Bayesian Unified Monte Carlo Method for Evaluating and Utilizing Nuclear Reaction Data

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Outline of This Talk

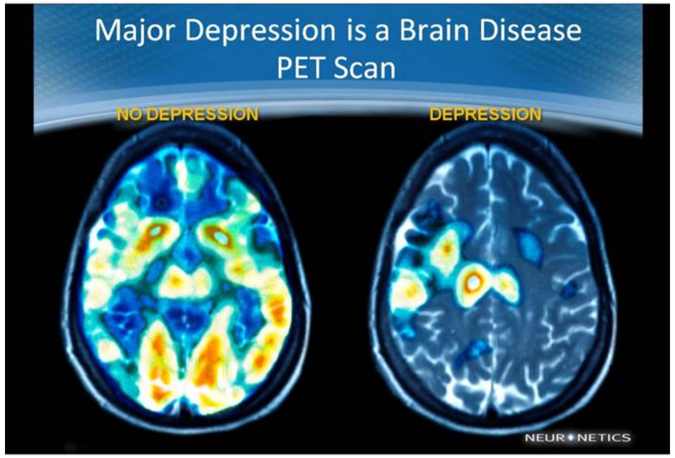
- Motivation and Background
- Historical Nuclear Data Evaluation
- Nuclear Data Evaluation in a Linear(ized) World
- Unified Monte Carlo: Beyond Linearity
- Evaluated Data Validation
- Wrap-up

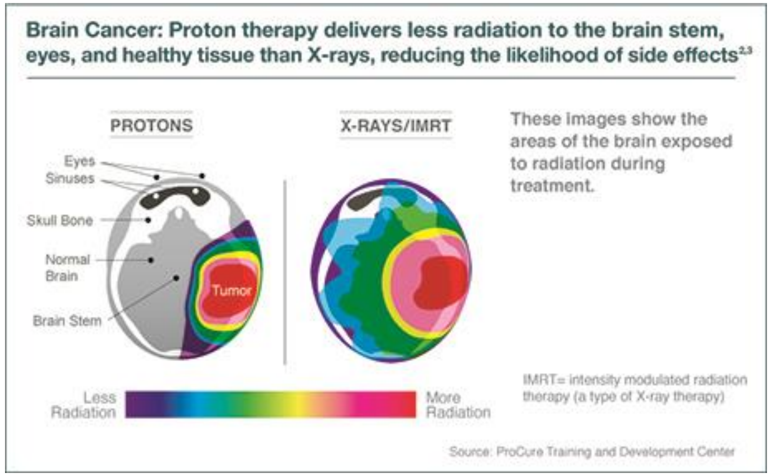
MOTIVATION AND BACKGROUND

Motivation

To develop comprehensive and accurate numerical data libraries containing recommended values for nuclear physics observables that are to be employed for computational analyses in a wide range of nuclear applications, and to accomplish this by using the best available theoretical and experimental information and mathematically well-justified data evaluation methods.

