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Title: Going beyond generalized least squares algorithms for estimating nuclear data observables

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Going beyond generalized least squares algorithms for estimating nuclear data observables

INT16-2a, Seattle, WA June 13-17, 2016

Speaker: D. Neudecker (Los Alamos National Laboratory)
P. Helgesson (Uppsala University),
D.L. Smith (Argonne Associate of Seville),
R. Capote (International Atomic Energy Agency),
P. Talou (Los Alamos National Laboratory)

Questions to the audience:

- **Are our statistical analysis methods mathematically sound?**

- **Are there better suited statistical methods to solve our physics problem?**

- **Can we use third (skewness) or fourth (kurtosis) moment of a probability distribution function as a measure to quantify how adequate a generalized least square technique is?**

Outline:

Introduction:

- The question we want to answer
- The physics problem
- The statistics problem

The study undertaken:

- Modeling the physics problem
- Preliminary results and conclusions

Introducing the physics and statistics problem:

The physics problem:

- Aim of a nuclear data evaluation at the example of prompt fission neutron spectra.
- The prompt fission neutron spectrum and challenges in quantifying it.

The statistics problem:

- Why is the generalized least squares technique insufficient for our needs?
- Alternative methods we are looking at.

What is the aim of the field of nuclear data evaluation?

Aim of nuclear data evaluations:

We provided **one recommended (i.e., evaluated) data set of a nuclear physics observable of interest for nuclear data application areas**.

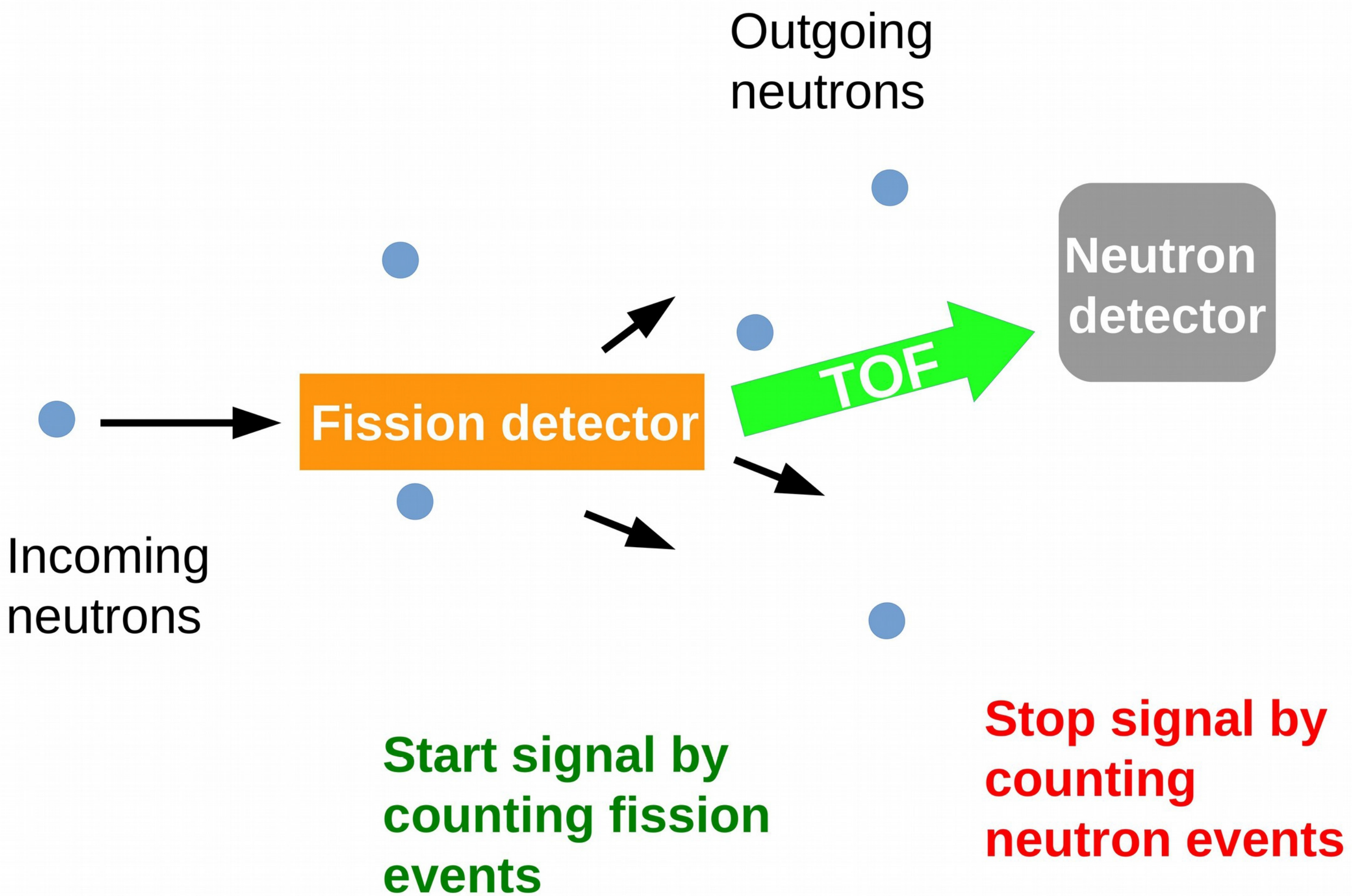
This recommended data set is often **obtained by a statistical analysis of experimental data and their covariances as well as model predicted values and their covariances.**

We provide recommended data in the form of **evaluated mean values and covariances.**

Here, **we look at prompt fission neutron spectra** as a representative example.

What is a prompt fission neutron spectrum (PFNS) & what is it needed for?

A PFNS gives the energy distrib. of neutrons emitted after scission & before β-decay



