# Model defects for nuclear data evaluation

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# Introduction

-) Energy range of evaluated files normally limited up to 20 MeV

-) novel nuclear technologies and radioactive waste incineration methods require extension to higher energies

-) in general nuclear data evaluation is a statistical process within BAYESIAN statistics

-) unfortunately experimental data is scarce for neutron induced reactions at higher energies

-) PRIOR becomes important due to scarcity of data

-) Model defects cause great impact on prior

# Bayes theorem

**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

# Prior

The contributions to the covariance matrix of the model are:

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

**Parameter uncertainties**

**Numerical implementation errors**

**Deficiencies of the model, is of non-statistical nature**

# Prior

The contributions to the covariance matrix of the model are:

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

**-) cannot be determined within the considered nuclear model**

**-) It is requiered to involve experimental data in the procedure.**

**-) Only corresponding data from neighbouring nuclei is considered.**

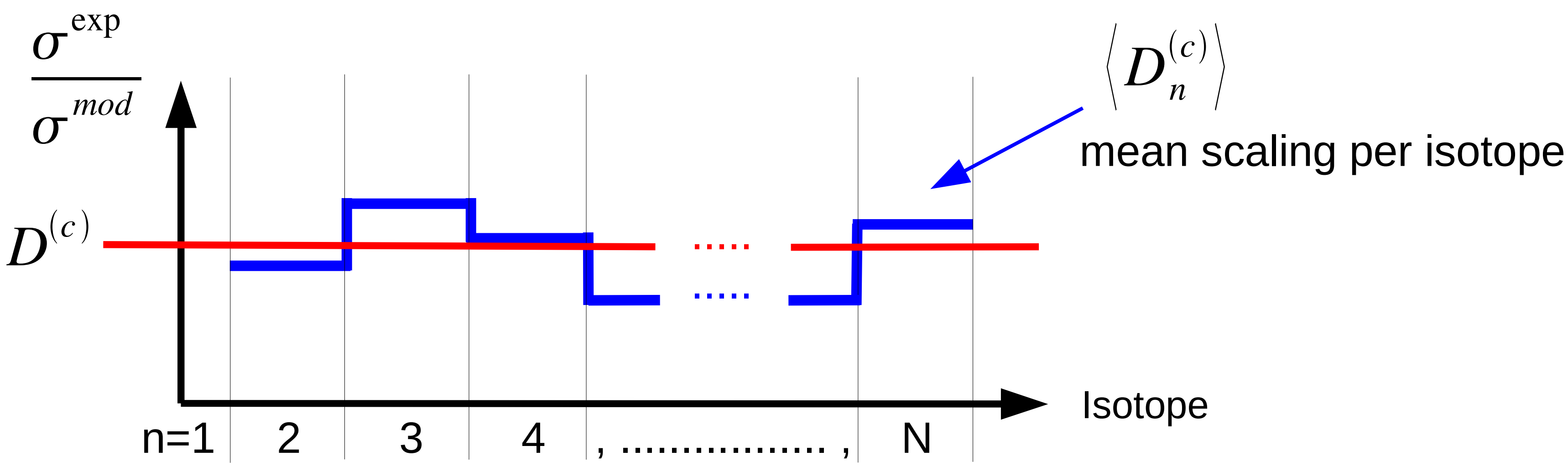
# Formulation of model defects

The basic idea is to introduce an overall scaling factor:

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

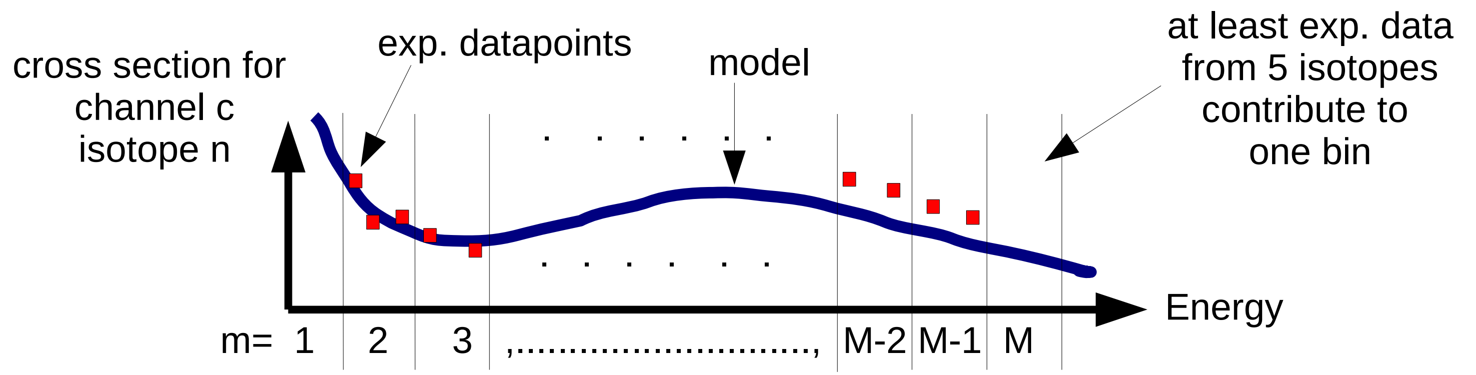
for the reaction channel c

which is a mean quotient between experiment and theory $\frac{\sigma^{\exp}}{\sigma^{mod}}$




energy independent scaling factors => deficiencies of model are directly reflected

# Formulation of model defects




scaling factor in the energy bin M

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

chosen weights emphasize values at the highest cross section

$$w_j^{(c,m,n)} = \frac{\sigma_{th}^{(c,n)}(E_j)}{\sum_{j'\in E_{bin}(m,n)} \sigma_{th}^{(c,n)}(E_{j'})}$$

scaling factor per isotope:

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

$$w_m^{(c,n)} = \frac{\sigma_{th}^{(c,n)}(E_m)}{\sum_{m'\in E_{bin}} \sigma_{th}^{(c,n)}(E_{m'})}$$

# Formulation of model defects

covariance matrix due to model defects we define by:

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

-) it's an assumption

-) that formulation is of non-statistical nature!

# Covariance matrix

covariance matrix due to model defects:

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

First term expresses systematical errors, represents the correlations

# Covariance matrix

covariance matrix due to model defects:

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

$N^{(c)}(E_m)$ is the number of isotopes for which $\langle D_n^{(c)}(E_m)\rangle$ can be evaluated

chosen normalization accounts for nonstatistical nature of the formulation

# Covariance matrix

covariance matrix due to model defects:

$$\left\langle \Delta^{(c)}(E_m)\Delta^{(c')}(E_{m'})\right\rangle = \sigma_{th}^{(c)}(E_m)\sigma_{th}^{(c')}(E_{m'})$$

$$\cdot \frac{1}{\sqrt{N^{(c)}(E_m)}\sqrt{N^{(c')}(E_m')}} \sum_{n=1}^{N} \left\{ \left[\left(\left\langle D_n^{(c)}(E_m)\right\rangle - D^{(c)}\right)\left(\left\langle D_n^{(c')}(E_{m'})\right\rangle - D^{(c')}\right)\right]\right.$$

$$\left. + \delta_{cc'}\delta_{mm'}\left[\left\langle \left(D_n^{(c)}(E_m)\right)^2\right\rangle - \left(\left\langle D_n^{(c)}(E_m)\right\rangle\right)^2\right]\right\}$$

$$\left\langle \left(D_n^{(c)}(E_m)\right)^2\right\rangle = \sum_{j\in E_{bin}(m,n)} w_j^{c,m,n}\left(\frac{\sigma_{ex}^{(c)}(E_j)}{\sigma_{th}^{(c)}(E_j)}\right)^2$$

Second term is a real covariance term as defined in statistics due to fluctuations of the experimental data

# Correlation matrix

covariance matrix due to model defects:

$$\left\langle \Delta^{(c)}(E_m)\Delta^{(c')}(E_{m'})\right\rangle = \sigma_{th}^{(c)}(E_m)\sigma_{th}^{(c')}(E_{m'})$$

$$\cdot \frac{1}{\sqrt{N^{(c)}(E_m)}\sqrt{N^{(c')}(E_m{}')}} \sum_{n=1}^{N} \Big\{ \Big[ \Big( \left\langle D_n^{(c)}(E_m) \right\rangle - D^{(c)} \Big) \Big( \left\langle D_n^{(c')}(E_{m'}) \right\rangle - D^{(c')} \Big) \Big]$$

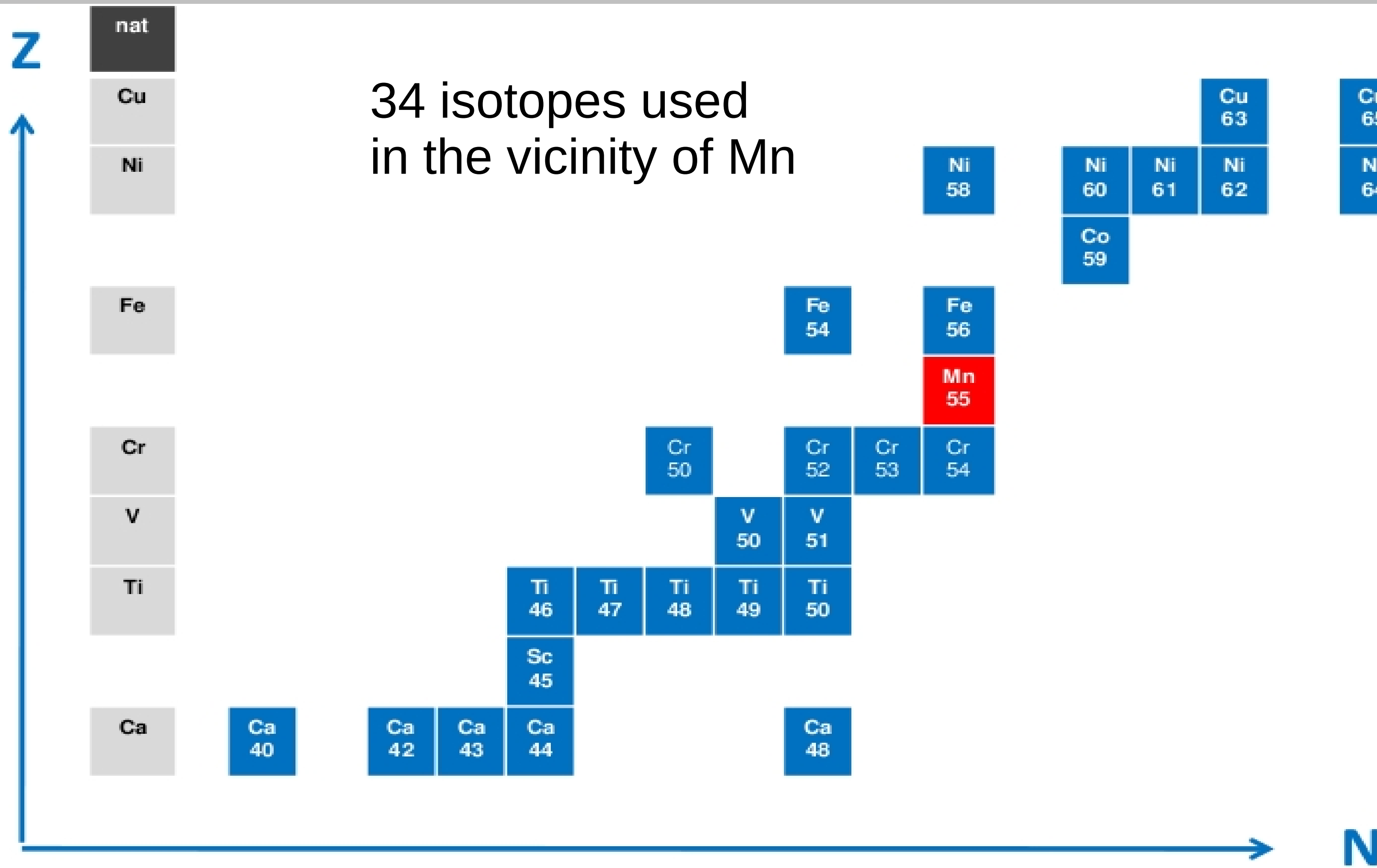
$$+ \delta_{cc'}\delta_{mm'} \Big[ \left\langle \left( D_n^{(c)}(E_m) \right)^2 \right\rangle - \left( \left\langle D_n^{(c)}(E_m) \right\rangle \right)^2 \Big] \Big\}$$