Medical Diagnostics



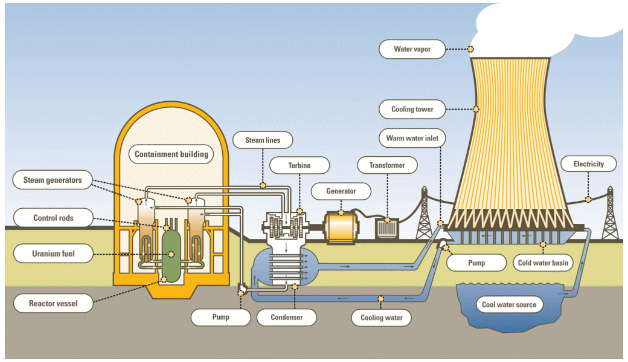


Medical Radiation Therapies

Nuclear Non-Proliferation

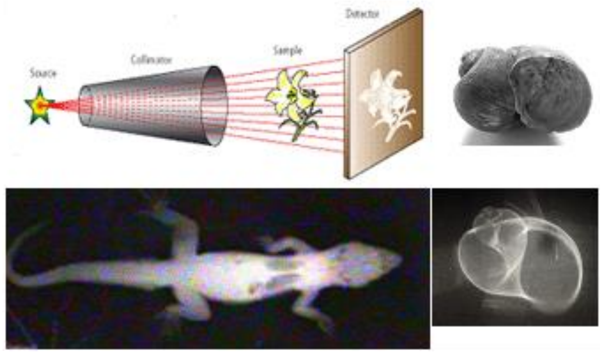
Nuclear Data Applications in Nuclear Technology

- System **modeling** plays a large role in system development by reducing time and cost.
- Broad scope of nuclear data needs: many elements, isotopes, reaction types, energy ranges, etc.
- Important societal implications:
  - Safety
  - Reliability
  - Cost



Nuclear Energy and Safety Technologies

Nuclear Propulsion



Neutron Radiography

Nuclear Data Library Requirements for Applications

- Provide recommended quantitative information on mean values and uncertainties for many elements and isotopes, nuclear processes, particles, angles, and energy ranges.
- Data sufficiently accurate and detailed for system modeling.
- Readable by system modeling codes (i.e., uses standard formats).
- Well validated by C/E comparisons with available nuclear system performance data from well-characterized integral benchmarks.
- Readily accessible to a wide range of users (i.e., not classified).

The following nuclear data libraries are intended to satisfy these requirements: **ENDF/B** (U.S.), **JEFF** (Europe), **JENDL** (Japan), **ROSFOND** (Russia), and **CENDL** (China). In reality there is a considerable degree of overlap in their content.

National Nuclear Data Center

ENDF/B Libraries are developed in the U.S. by CSEWG (National Lab, university, and foreign contributions).

ENDF B-VII.1

Formally Released: December 22, 2011

No.	NSUB	Sublibrary name	Short name	VII.1	VII.0	VI.8
1	0	Photonuclear	g	163	163	-
2	3	Photo-atomic	photo	100	100	100
3	4	Radioactive decay	decay	3817	3838	979
4	5	Spont. fis. yields	s/fpy	9	9	9
5	6	Atomic relaxation	ard	100	100	100
6	10	Neutron	n	**423**	393	328
7	11	Neutron fis.yields	n/fpy	31	31	31
8	12	Thermal scattering	tsl	21	20	15
9	19	Standards	std	8	8	8
10	113	Electro-atomic	e	100	100	100
11	10010	Proton	p	48	48	35
12	10020	Deuteron	d	5	5	2
13	10030	Triton	t	3	3	1
14	20030	^{3}He	he3	2	2	1

NOTE: ENDF/B-VIII.0 will be available for formal release in about a year.

Neutron Reaction Sub-library
[216.0 Mb zipfile]

Thermal Neutron Scattering Sub-library
[10.0 Mb zipfile]

Proton Reaction Sub-library
[13.6 Mb zipfile]

Triton Reaction Sub-library
[145.3 kb zipfile]

Neutron Induced Fission Product Yields Sub-library
[1.6 Mb zipfile]

Decay Reaction Sub-library
[13.7 Mb zipfile]

Atomic Relaxation Reaction Sub-library
[1.6 Mb zipfile]

Full ENDF/B-VII.1 Library

[325.82 Mb tarball]

All these files are highly compressed!