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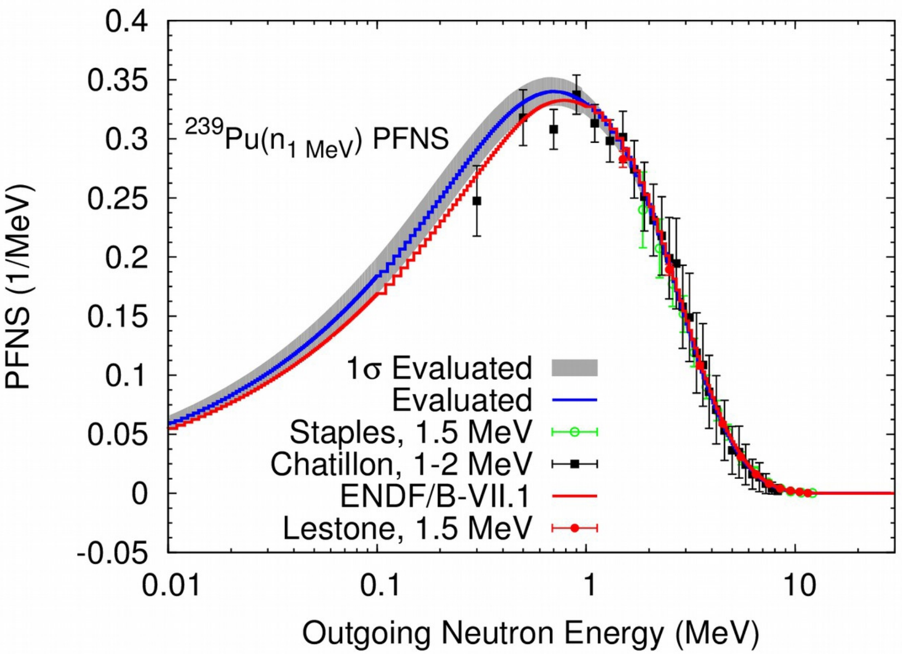
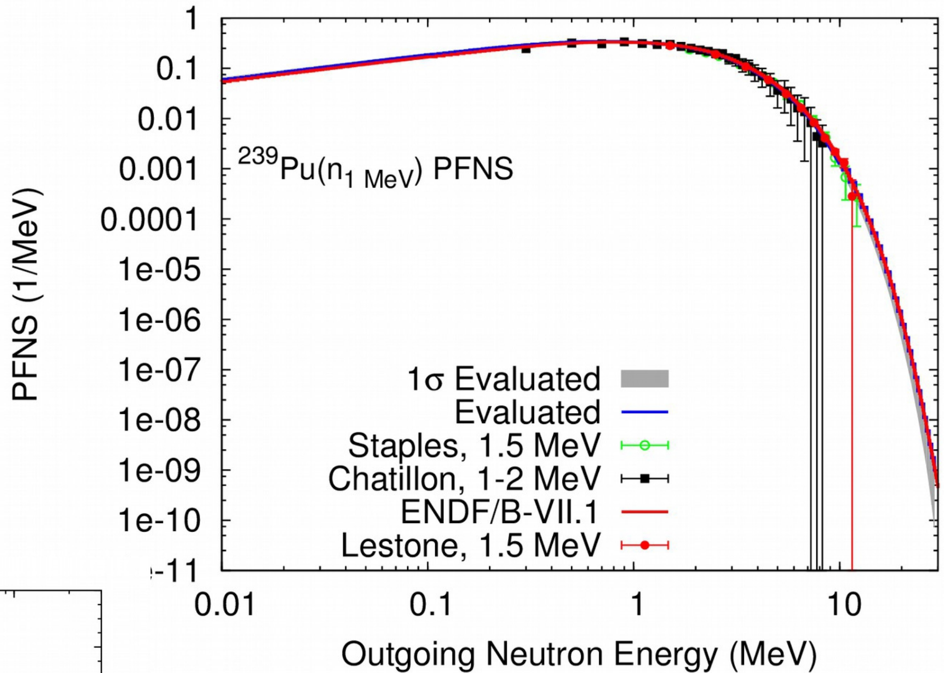
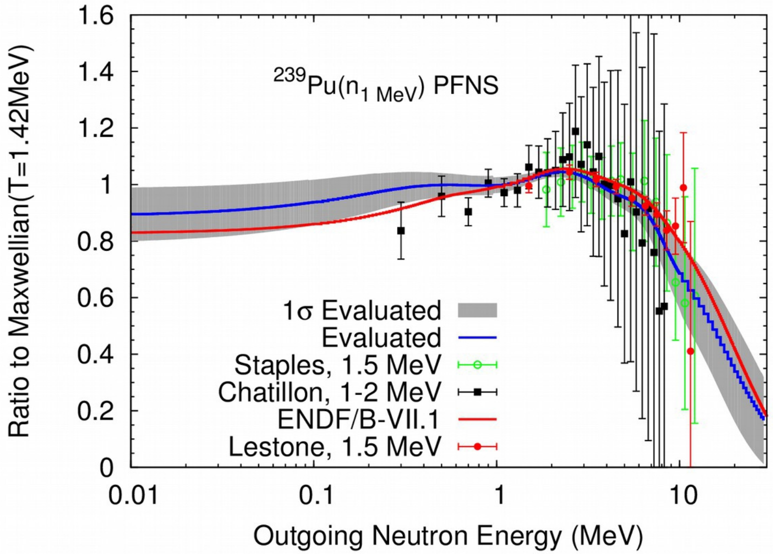
A PFNS covers many orders of magnitude.







$$Maxw \propto \sqrt{E} \exp(-E/T)$$

We need to provide a realistic evaluated PFNS and cov. for application needs:

- Development of innovative nuclear reactors (Generation IV reactors, small and modular reactors)
- Neutron Dosimetry
- Global Security
- Non-proliferation …

Not only mean values but also covariance matrices are needed!

What are the challenges encountered in evaluations of a PFNS?

