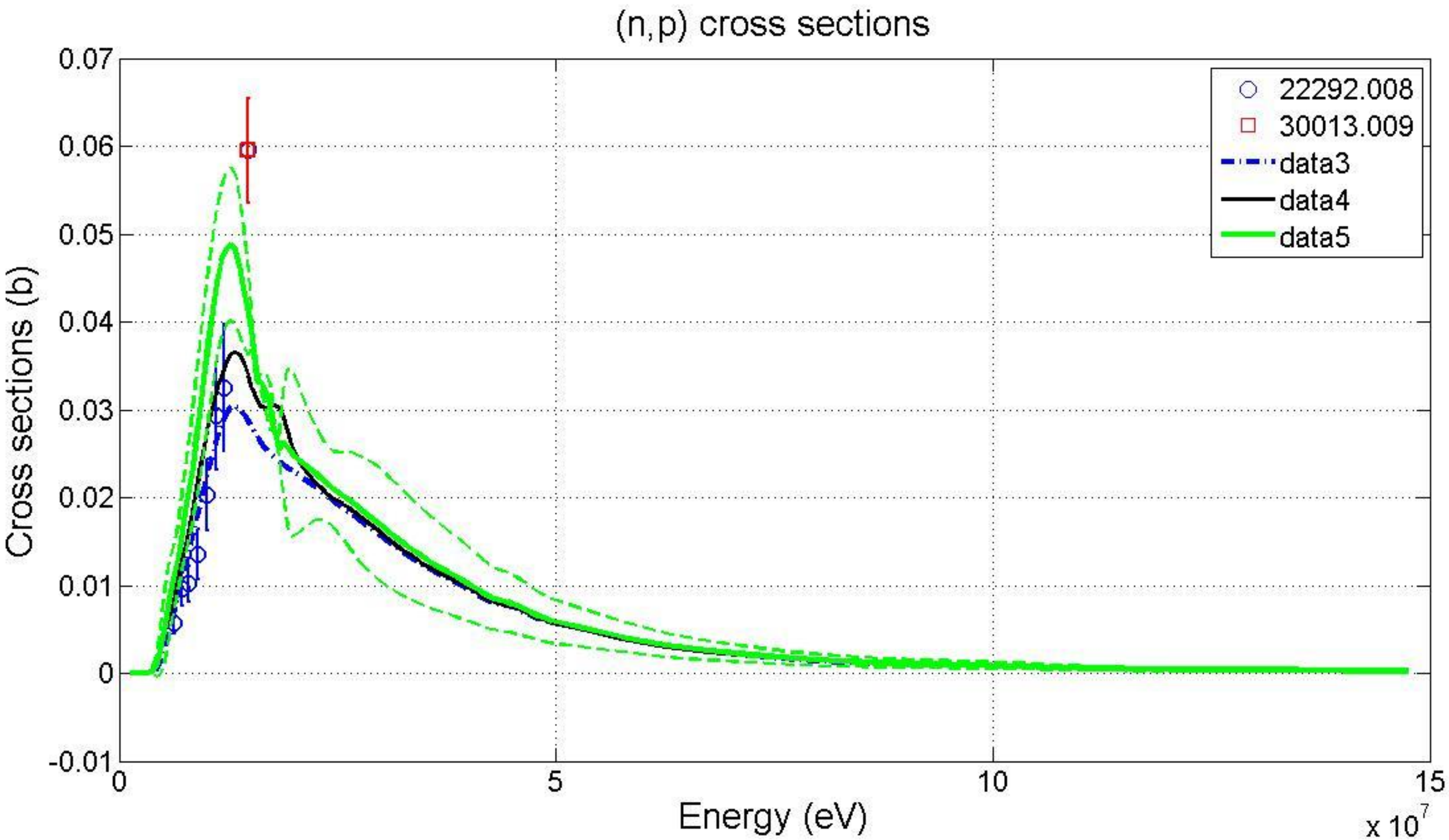
NEW EVALUATION

$<\Delta\sigma_{ela}(E)\ \Delta\sigma_{inl}(E')>$

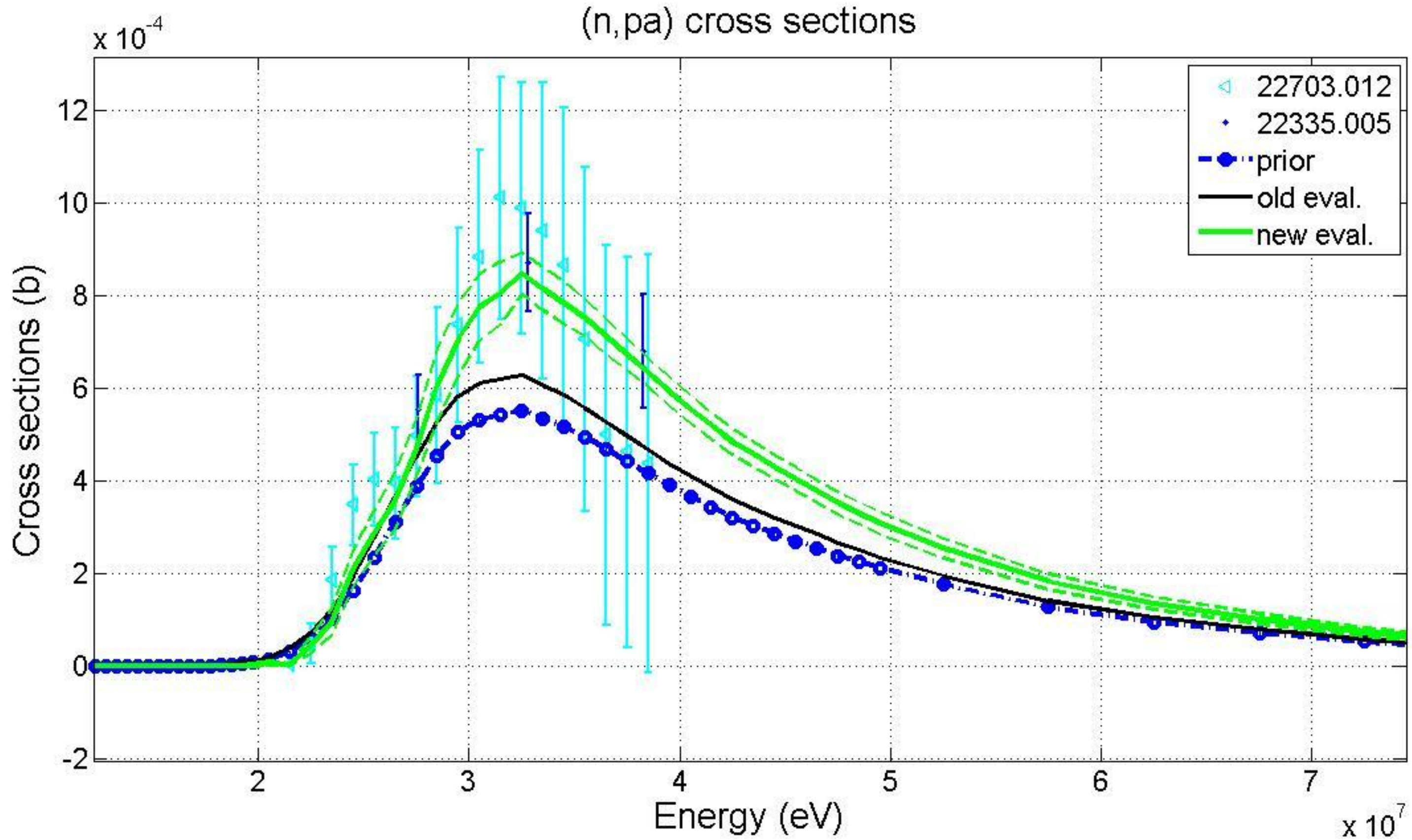