Correlations are defined in the usual way:

$$C^{(cc')}(E_m, E_n) = \frac{\left\langle \Delta\sigma^{(c)}(E_m)\Delta\sigma^{(c')}(E_n) \right\rangle}{\sqrt{\left\langle \Delta^2\sigma^{(c)}(E_m) \right\rangle}\sqrt{\left\langle \Delta^2\sigma^{(c')}(E_n) \right\rangle}}$$

# Used Data

34 isotopes used
in the vicinity of Mn




| 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 |

# Parametrisation

-) optical potential (Koning and Delaroche) and level densities (CTM - TALYS) were optimised

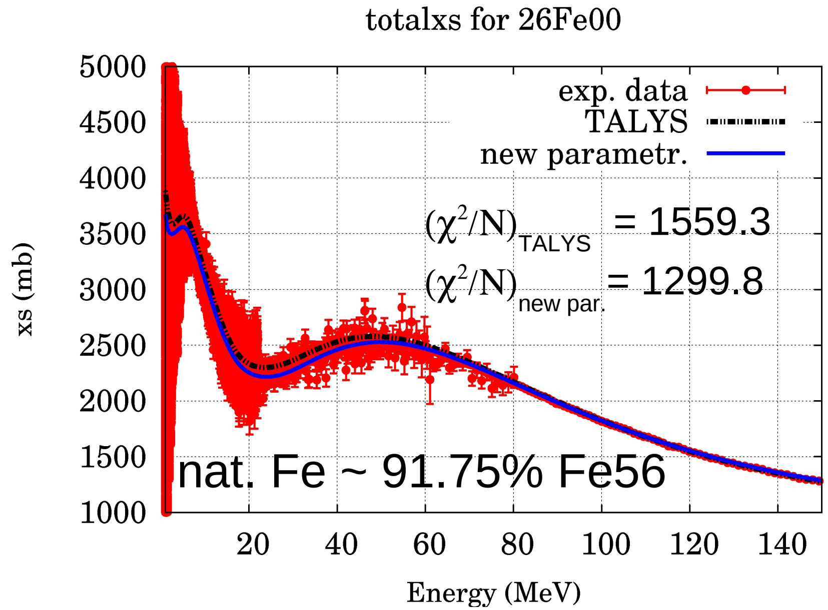
-) because global parameters in TALYS are optimised from A=12 to 339

-) secures that no exp. information of $^{55}Mn$ goes into global parametrisation

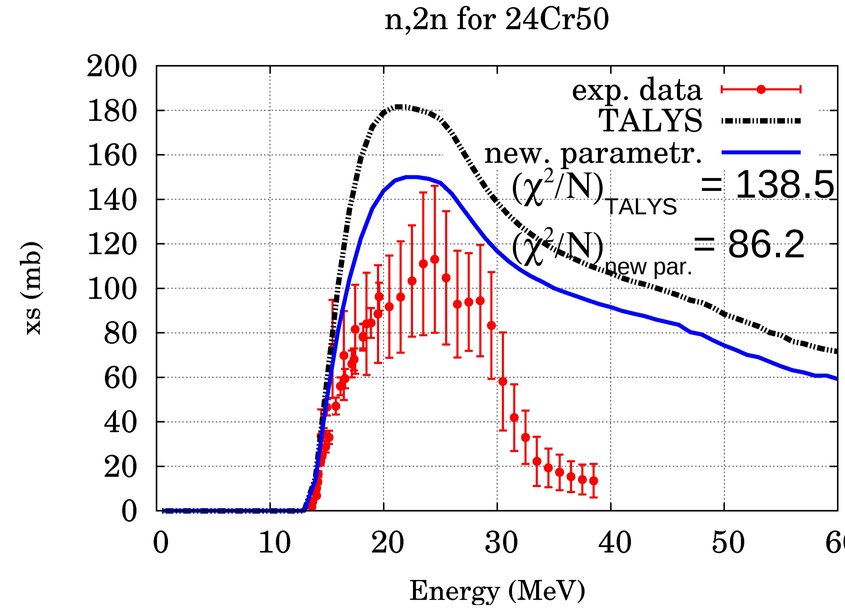
-) we have obtained a slightly different parametrisation

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

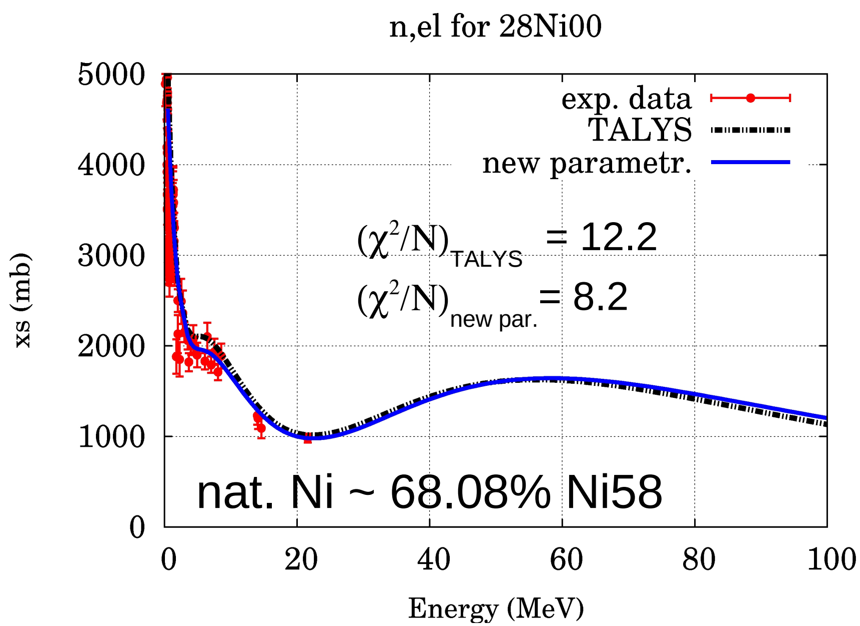
# Around Mn55



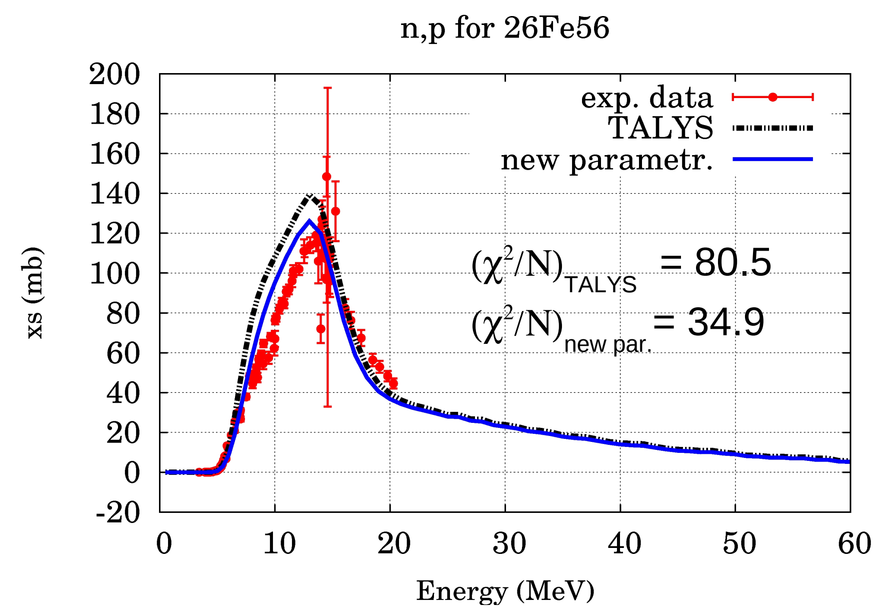
totalxs for 26Fe00
exp. data
TALYS
new parametr.
$(\chi^2/N)_{TALYS}$ = 1559.3
$(\chi^2/N)_{new\ par.}$ = 1299.8
nat. Fe ~ 91.75% Fe56
xs (mb)
Energy (MeV)

n,2n for 24Cr50
exp. data
TALYS
new. parametr.
$(\chi^2/N)_{TALYS}$ = 138.5
$(\chi^2/N)_{new\ par.}$ = 86.2
xs (mb)
Energy (MeV)