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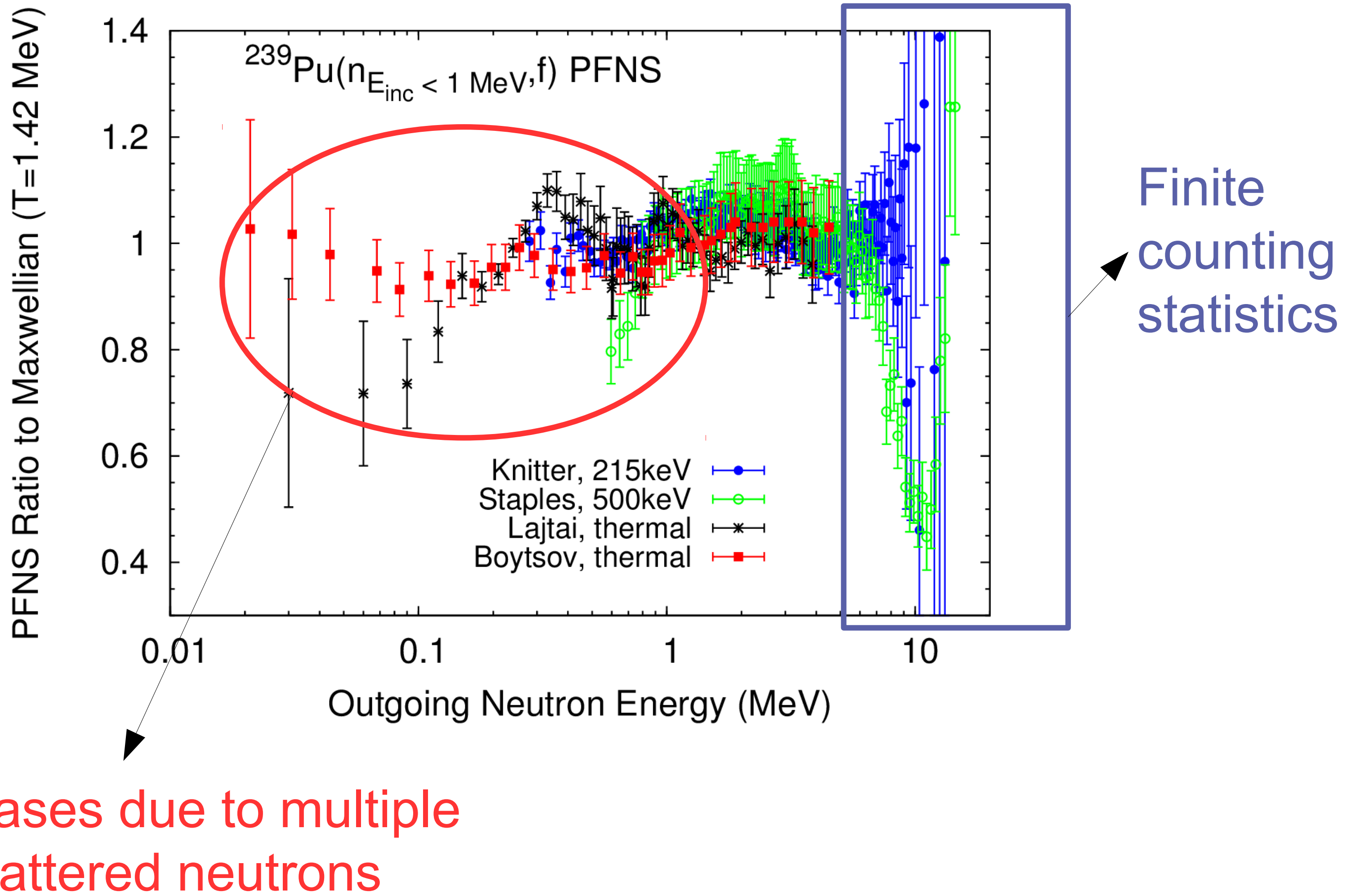
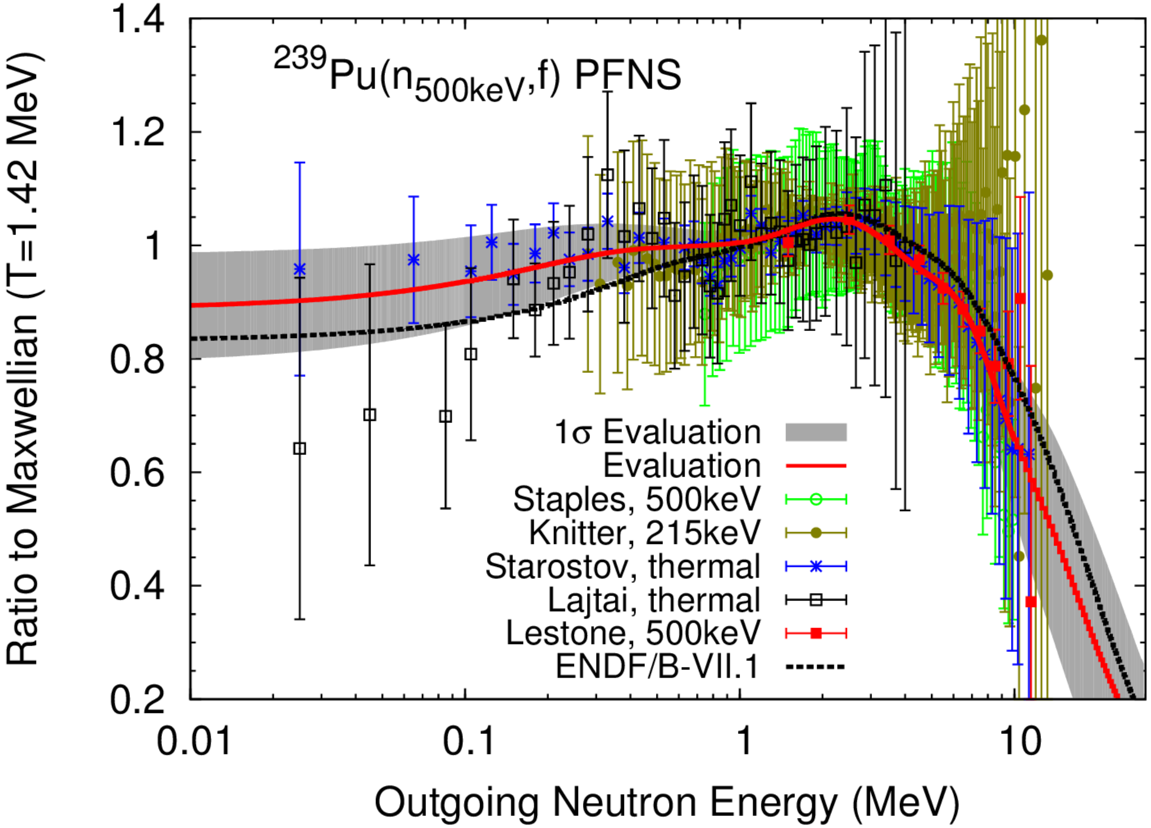
Experimental data are scarce and discrepant:



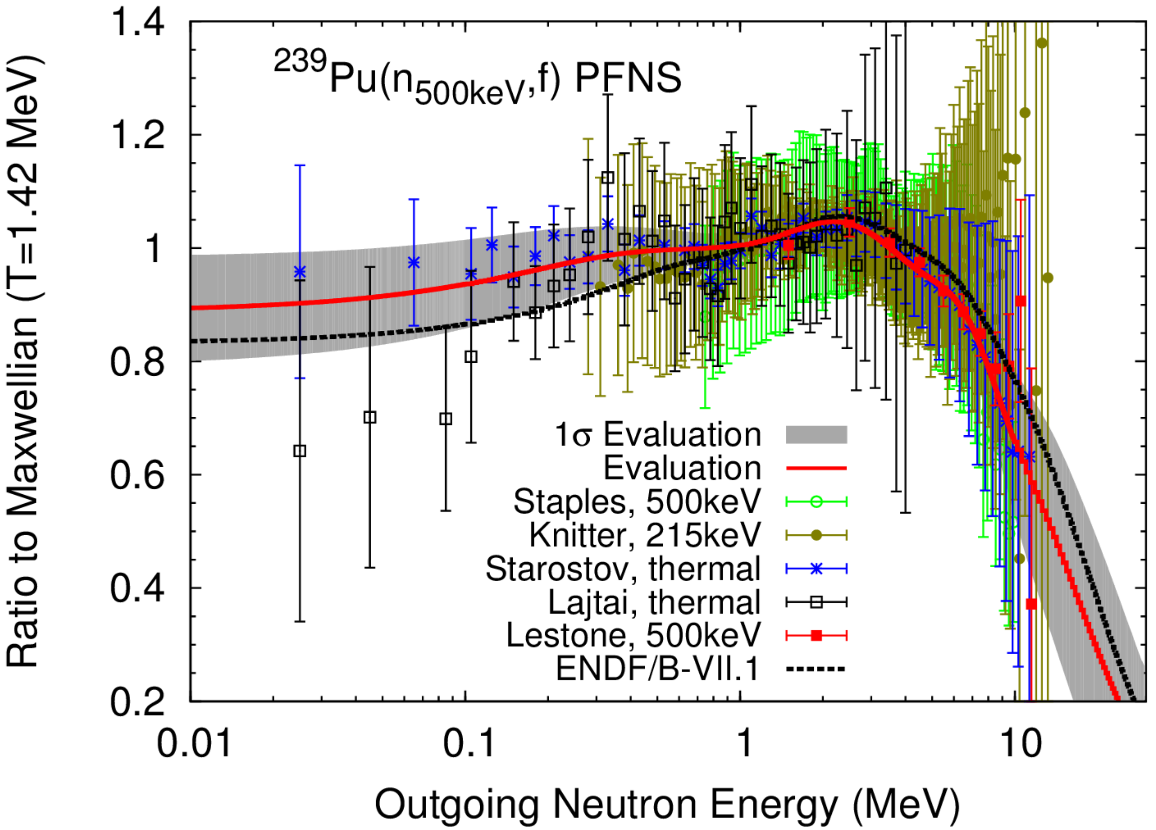
Currently used nuclear models are effective & their parameters fitted to exp. data.