OLD EVALUATION

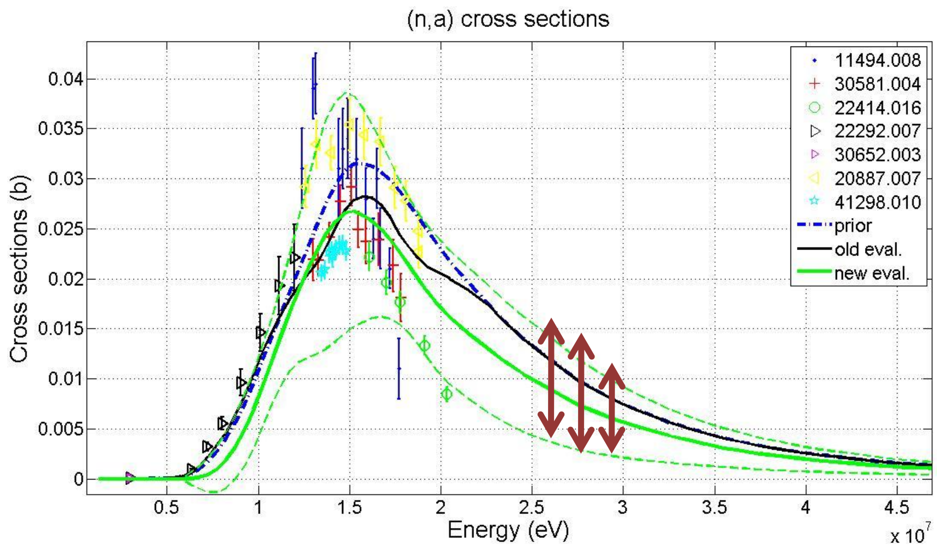
Evaluated (n,p)-cross section



Evaluated (n,pα)-cross section

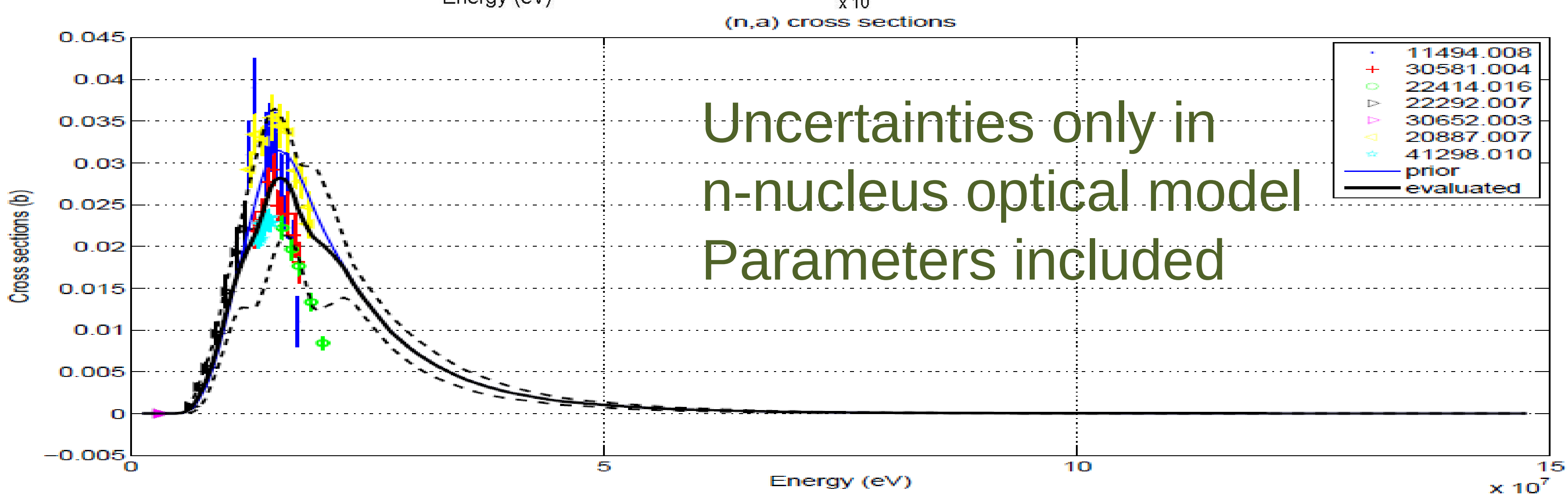


Impact of increased model space



(n,α) cross section

Uncertainties of n-, p-, d-, α-nucleus optical model parameters and level densities included