Neutron Standards Sub-library
[225.4 kb zipfile]

Photonuclear Sub-library
[56.2 Mb zipfile]

Deuteron Reaction Sub-library
[89.5 kb zipfile]

Helium-3 Reaction Sub-library
[115.4 kb zipfile]

Spontaneous Fission Product Yields Reaction Sub-library
[295.1 kb zipfile]

Photoatomic Reaction Sub-library
[7.5 Mb zipfile]

Electron Reaction Sub-library
[7.0 Mb zipfile]

The entire ENDF/B-VII.1 library or portions of it can be downloaded from the following website: **http://www.nndc.bnl.gov/endf/b7.1/download.html**

HISTORICAL NUCLEAR DATA EVALUATION

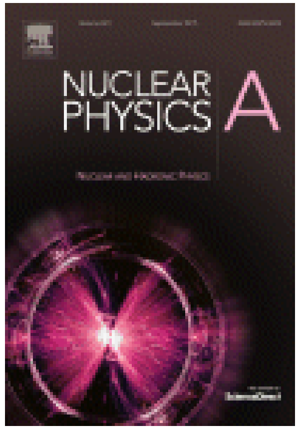
Persistent Challenges to Nuclear Data Evaluation

- Nuclear Theory and Modeling:
  - Even the best nuclear theories tend to have limited quantitative predictability.
  - Most theoretical models are known to have some unresolved defects.
  - A "unified" theory that applies for all nuclei and processes does not exist.

- Experimental Data:
  - Often not sufficiently comprehensive (sparse or lacking).
  - Data are excessive in some cases, and this too can introduce difficulties.
  - Unresolved discrepancies.

- Evaluation Procedures:
  - Required assumptions are often not satisfied.
  - Computational challenges (number crunching).
  - Difficulties in estimating and dealing with data correlations.
  - Difficulties in reconciling differential and integral data.

Nuclear Reaction Data Evaluation in the “Good Old Days” (≤ early 1970’s)



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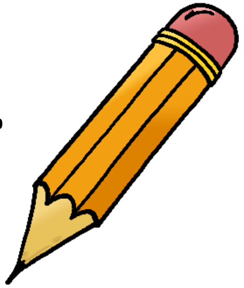

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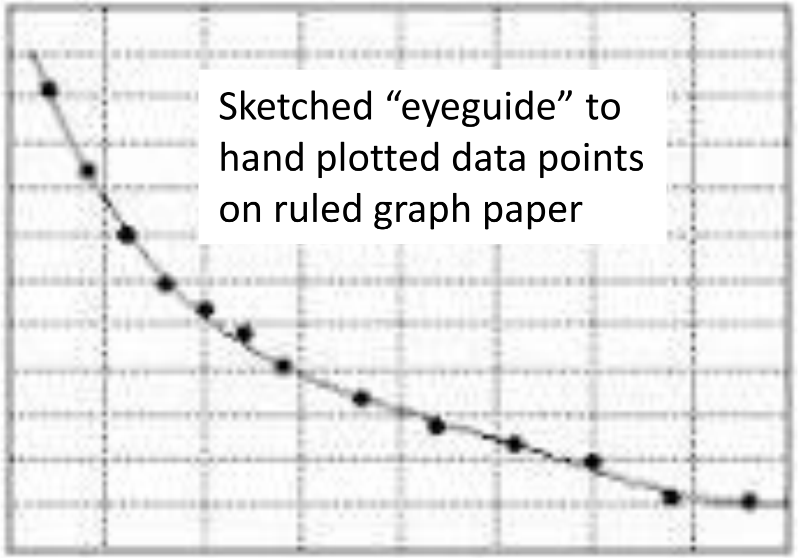
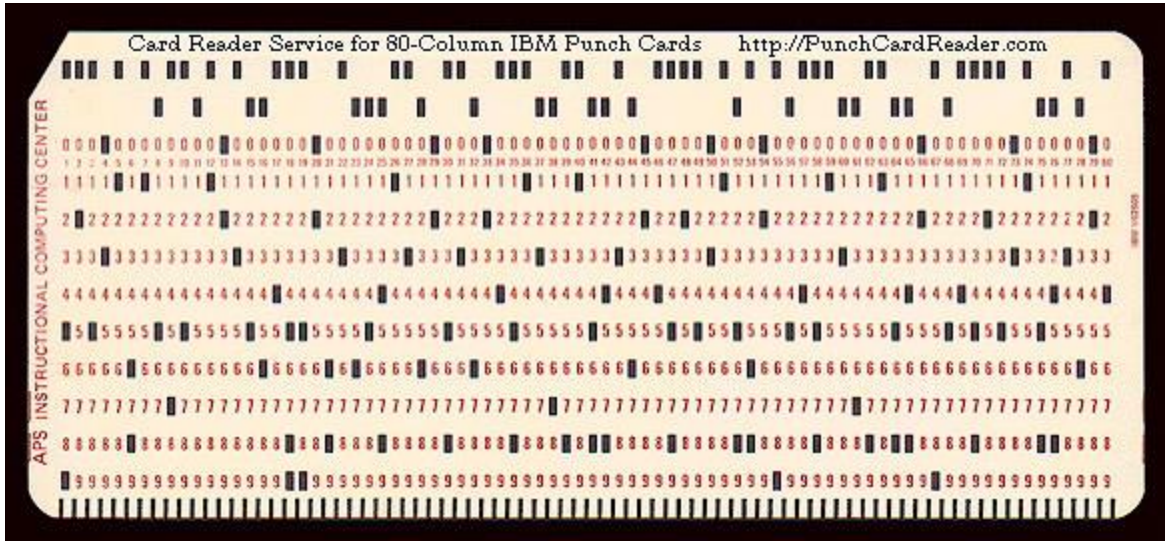