Both the "evaluation" and "ENDF/B-VII.1" were obtained with the same nuclear model ***…. The differences impact application calculations distinctly!!!***

AND the model might be defective!

So, what is truth now??!!??



Why is the generalized least squares algorithm insufficient?

Generalized least squares is an algorithm we often use for evaluations.

The generalized least squares algorithm combines model ("M") and experimental mean values ("x") and their associated covariances to evaluated mean values and covariances ("post").

$$\underline{\phi}^{post} = \underline{\phi}^{M} + \mathbf{Cov}^{post}\mathbf{S}^{+}(\mathbf{Cov}^{x})^{-1}\left(\underline{\phi}^{x} - \mathbf{S}\underline{\phi}^{M}\right),$$

$$\mathbf{Cov}^{post} = \mathbf{Cov}^{M} - \mathbf{Cov}^{M}\mathbf{S}^{+}\left(\mathbf{S}\mathbf{Cov}^{M}\mathbf{S}^{+} + \mathbf{Cov}^{x}\right)^{-1}\mathbf{S}\mathbf{Cov}^{M}$$

It requires:

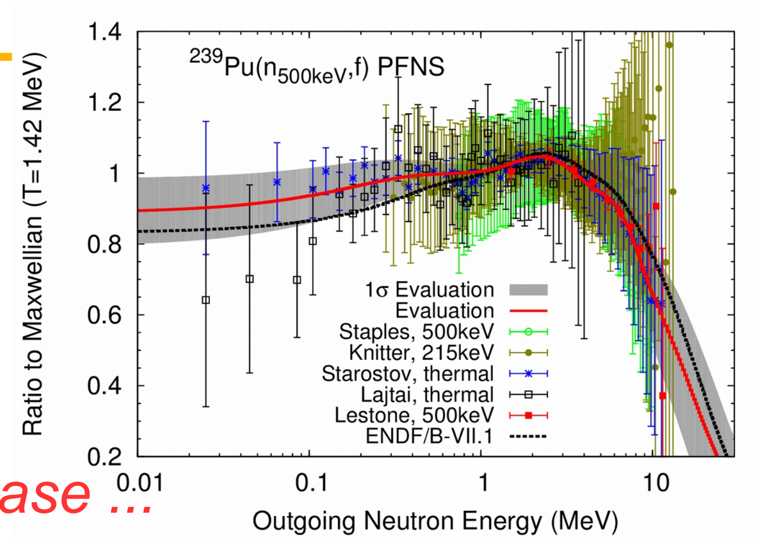
- ➢ Experimental data and model values to be normally distributed.
- ➢ Linear relationship between all observables.
- ➢ Non-discrepant data.
- ➢ Data that is less than ~30% uncertain.
- ➢ Data that should not cover many orders of magnitude.

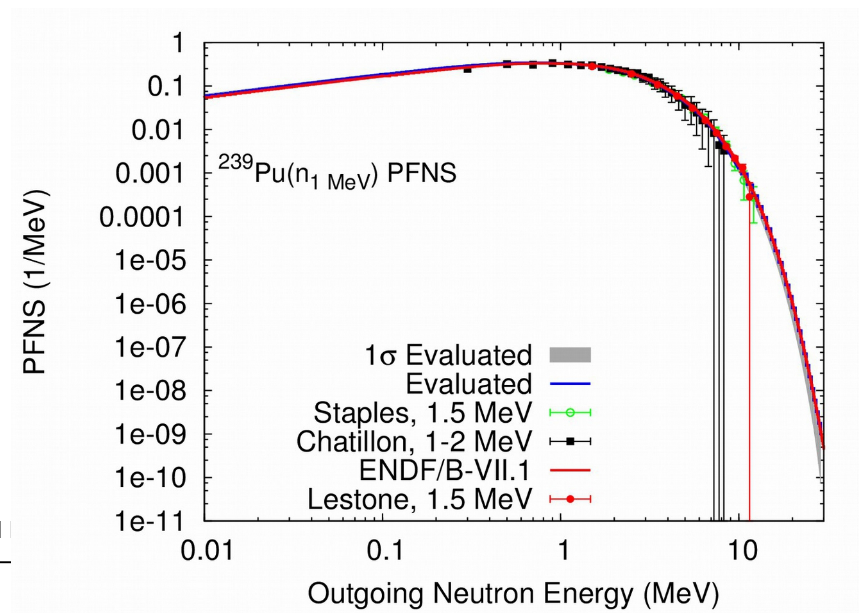
Generalized least squares is not ideal for evaluating PFNS.

It requires:

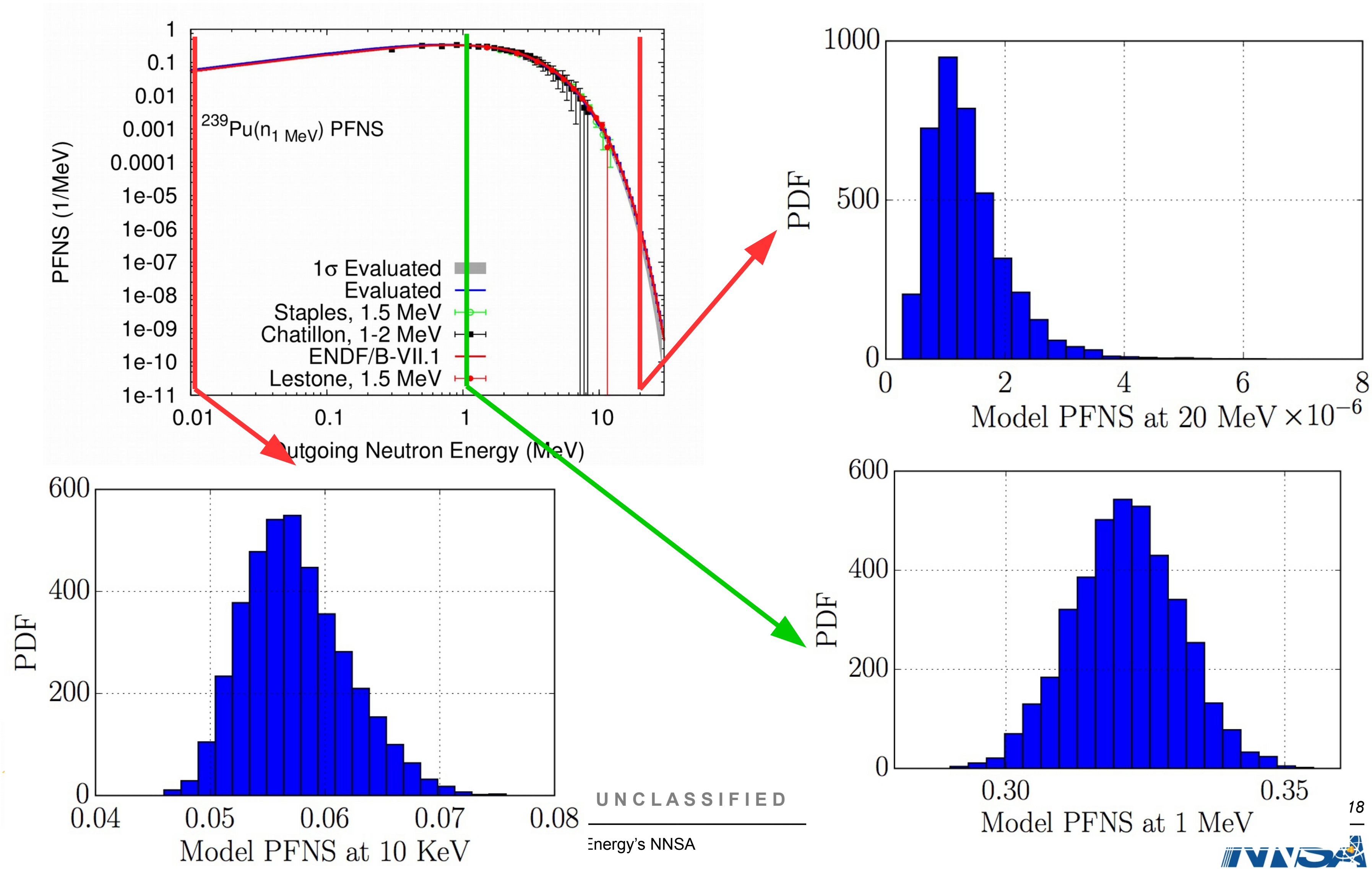
- Experimental data and model values are normally distributed.
- Linear relationship between all observables. ✔
- Non-discrepant data.
- Data that is less than ~30% uncertain.
- Data should not cover many orders of magnitude.