Uncertainties only in n-nucleus optical model Parameters included

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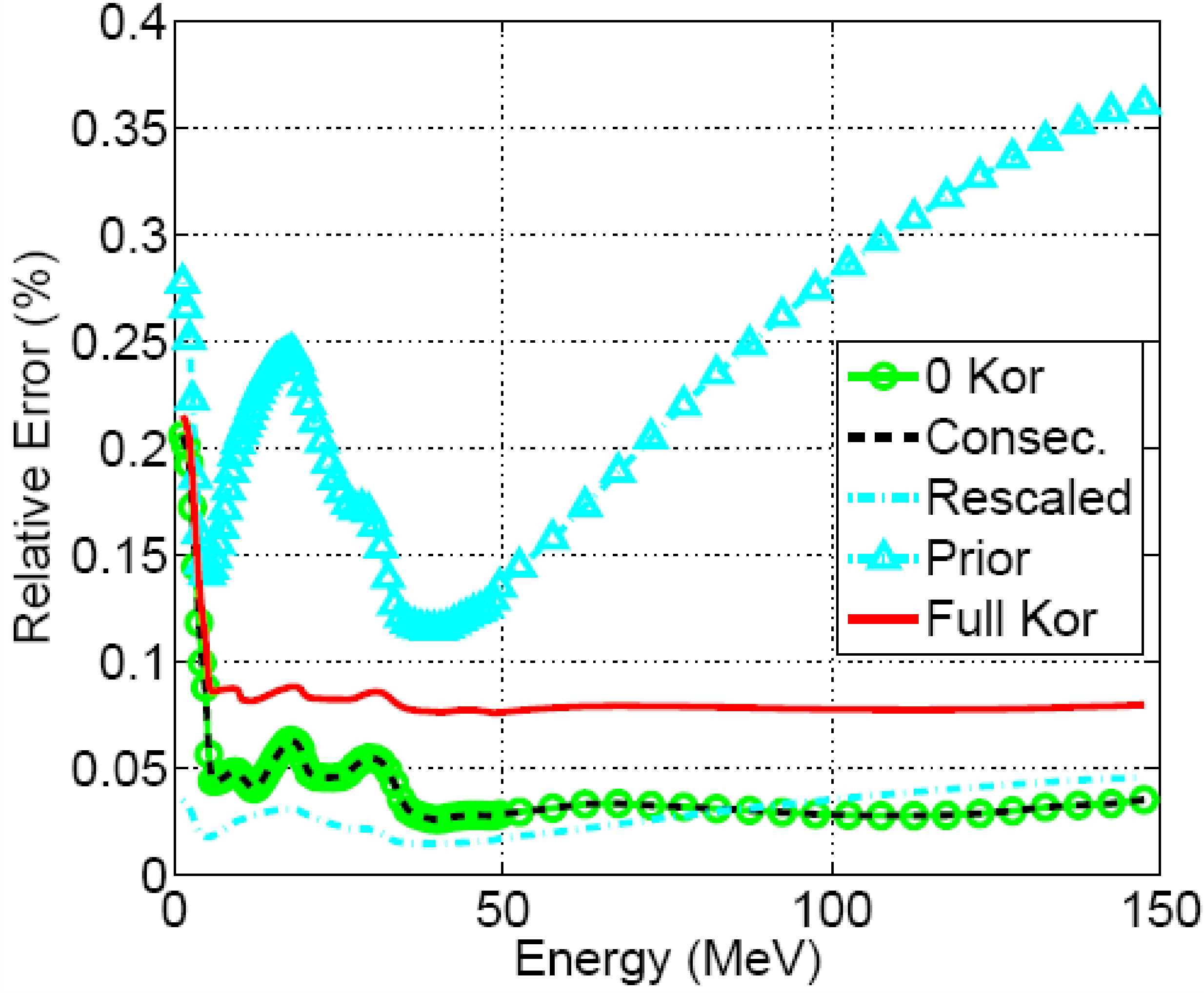
Importance of Prior correlations



elastic cross section

Summary

neutron-induced reaction cross section for ^{55}Mn in the energy range between 5-150 MeV have been re-evaluated within an **Improved Full Bayesian Evaluation Technique**