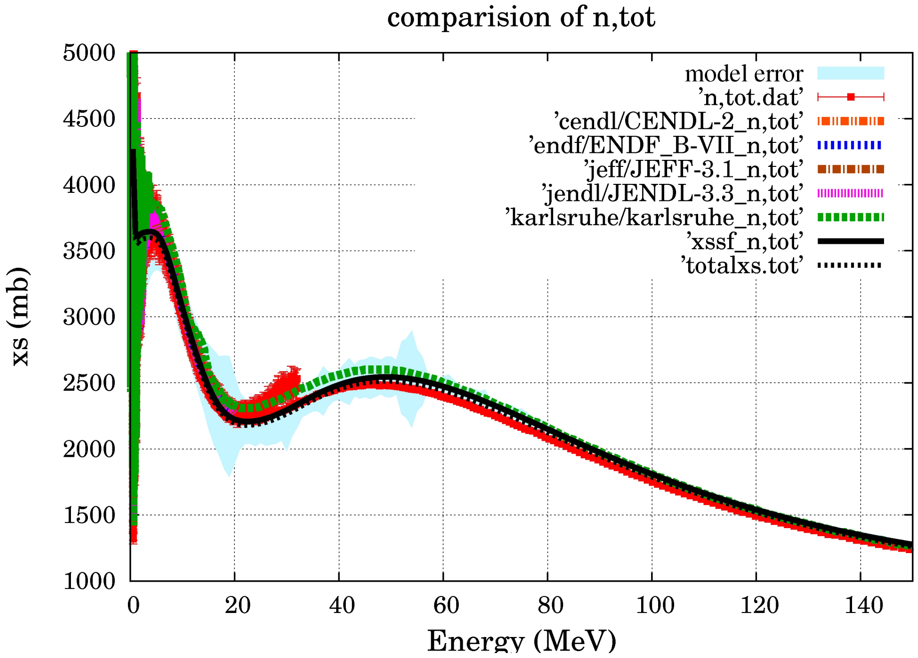
n,el for 28Ni00
exp. data
TALYS
new parametr.
$(\chi^2/N)_{TALYS}$ = 12.2
$(\chi^2/N)_{new\ par.}$ = 8.2
nat. Ni ~ 68.08% Ni58
xs (mb)
Energy (MeV)

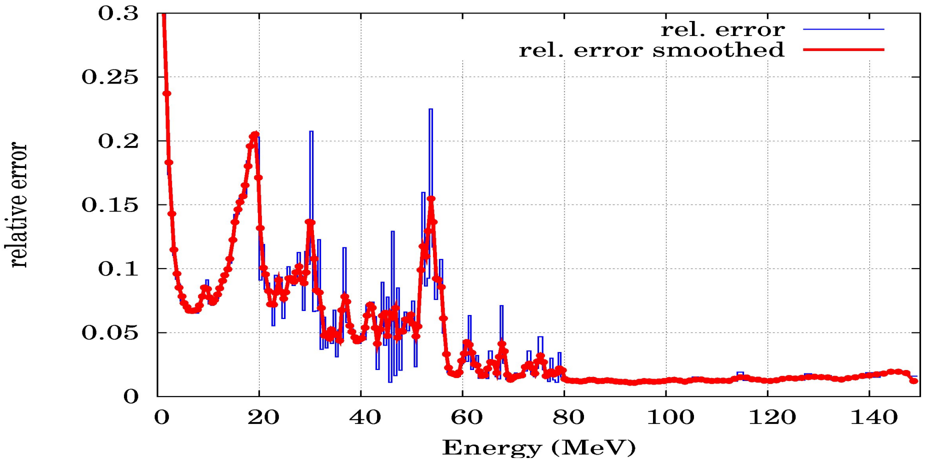



n,p for 26Fe56
exp. data
TALYS
new parametr.
$(\chi^2/N)_{TALYS}$ = 80.5
$(\chi^2/N)_{new\ par.}$ = 34.9
xs (mb)
Energy (MeV)