In this case ...

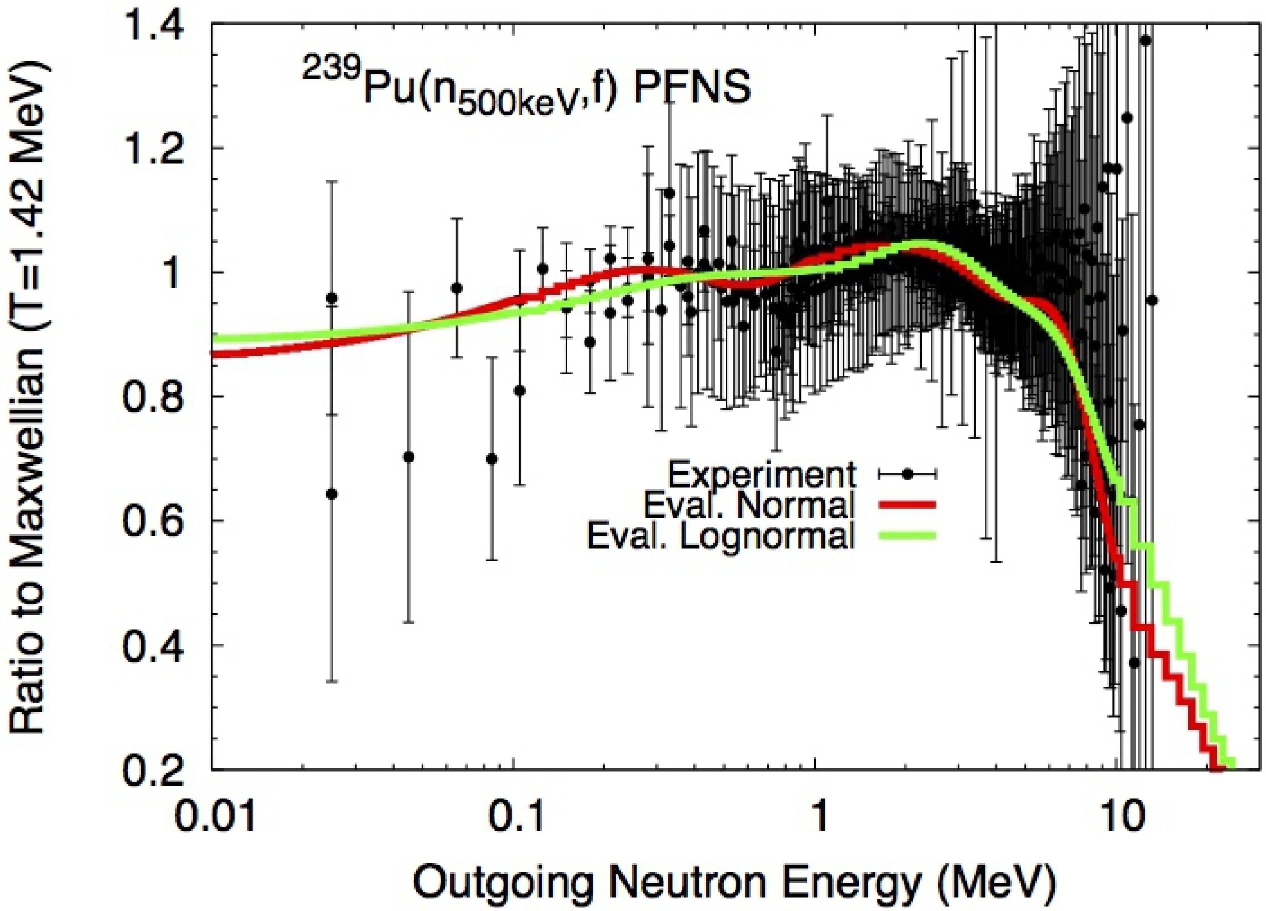




Model predicted values are NOT normally distributed.



We evaluate in log-space to get reasonable results … how close to truth is that?



Searching for alternative evaluation techniques based on Bayes theorem:

Unified Monte Carlo G (UMC-G) uses Bayes theorem and makes assumptions about pdfs.

Bayes Theorem: $p(\boldsymbol{\varphi}_{post}) = C\, L(\boldsymbol{\varphi}_X, Cov_X \,|\boldsymbol{\varphi}_M)\; p_0(\boldsymbol{\varphi}_M, Cov_M)$

For studies here, we assume:

Likelihood function L is normally distributed with exp. data φ_x & covariances Cov_x produced to mirror PFNS and its challenges

Prior pdf p_0 is normally distributed with prior mean values φ_M & covariances Cov_M calculated from model calculated values computed with sampled model parameters.

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Unified Monte Carlo B (UMC-B) weights model values compared to experimental data.

A set of model values $\varphi_M(p_k)$ is calculated by the model using a set of sampled parameters p_k.