- Angle integrated cross sections (MF=3)
- Covariance matrices for cross section uncertainties (MF=33)

  total, elastic, inelastic, (n,2n),(n,3n),(n,4n),(n,p),(n,t),(n,pα),(n,α)

- Parameter uncertainties for n-, p-, d- and α-nucleus optical potentials as well as level densities are taken into account
- Model defects are taken into account – improved extrapolation
- Covariance matrices of experiments are estimated
- ENDF Files (MF=3 and 33) have been generated

Outlook

Further improvements are in progress:

- Extension to fissionable nuclei within ANDES
- Inclusion of angle differential data into the evaluation
- Improve method for determination of correlations of exp.
- Improved automatisation of determination of model defects

Co-workers

Denise NEUDECKER

Thomas SRDINKO

Thank you for your attention

Stefan GUNDACKER

Volker WILDPANER

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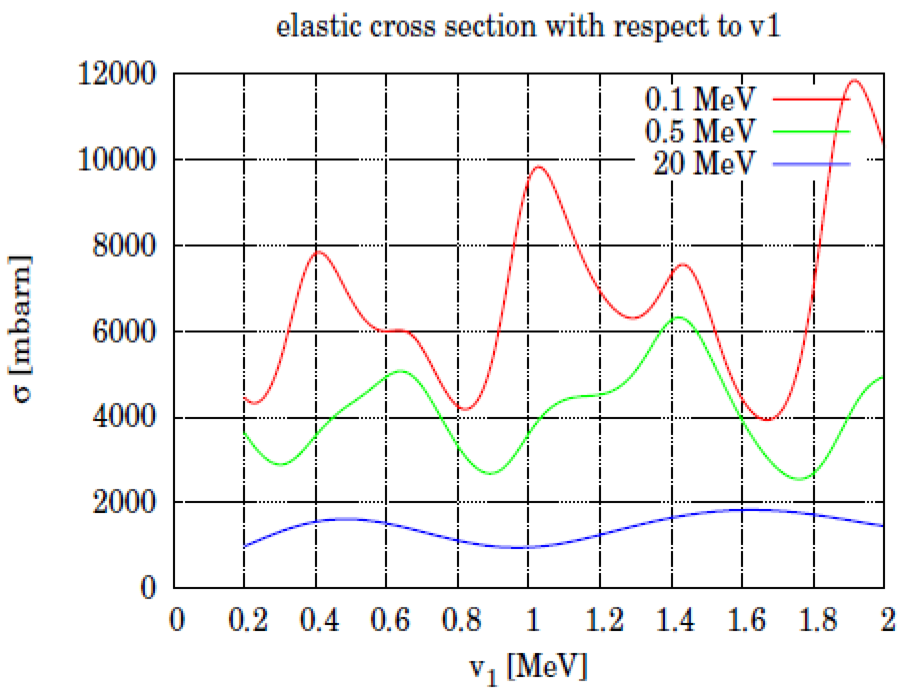
Parameter boundaries: potential depths



Potential should be within one family characterized by the number of bound states sustained by the potential