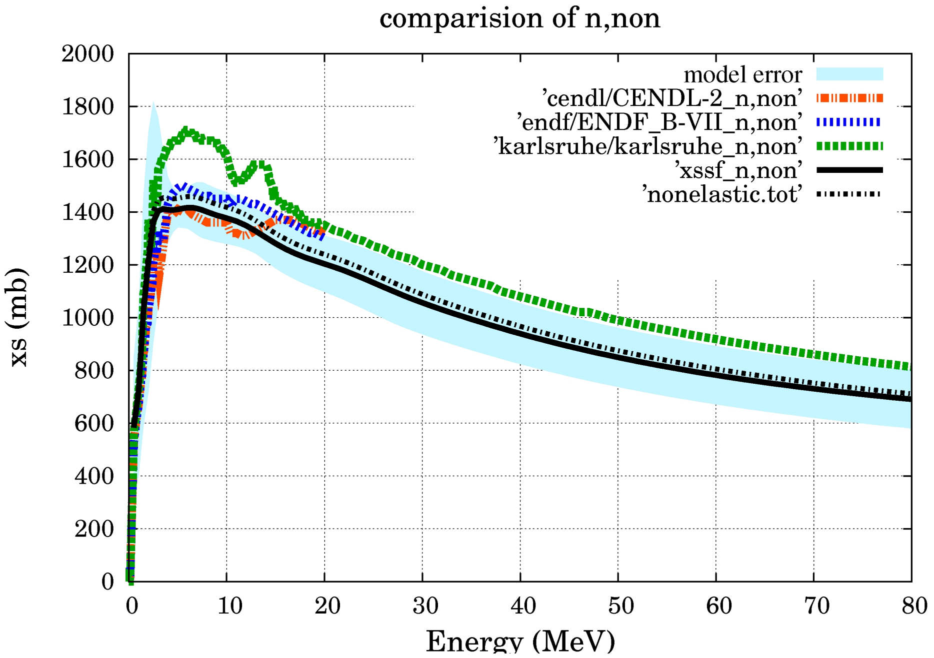
# Uncertainties due to model defects

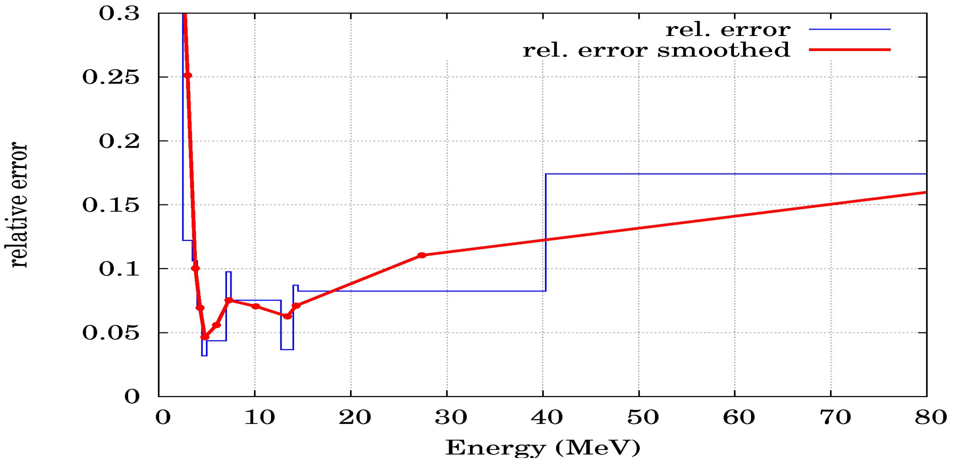
overall scaling factor (n,tot): 1.013



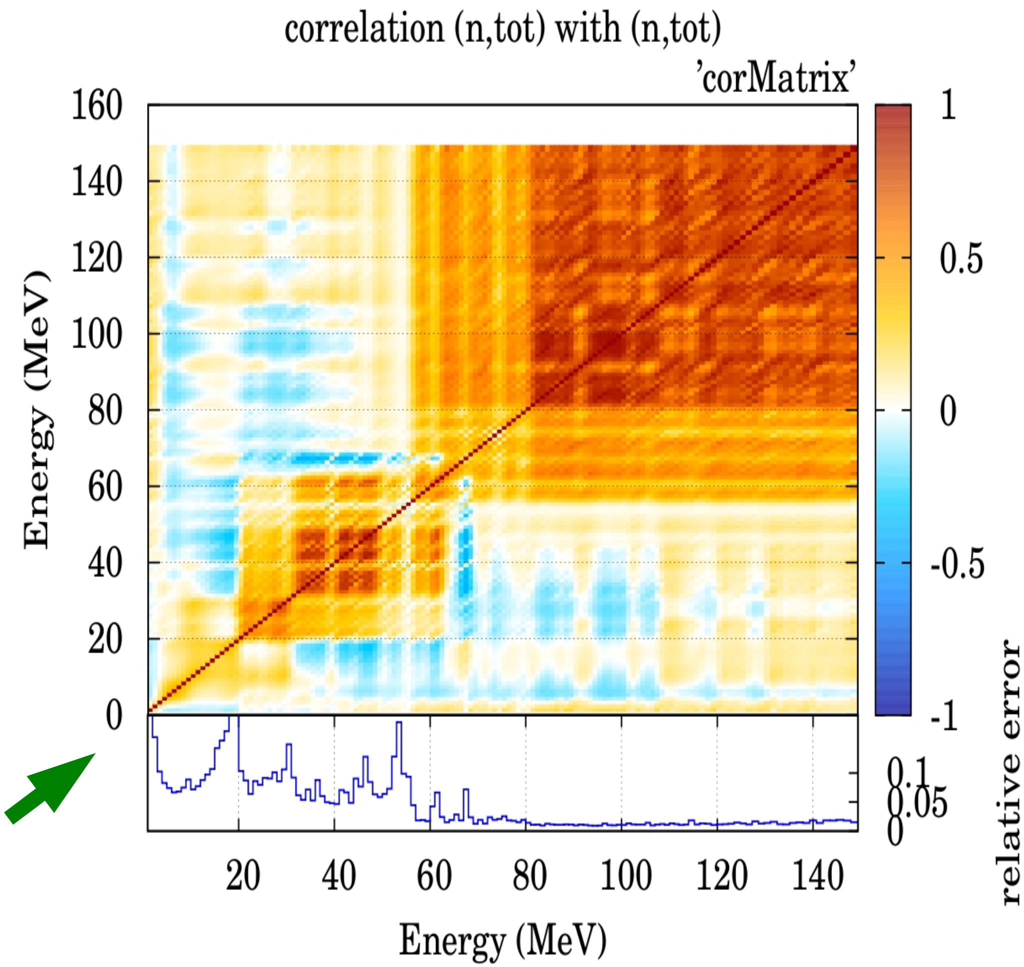



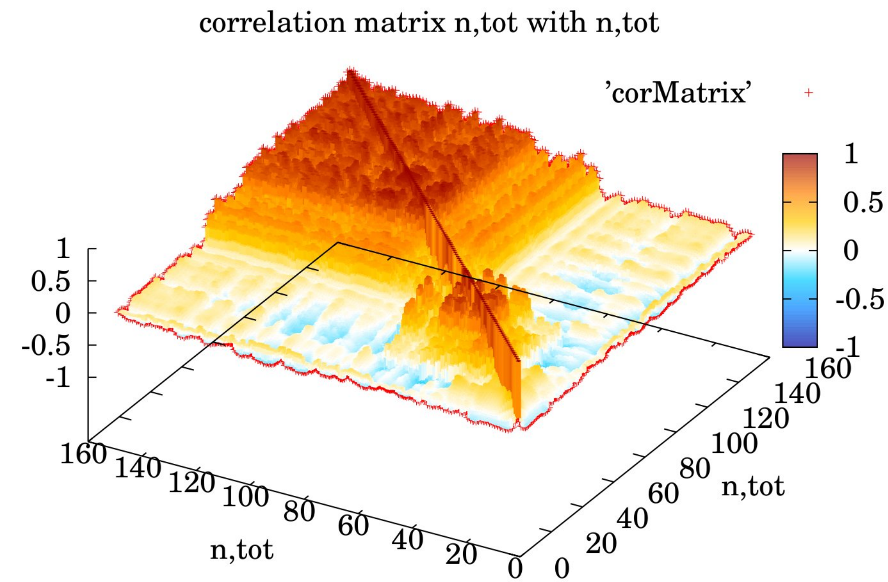

overall scaling factor (n,non): 0.971

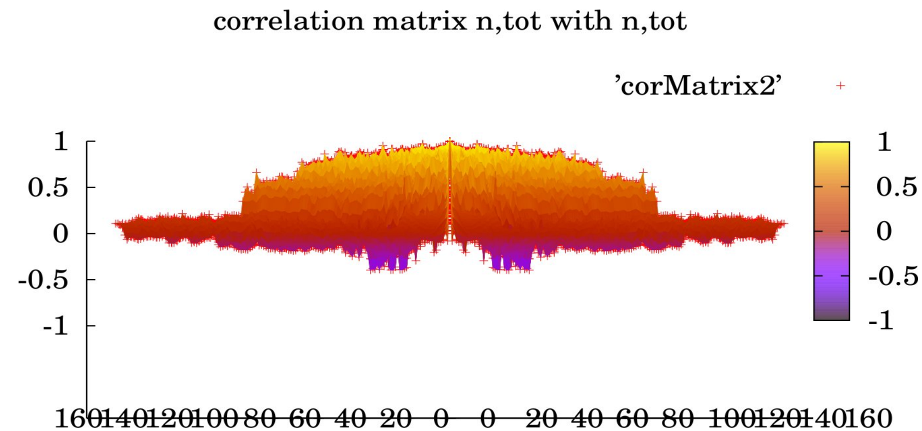


# Correlation Matrix n,tot with n,tot



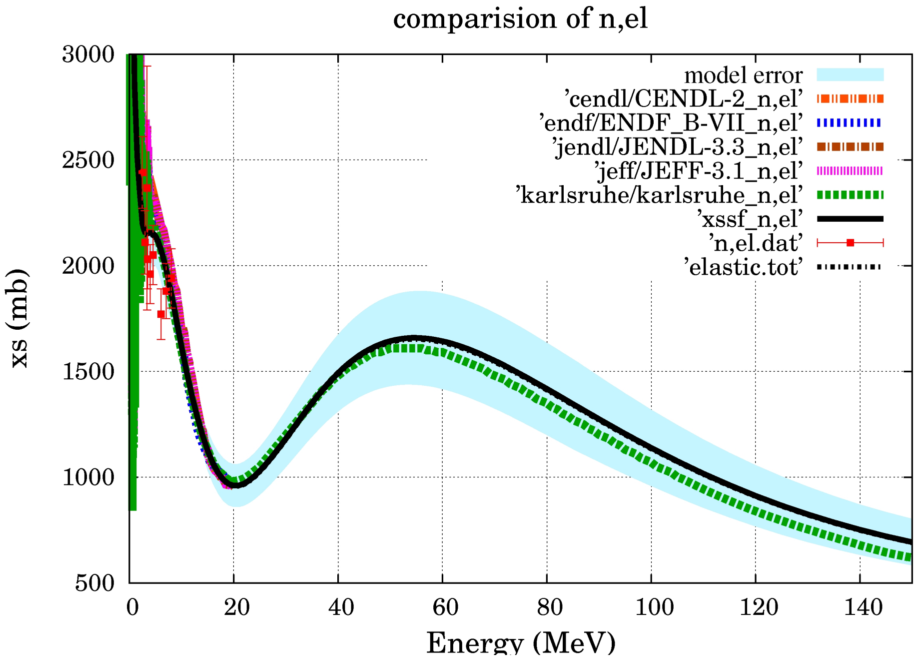



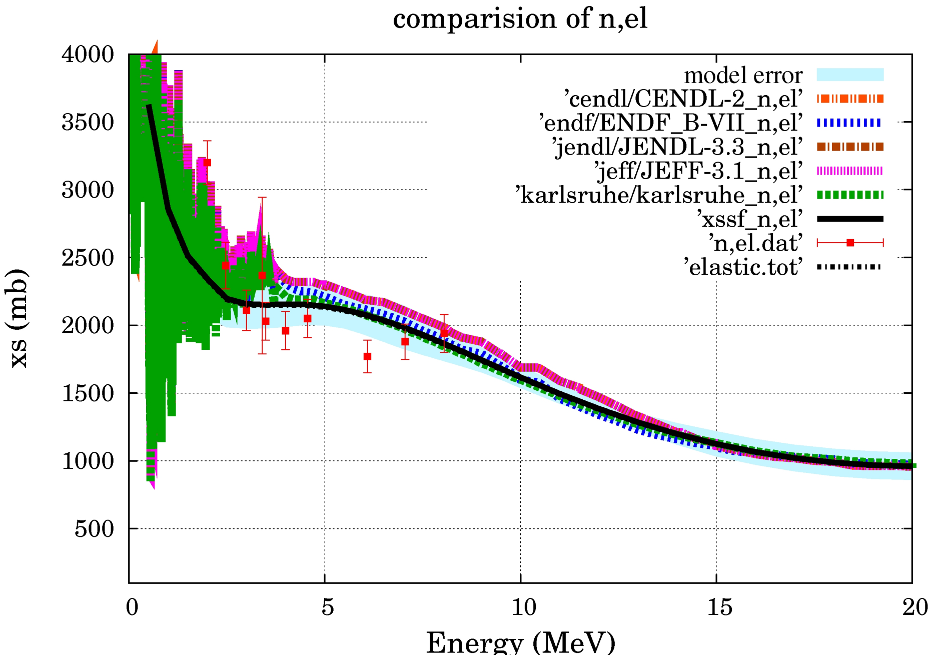