Weights ω_k are calculated by comparing $\varphi_M(p_k)$ & experiment:

$$\omega_k = \exp\{-(1/2)[(\boldsymbol{\varphi}_{Mk} - \boldsymbol{\varphi}_x)^T \bullet \mathbf{Cov}_x^{-1} \bullet (\boldsymbol{\varphi}_{Mk} - \boldsymbol{\varphi}_x)]$$

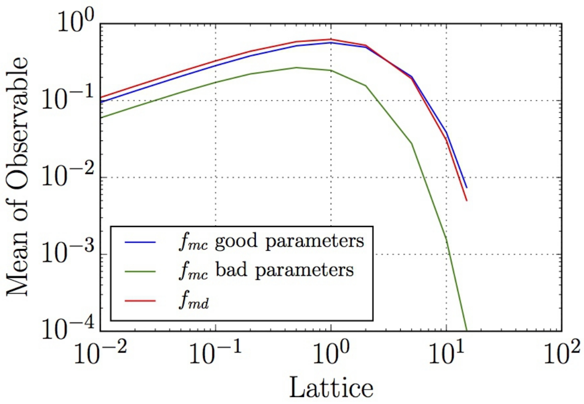
Posterior mean values and covariances are calculated by weighting $\varphi_M(p_k)$ with ω_k:

$$\langle\varphi_{post,i}\rangle \approx [\Sigma_{k=1,K}\, \omega_{k,i}\, \varphi_{Mk,i}] / [\Sigma_{k=1,K}\, \omega_k]\ , \ (i,j=1,m)$$

$$(\mathbf{Cov}_{post})_{ij} = [\Sigma_{k=1,K}\, \varphi_{Mk,j}\, \varphi_{Mk,i}\, \omega_k] / [\Sigma_{k=1,K}\, \omega_k] - \langle\varphi_{post,i}\rangle \langle\varphi_{post,j}\rangle\ .$$

Testing GLS, UMC-G & UMC-B and results.

- Building a test-case similar to a PFNS & its challenges

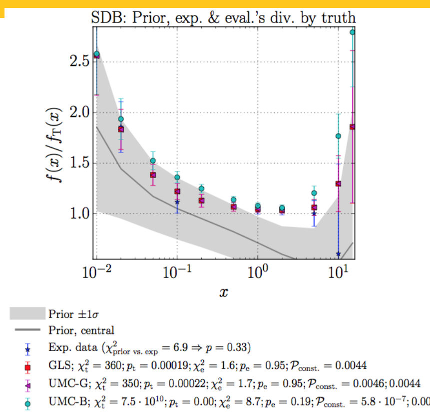


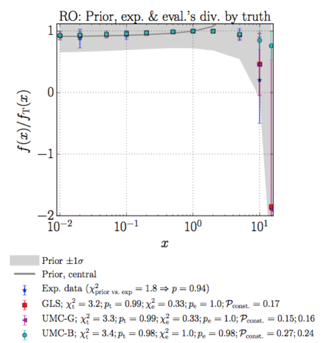
Experiment \ Model	$f_{E,r}$	$f_{E,r+s}$ with good experimental covariances	$f_{E,r+s}$ with bad experimental covariances
$f_{M,c}$ with overlapping parameter space			
$f_{M,c}$ with non-overlapping parameter space			
$f_{M,d}$			

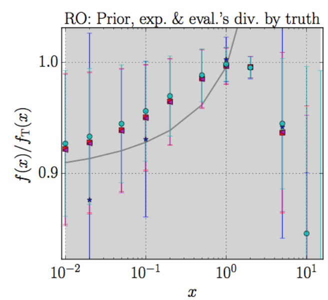
Question: *Which evaluation algorithm gives evaluated results closest to truth?*

- Testing how close GLS, UMC-G and UMC-B come to truth.

- Results







Generating a test surrounding similar to PFNS with a model close to truth and with defects.

Truth: $f_{\mathrm{T}}(x;\mathbf{a}) = \left(a_1\sqrt{x} + a_2 x\right)\exp(-x/a_3).$

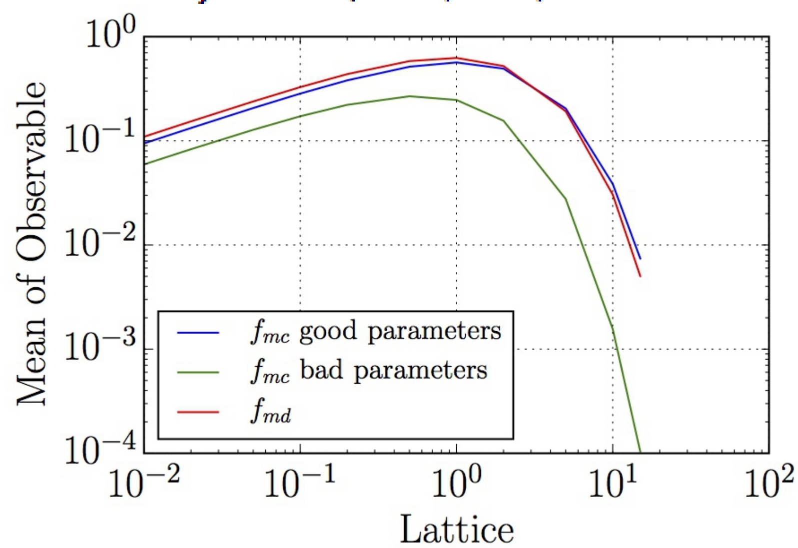
We test:

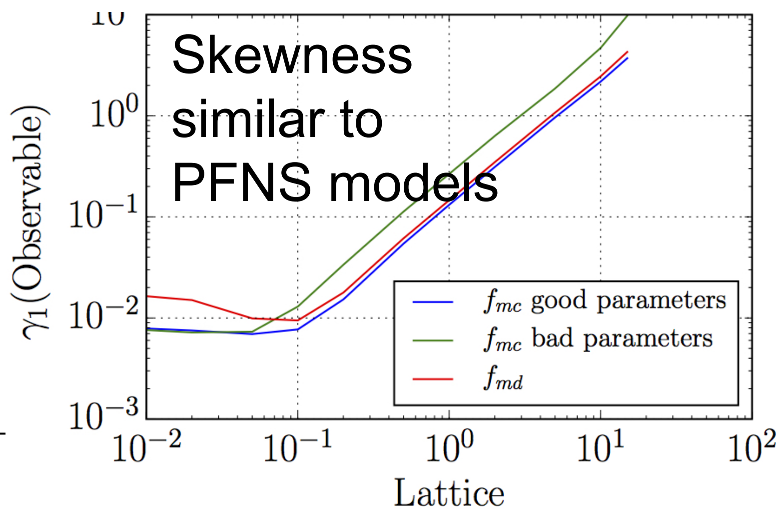
- **Model function = truth** & parameter space enclosing truth

- Model function = truth & **parameter space far from truth**

- Model function suffers from **model defect**

$$f_{\mathrm{M,d}}(x;\mathbf{c}) = \left(c_1\sqrt{x} + c_2/\sqrt{x}\right)\exp(-x/c_3),$$





Generating a test surrounding similar to PFNS with exp. Data close to truth and with biases

Truth: $f_{\mathrm{T}}(x;\mathbf{a}) = \left(a_1\sqrt{x} + a_2 x\right)\exp(-x/a_3).$

We test:

- **Experiment = truth+random error** $f_{\mathrm{E,r}}(x) = f_{\mathrm{T}}(x;\mathbf{a}) + \mathcal{E}_{\mathrm{r}}(x)$

- **Experiment = truth+random error+systematic biases & Cov_x accounting for it**

- **Experiment = truth+random error+systematic biases & Cov_x underestimated**

$$f_{\mathrm{E,r+s}}(x;\mathbf{d}) = f_{\mathrm{T}}(x,\mathbf{a}) + d_1 x^{-(d_2+1/4)}\exp(-x/a_3) + d_3 + \mathcal{E}_{\mathrm{r}}(x)$$

"Multiple scattering" "Background" "Counting statistics"