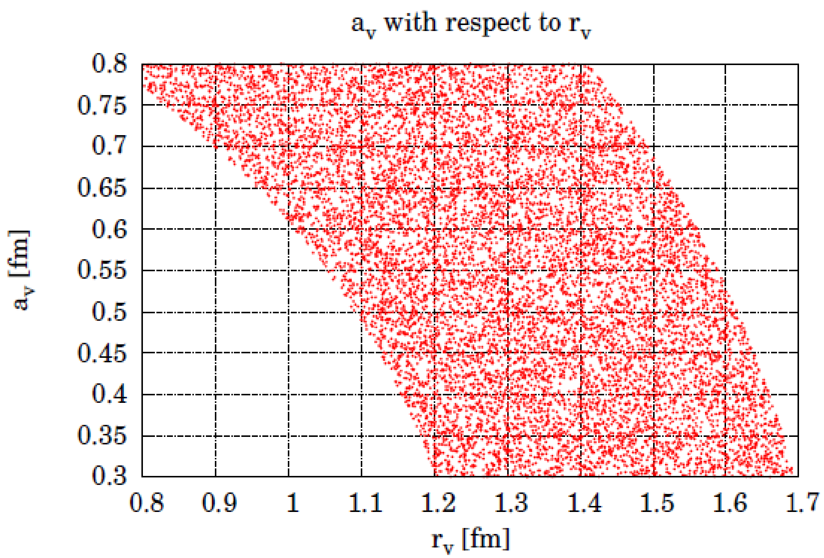
		$v^<$	$v^>$	$v^<$ (%)	$v^>$ (%)
v_1	56.4	47.9	64.9	15.0	15.0
v_2	0.0072	0.0058	0.0086	20.0	20.0
v_3	0.000020	0.000016	0.000024	20.0	20.0
v_{so1}	7.4	5.9	8.9	20.0	20.0
v_{so2}	0.0038	0.0030	0.0046	20.0	20.0

Parameter boundaries: geometry

Physics constraints on the geometry:
rms-radius must lie between
charge radius and
charge radius + 2 nuclear range

		$r^<$ (fm)	$r^>$ (fm)	$r^<$ (%)	$r^>$ (%)
r_v	1.194	0.967	1.536	19.0	28.6
r_{vd}	1.266	1.026	1.628	19.0	28.6
r_{so}	1.000	0.810	1.286	19.0	28.6

		$a^<$ (fm)	$a^>$ (fm)	$a^<$ (%)	$a^>$ (%)
a_v	0.639	0.543	0.791	15.0	23.8
a_{vd}	0.529	0.450	0.655	15.0	23.8
a_{so}	0.665	0.565	0.823	15.0	23.8



These uncertainties are transferred to other parameters

		$w^<$	$w^>$	$w^<$ (%)	$w^>$ (%)
w_1	11.6	9.9	13.3	15.0	15.0
w_2	80.0	64.0	96.0	20.0	20.0
w_{so1}	−3.5	−2.8	−4.2	20.0	20.0
w_{so2}	160.0	128.0	192.0	20.0	20.0

		$d^<$	$d^>$	$d^<$ (%)	$d^>$ (%)
d_1	13.7	11.6	15.8	15.0	15.0
d_2	0.0236	0.0189	0.0283	20.0	20.0
d_3	10.09	8.07	12.11	20.0	20.0