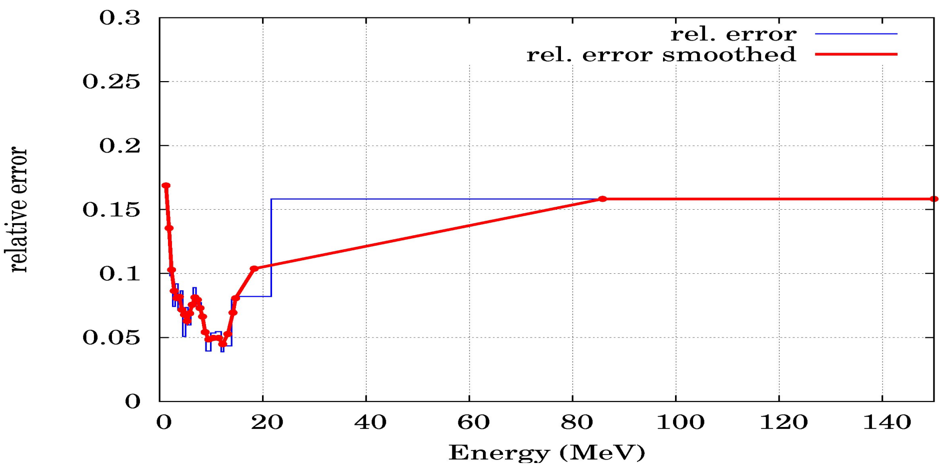

$E_m + E_{m'} = \text{const.}$

# Uncertainties due to model defects

overall scaling factor (n,el): 1.004



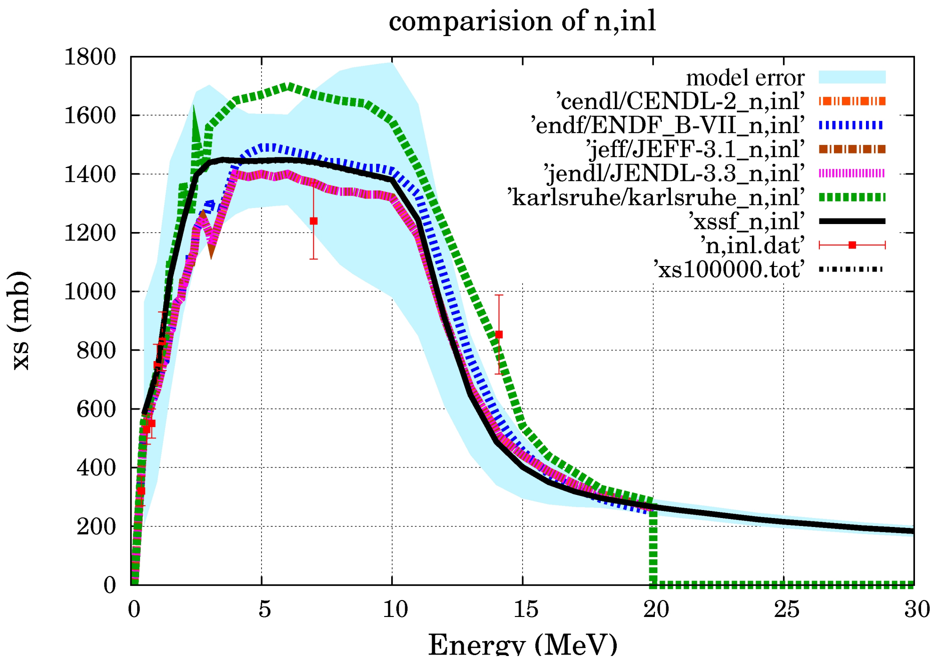



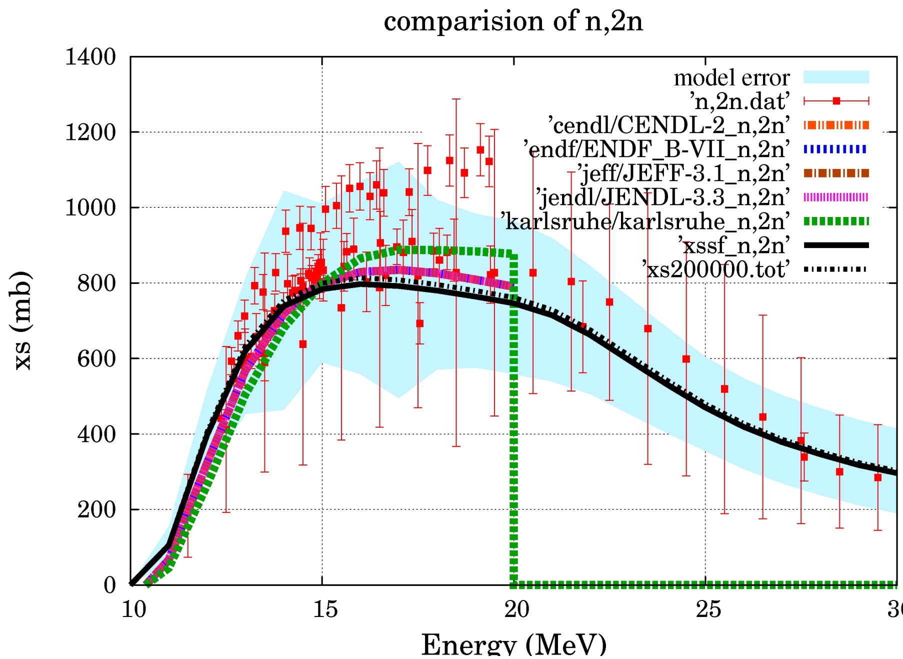



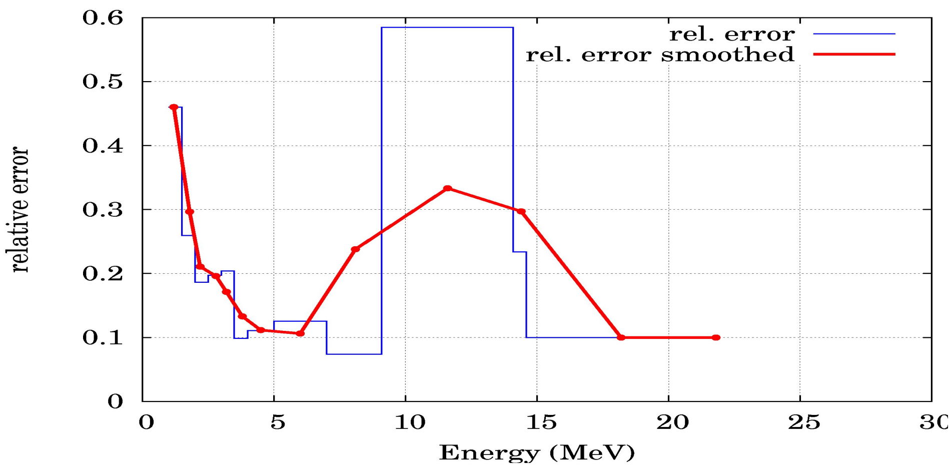
# Uncertainties due to model defects

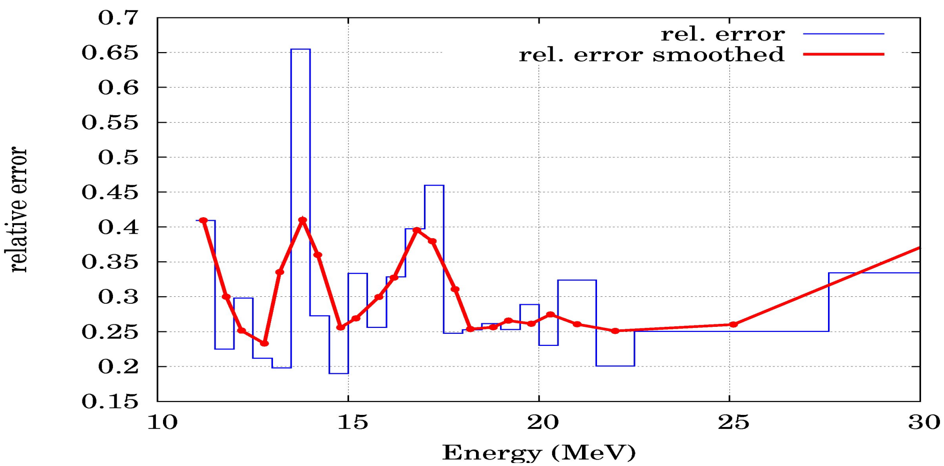
overall scaling factor (n,inl): 1.002

overall scaling factor (n,2n): 0.980

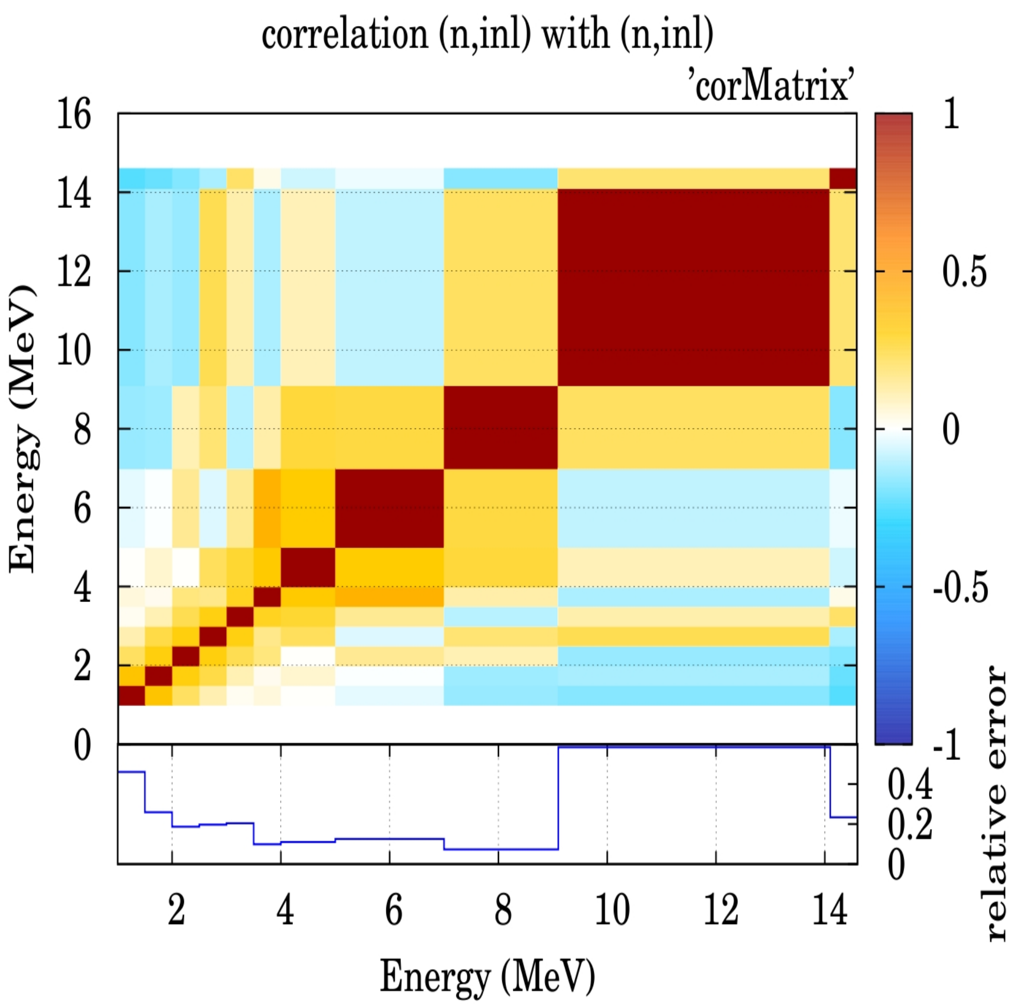