Generating a test surrounding similar to PFNS and testing how close we get to truth

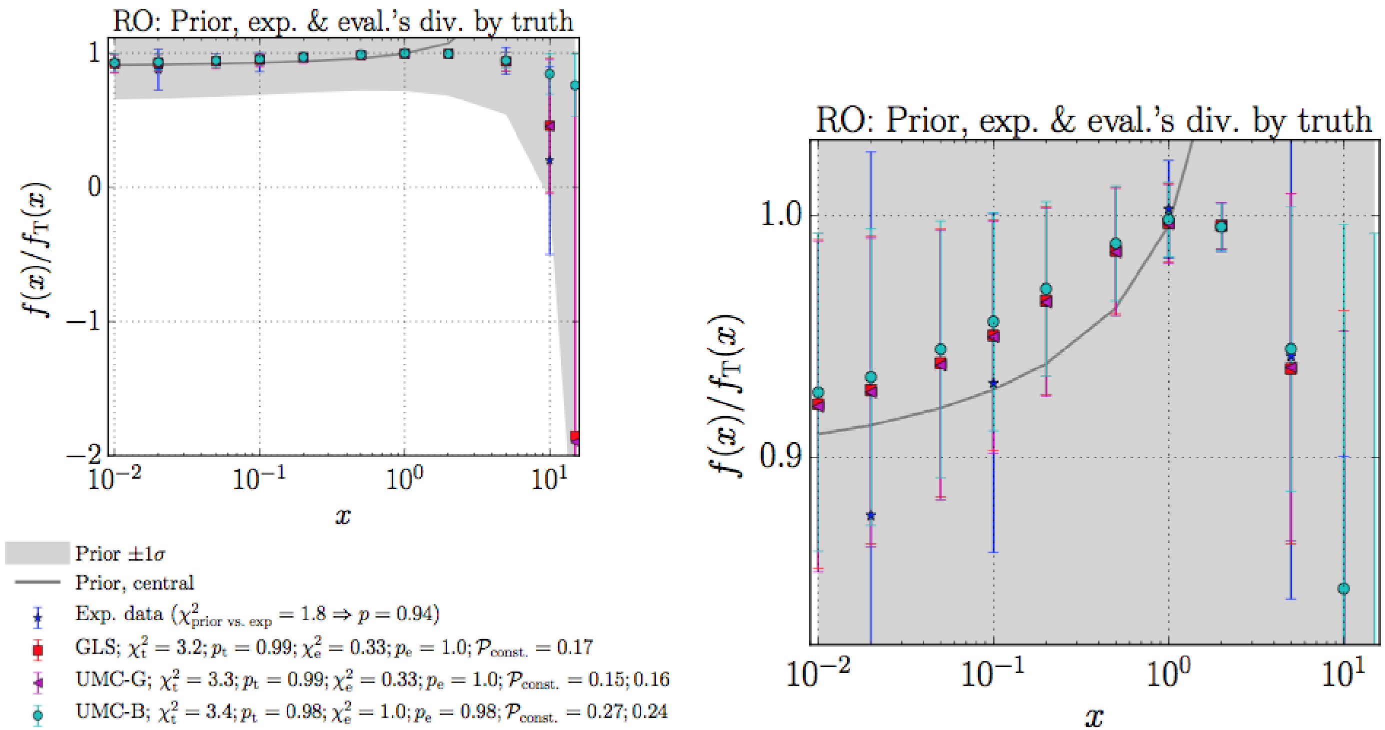
Experiment \ Model	$f_{E,r}$	$f_{E,r+s}$ with good experimental covariances	$f_{E,r+s}$ with bad experimental covariances
$f_{\mathrm{M,c}}$ with overlapping parameter space			
$f_{\mathrm{M,c}}$ with non-overlapping parameter space			
$f_{\mathrm{M,d}}$			

Study: Evaluating each case with GLS, UMC-G & UMC-B.

Question: *Which evaluation algorithm gives evaluated results closest to truth?*

RESULTS AND CONCLUSIONS ARE PRELIMINARY

Preliminary conclusion:UMC-B closest to truth if model=truth&parameter space good



<u>Experiment:</u> random experimental errors, no systematic biases,

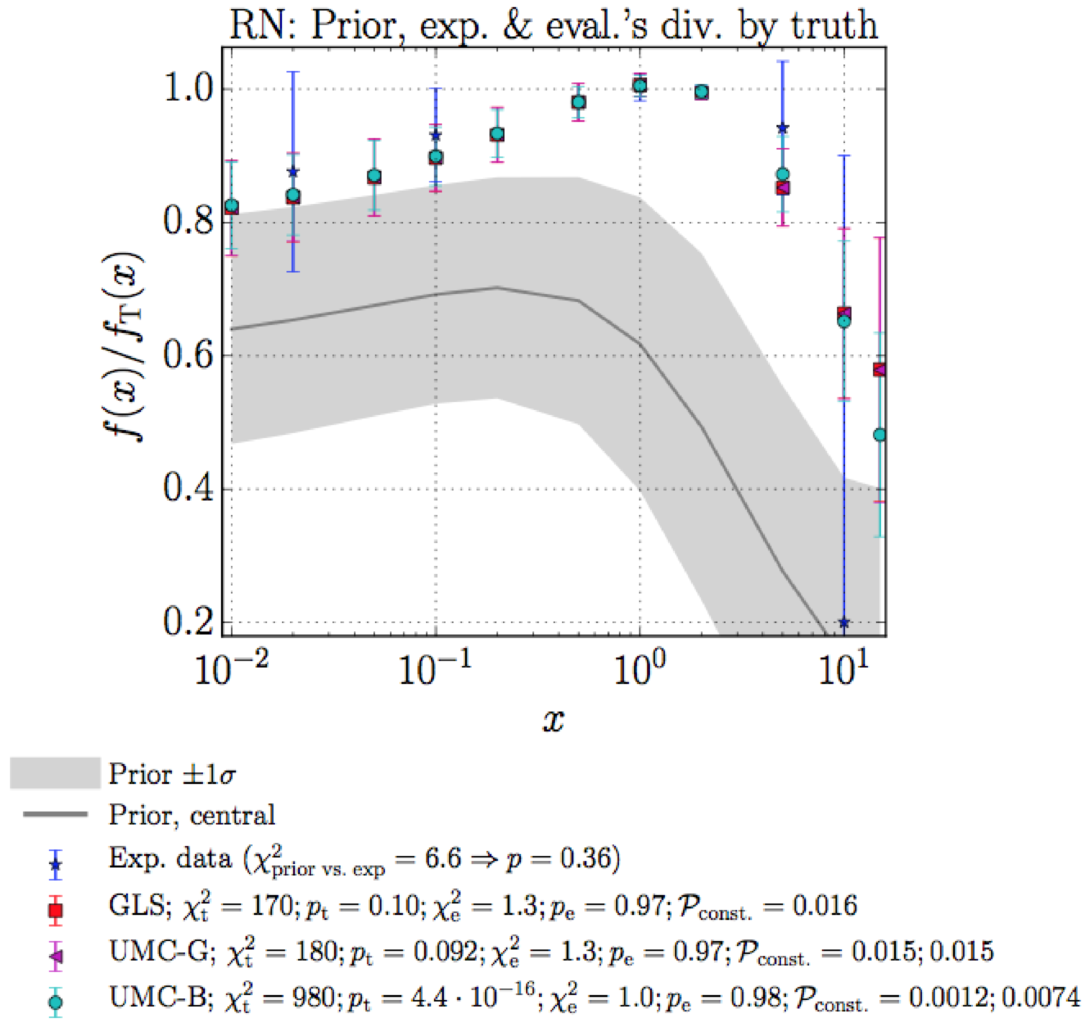
<u>Model:</u> same function as truth, parameter space encloses truth