Scaling factors and uncertainties

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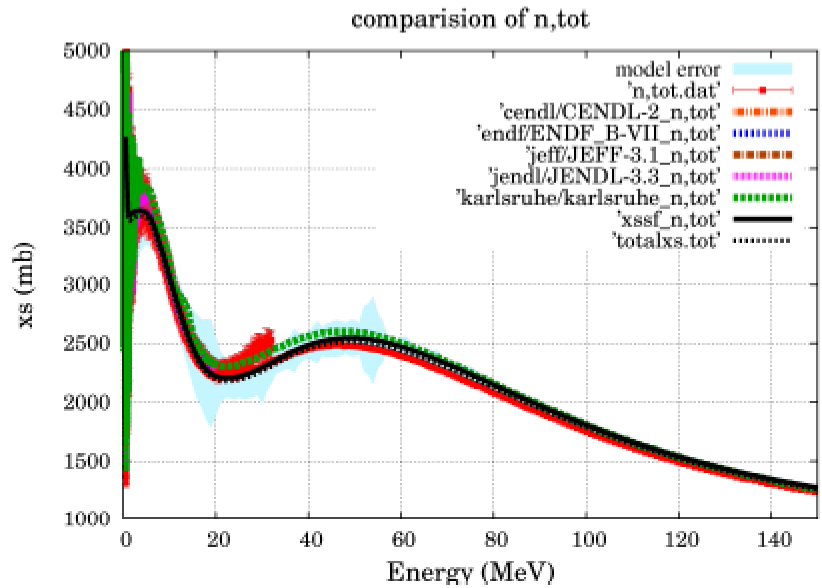
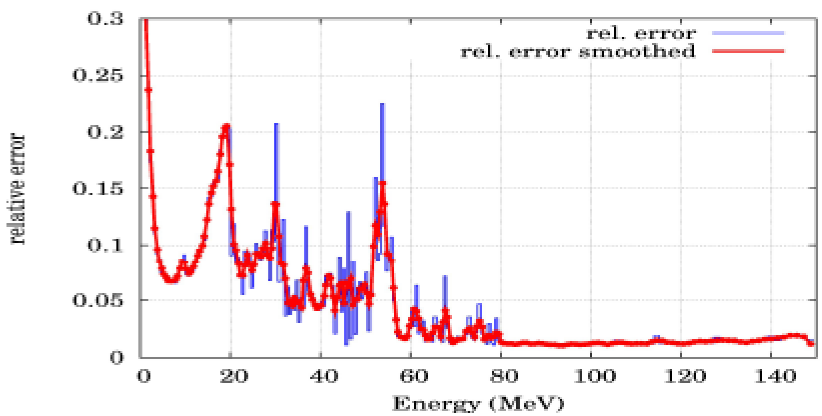
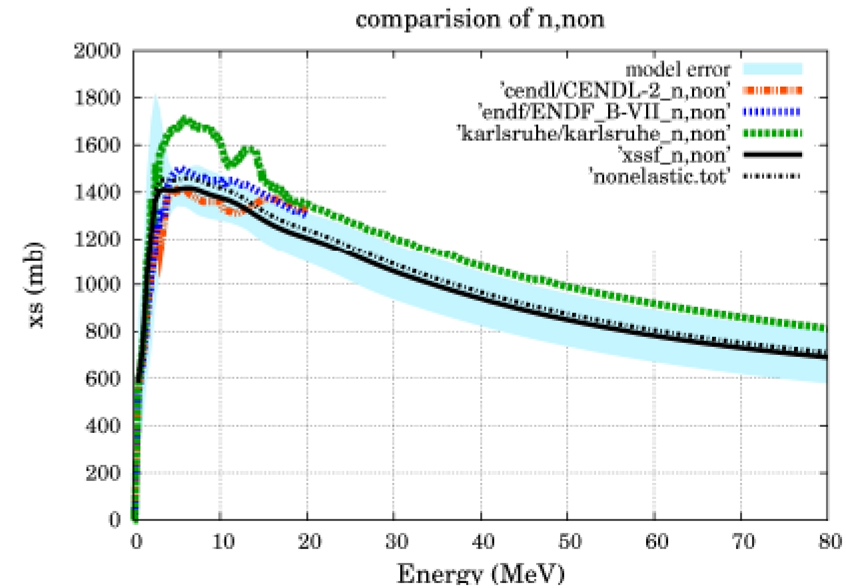
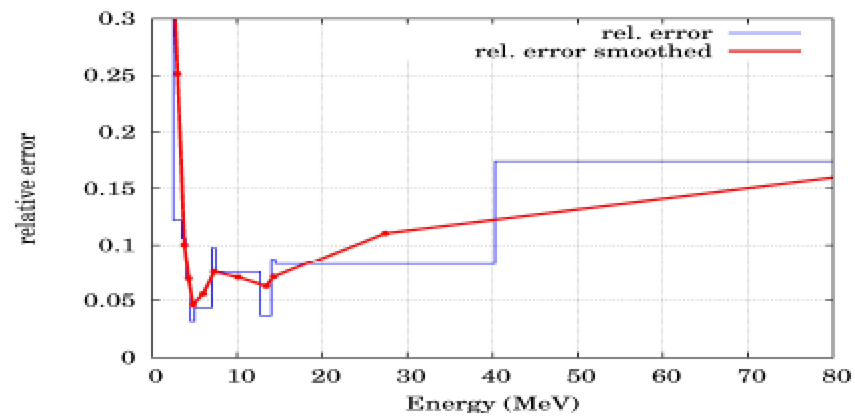
overall scaling factor (n,tot): 1.013





overall scaling factor (n,non): 0.971





Scaling factors and uncertainties

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overall scaling factor (n,el): 1.004