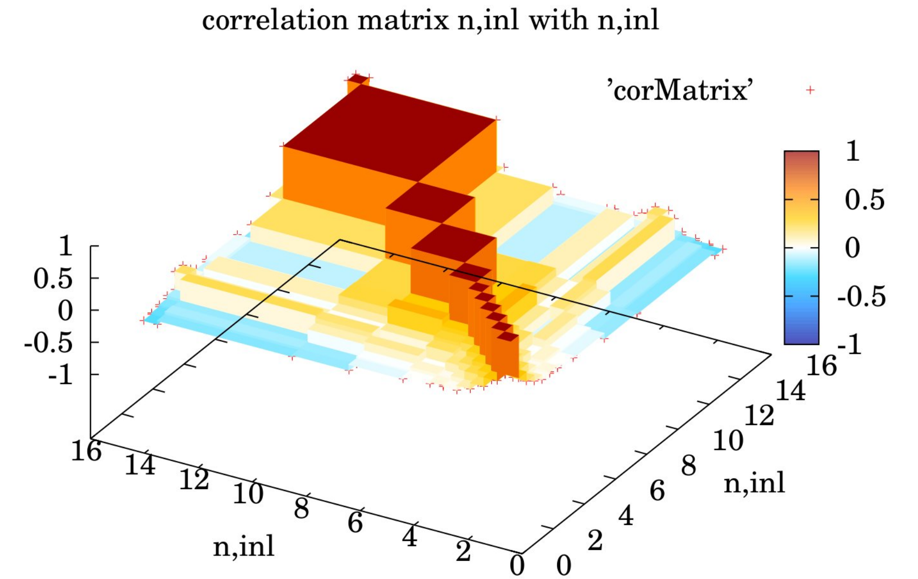



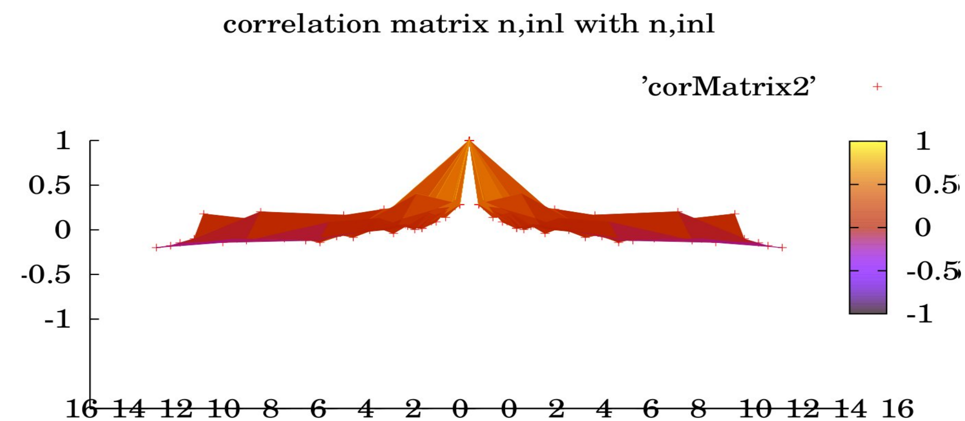



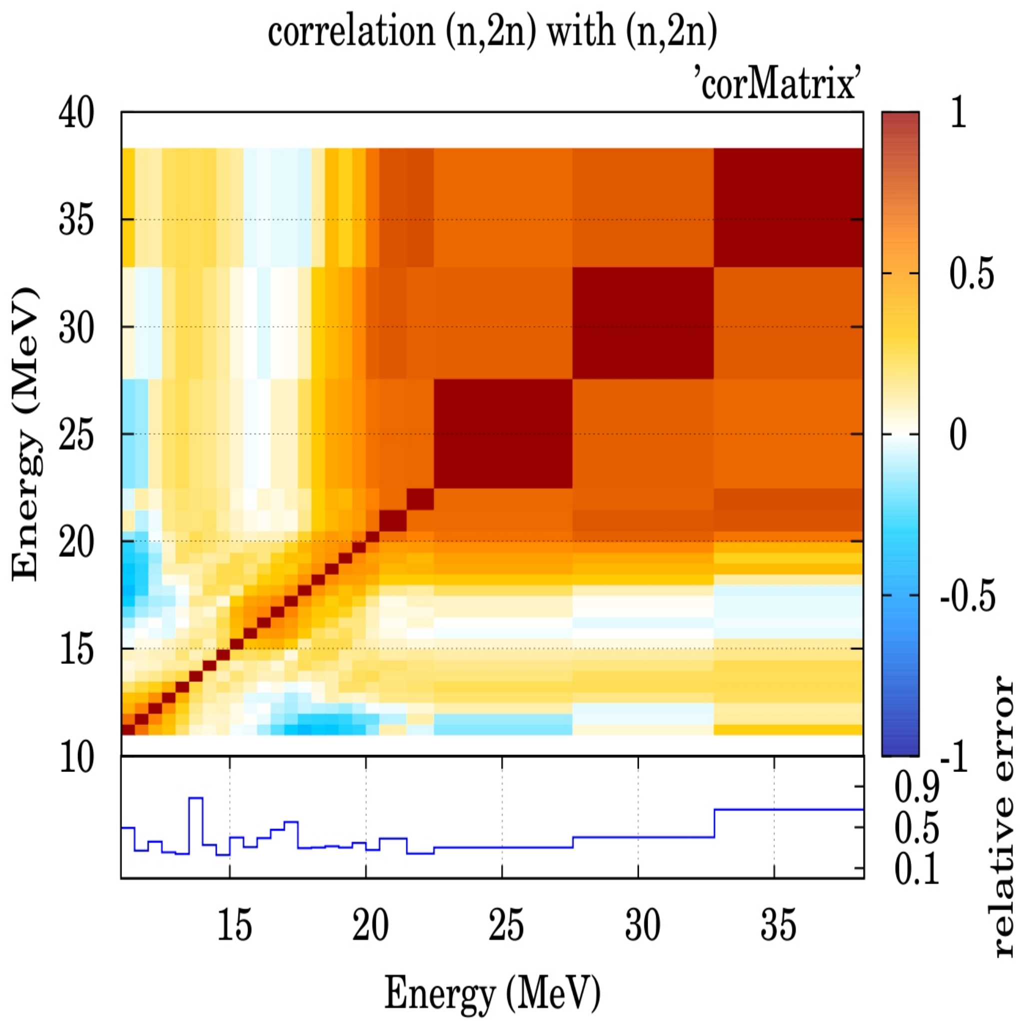
# Correlation Matrix n,inl with n,inl

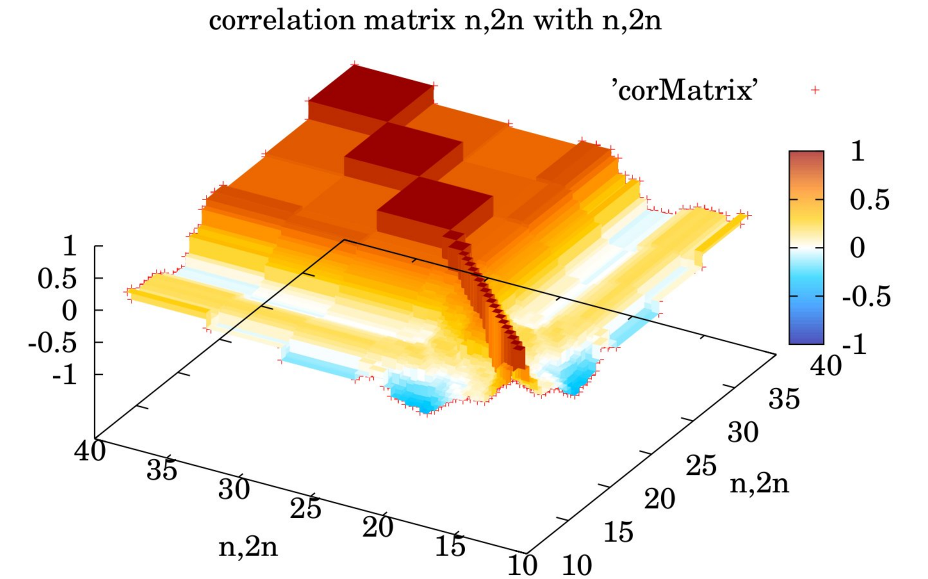


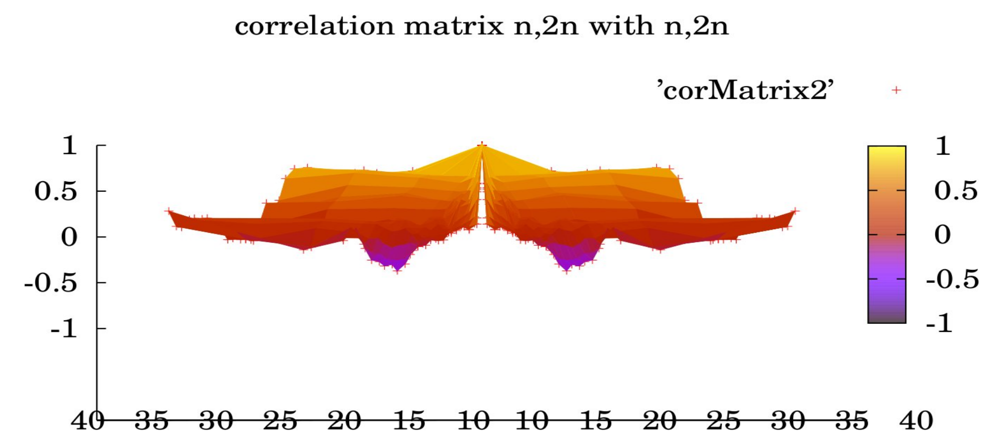



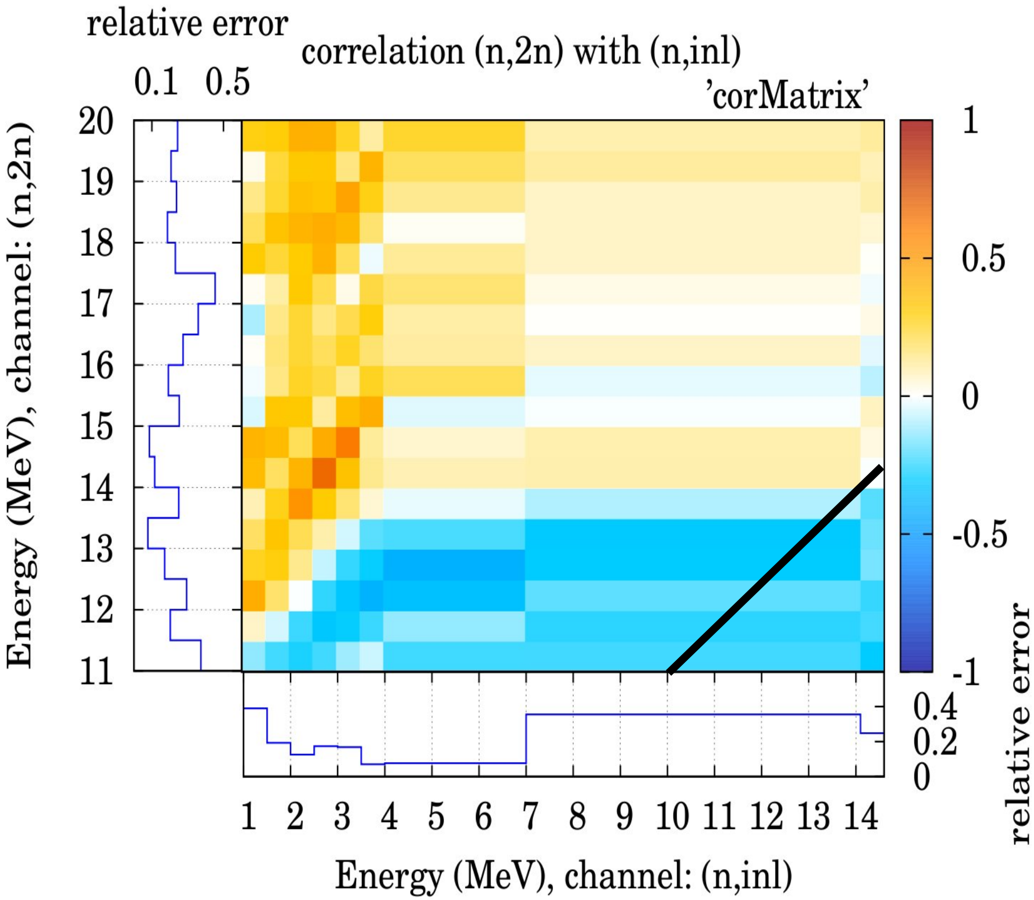
# Correlation Matrix n,2n with n,2n

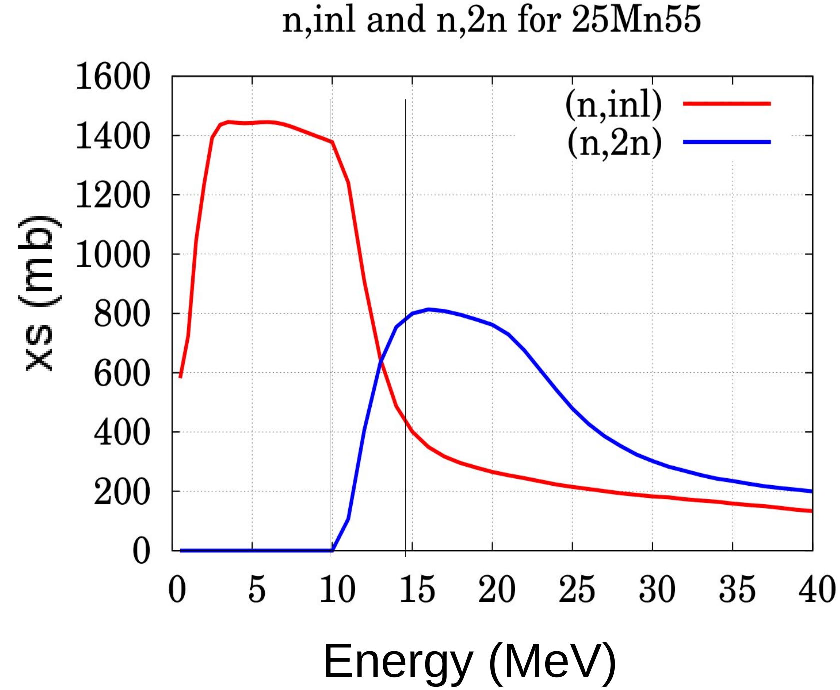


# Correlation Matrix n,inl with n,2n

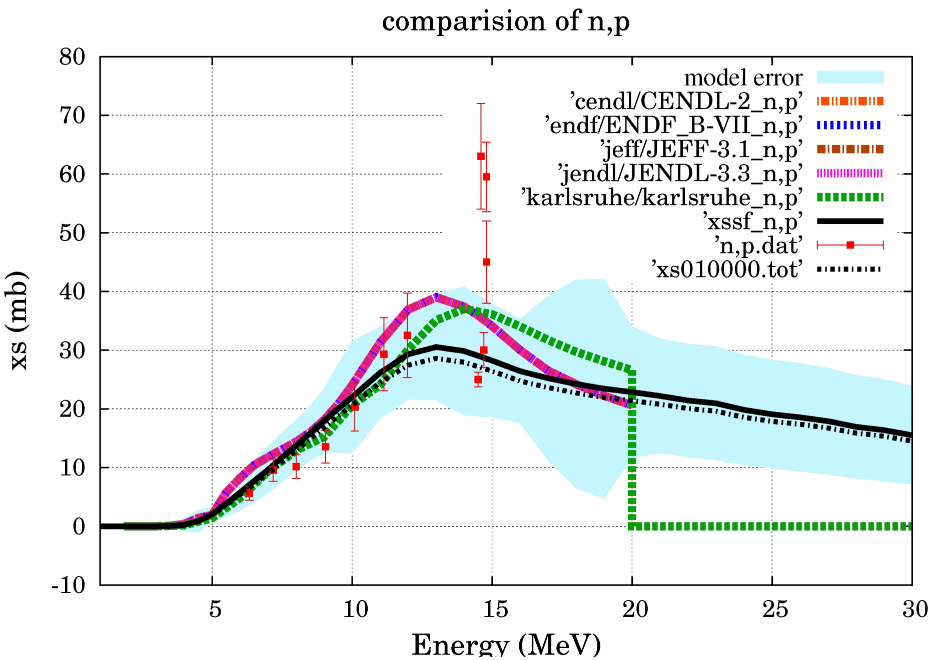