Preliminary conclusion:UMC-B, GLS and UMC-G similar if model=truth&par. space bad

<u>Experiment:</u> random experimental errors, no systematic biases,

<u>Model:</u> same functional form as truth, parameter space does not enclose true parameters

“eval. Parameters” far from true ones → local maximum

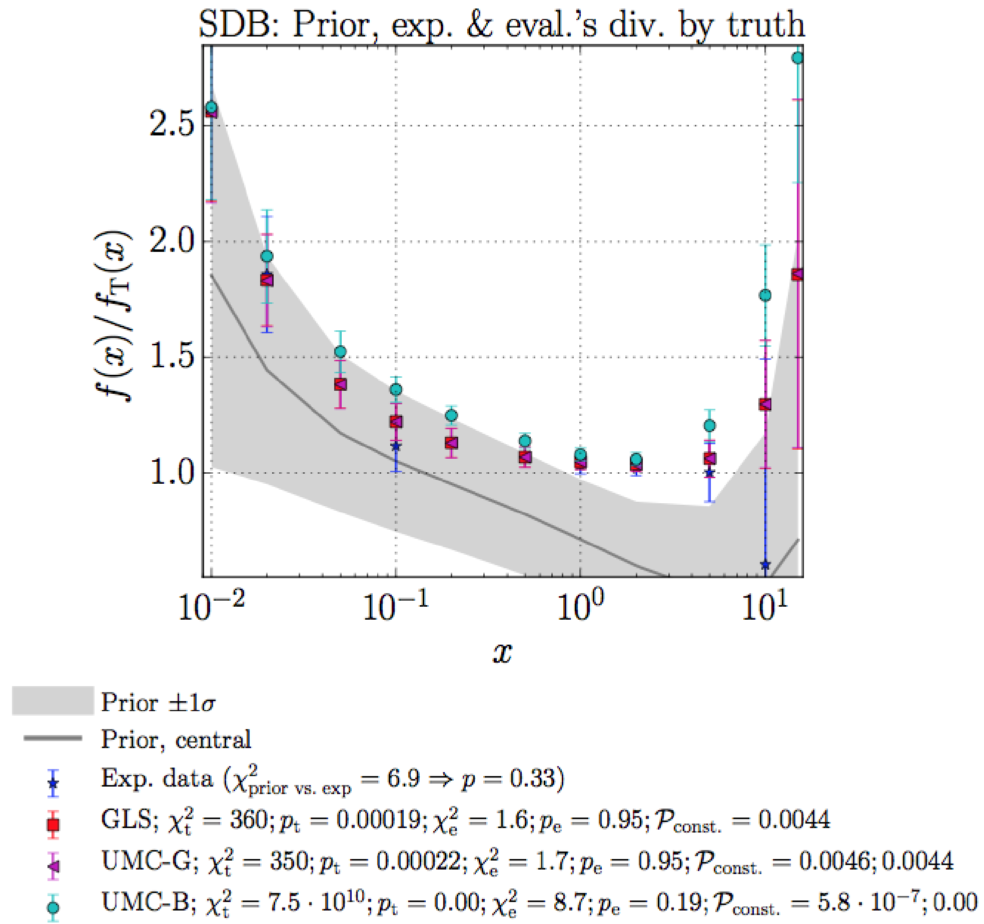


Preliminary conclusion:UMC-B farthest from truth if model defective

<u>Experiment:</u> random experimental errors, systematic biases, bad cov.

<u>Model:</u> defective

χ for UMC-B distinctly worse compared to model = truth



Preliminary conclusion:can we identify model defects by comparing GLS, UMC-B/G results?

- If model is good and a good parameter space was initially chosen → UMC-B best and comparable χ

- If model is good and a bad parameter space was initially chosen → UMC-B/G and GLS have similar χ and end up in local maximum

- If model is defective → UMC-B has the (distinctly!!) highest χ

→ can we use a comparison of evaluation results for UMC-B/G & GLS to diagnose model defects??

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- **Are our statistical analysis methods mathematically sound?**
- **Are there better suited statistical methods to solve our physics problem?**
- **Can we use third (skewness) or fourth (kurtosis) moment of a probability distribution function as a measure to quantify how adequate a generalized least square technique is?**

Thank you for your attention and your answers!

Literature:

UMC-G:

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D.L. Smith, Report ANL/NDM-166 (2008).
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UMC-B:

R. Capote et al., Proc. ISRD-14, Bretton Woods, ASTM STP-1550, 179 (2012).
See also: Journal of the ASTM International 9(4), JAI 104119 (2012).
P. Helgesson, Licenciate thesis, Uppsala Univ. (2015).
D.L. Smith et al., IAEA Report INDC(NDS)-0709 (2016).

PFNS:

R. Capote et al., Nuclear Data Sheets, Vol. 131, p. 1 (2016);
D. Neudecker et al., Nuclear Data Sheets, Vol. 131, p. 289 (2016);
D. Neudecker et al., Nucl. Instruments and Methods A, Vol. 791, p. 80 (2015).

Backup: Parameters for study shown

Truth: $f_\mathrm{T}(x;\mathbf{a}) = \left(a_1\sqrt{x} + a_2 x\right)\exp(-x/a_3).$ $a_1=1$; $a_2=0.5$; $a_3=2$

Model=Truth & good par. space: $b_1=0.9a_1$; $b_2=1.1a_2$; $b_3=1.15a_3$

Model=Truth & bad par. space: $b_1=0.6a_1$; $b_2=1.5a_2$; $b_3=0.6a_3$

Defective model: $f_\mathrm{M,d}(x;\mathbf{c}) = \left(c_1\sqrt{x} + c_2/\sqrt{x}\right)\exp(-x/c_3)$, $c_1=1.15$; $c_2=0.008$; $c_3=1.85$

Parameter uncertainties: 30% for b_1, b_2, b_3, c_1, c_3; 100% for c_2.

Exp.=Truth & random error: $f_\mathrm{E,r}(x) = f_\mathrm{T}(x;\mathbf{a}) + \mathcal{E}_\mathrm{r}(x)$ Random error is sampled around 0 with smallest unc. (~1%) at 1 MeV & largest unc. (~70%) at 10 MeV

Exp.=Truth & random+systematic error: $d_1=0.005$; $d_2=0.2$; $d_3=0.02$

$$f_\mathrm{E,r+s}(x;\mathbf{d}) = f_\mathrm{T}(x,\mathbf{a}) + d_1 x^{-(d_2+1/4)}\exp(-x/a_3) + d_3 + \mathcal{E}_\mathrm{r}(x)$$

Adequate systematic unc: Δd = (0.01, 0.5, 0.03)

Underestimated systematic unc: Δd = (0, 0, 0.03)