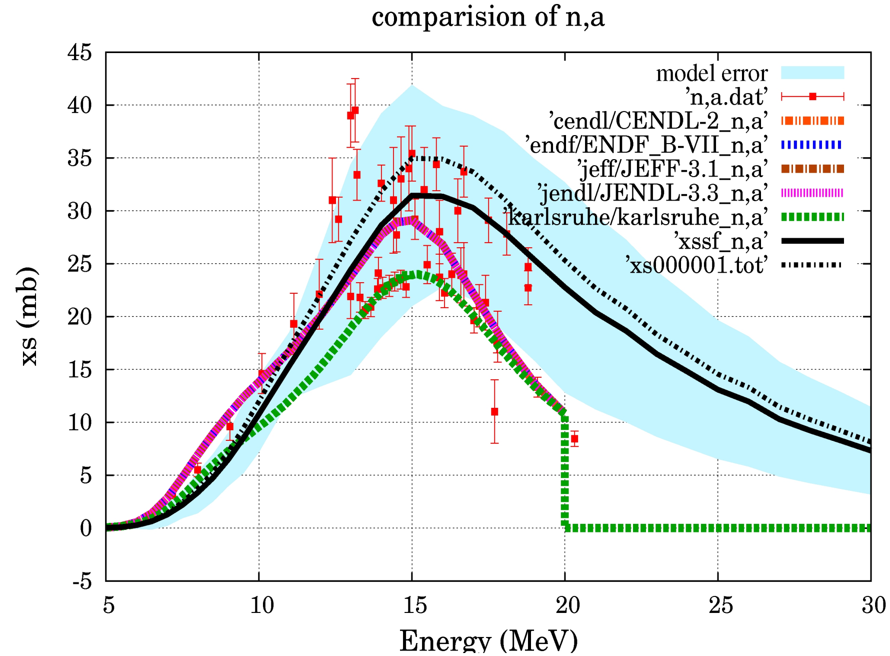



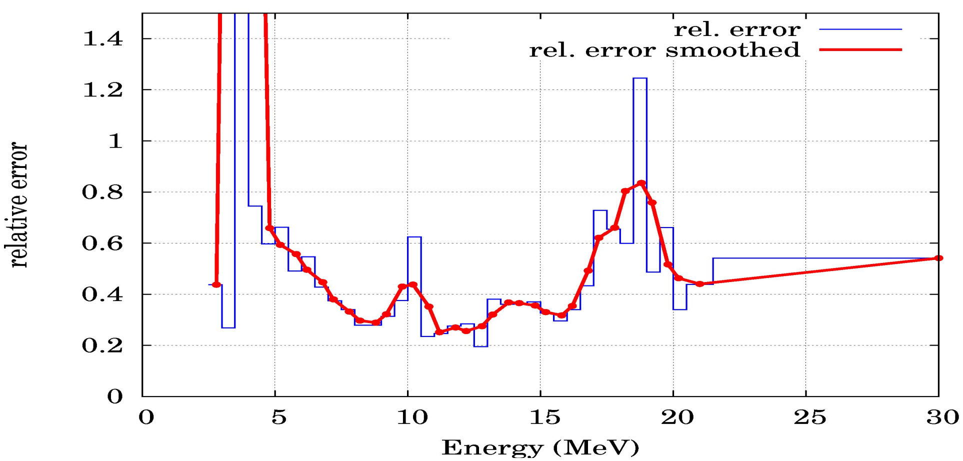
# Uncertainties due to model defects

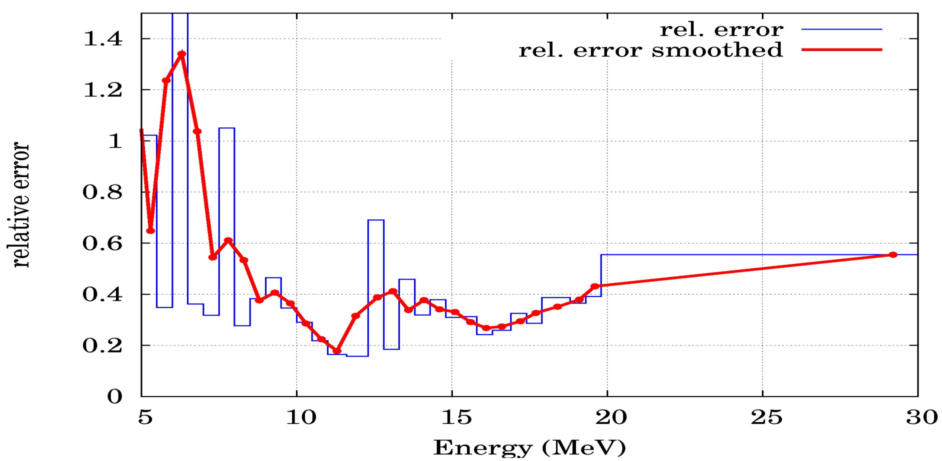
overall scaling factor (n,p): 1.068

overall scaling factor (n,α): 0.899

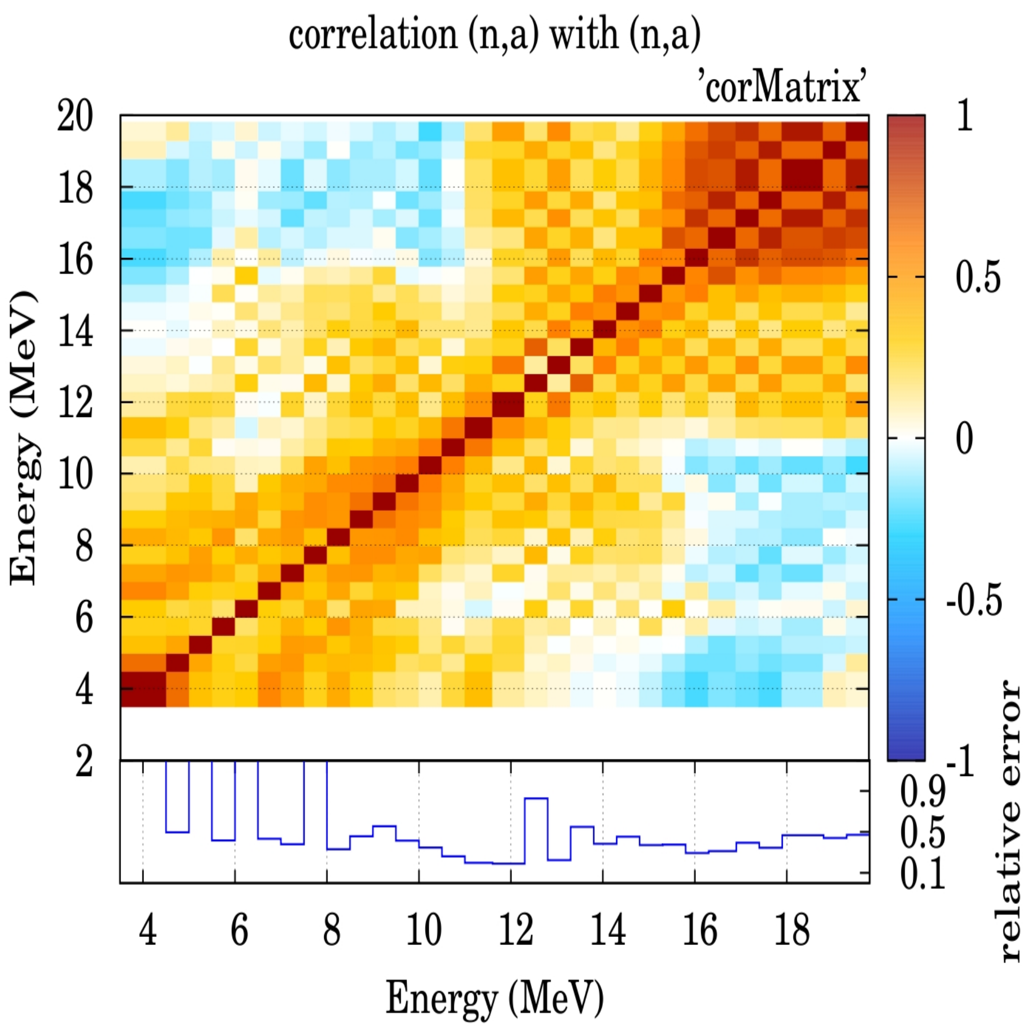


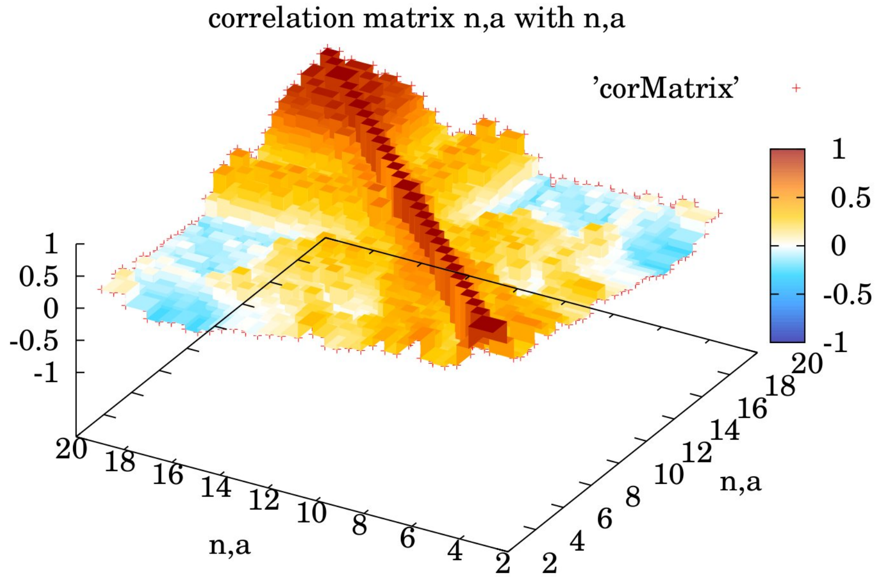



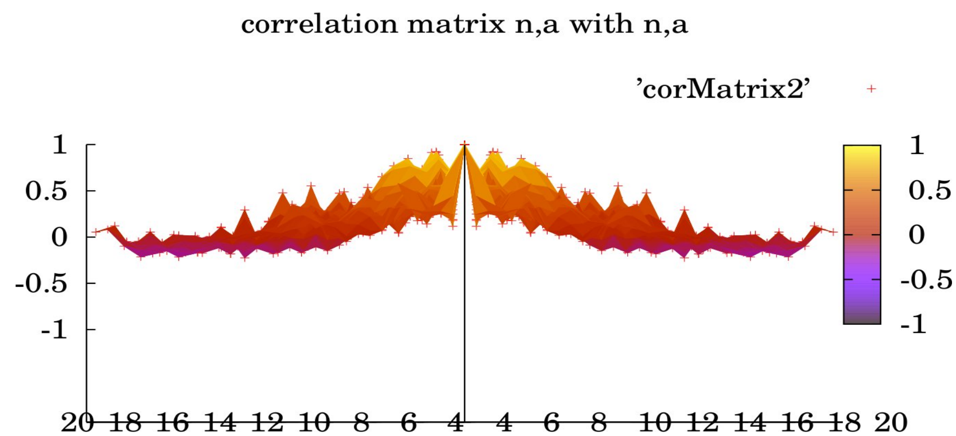



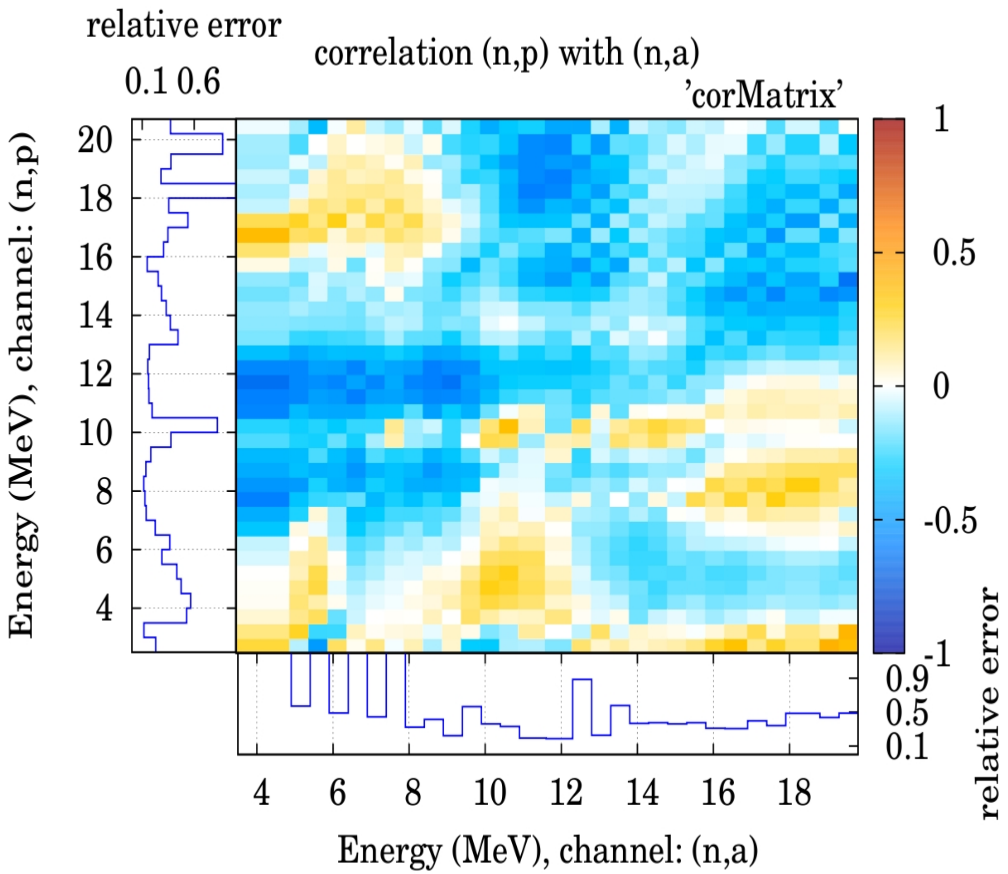
# Correlation Matrix n,α with n,α

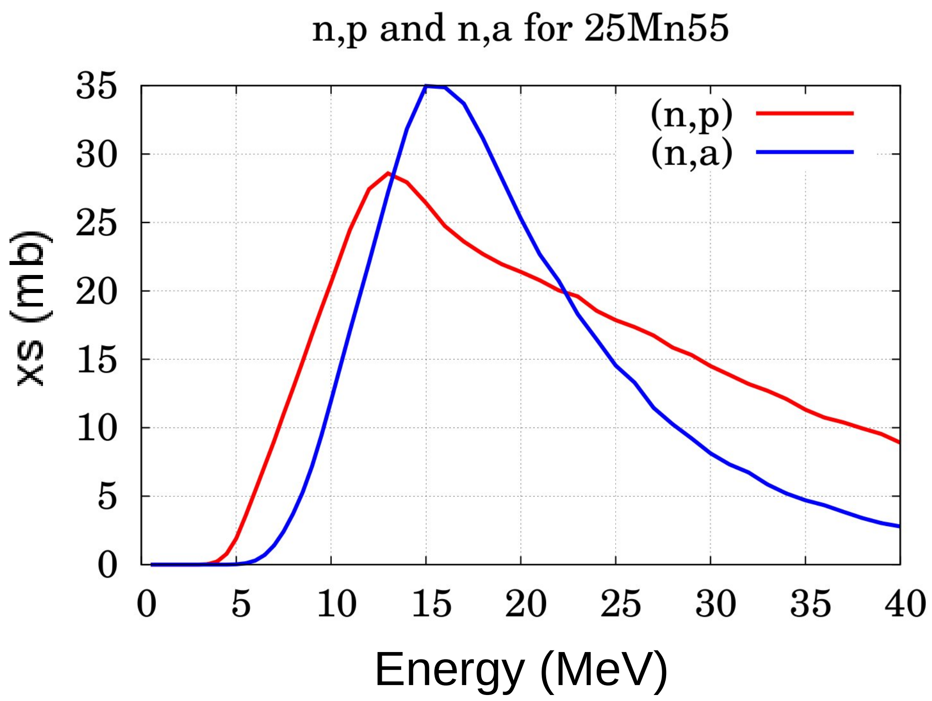


# Correlation Matrix n,p with n,α



# Outlook

-) calculation of parameter uncertainties are in progress

-) Full prior is starting point for Bayesian update procedure together with exp. information of Mn55

-) errors will go down, if good experimental data available

-) evaluation of $^{55}Mn$ which will be performed in our workgroup under the supervision of Prof. H. Leeb in Vienna

**Thank you for your attention!**