E(1)	Sigma(1)
E(2)	Sigma(2)
….	
E(n)	Sigma(n)



NUCLEAR DATA EVALUATION IN A LINEAR(IZED) WORLD

Deterministic Linear Model Data Uncertainty Propagation

<u>Single Variable</u>

If "model" function "$\mathcal{M}$" is truly linear in parameter "x":

$y = \mathcal{M}(x) = a\,x + b$ ("a" and "b" are constants)

$\Delta y = a\,\Delta x$

➔ $\mathrm{var}(y) = a\,(\Delta x)^2\,a = a\,\mathrm{var}(x)\,a$

If "$\mathcal{M}$" is non-linear in x:

$y = \mathcal{M}(x) = \mathcal{M}(x_0) + (d\mathcal{M}/dx)_0\,(x - x_0) +$ higher-order terms

$\mathrm{var}(y) \approx (d\mathcal{M}/dx)_0\,\mathrm{var}(x)\,(d\mathcal{M}/dx)_0 +$ higher-order terms

<u>Multiple Variables</u> (**"Law" of Error Propagation**)

y (dimension "m") :: **x** (dimension "n")

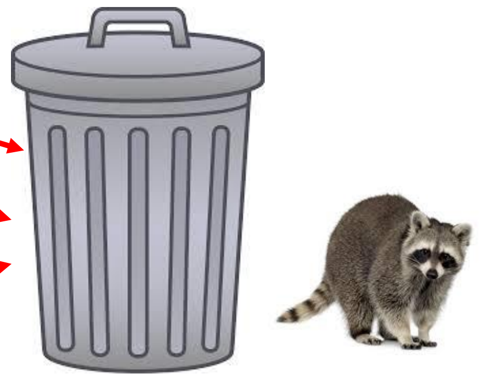
$\mathcal{M}$ (a model algorithm, e.g., "m" model functions)

$\mathbf{y} = \mathcal{M}(\mathbf{x})$ :: $\mathbf{y}_0 = \mathcal{M}(\mathbf{x}_0)$

$\mathbf{V}_y = \mathbf{A}^+\,\mathbf{V}_x\,\mathbf{A} +$ higher-order terms

$(\mathbf{A})_{ij} = [\partial\mathcal{M}_i(\mathbf{x})/\partial x_j]_0$ :: **A** (n x m "sensitivity" or "model design" matrix)

If $\mathcal{M}$ is a collection of functions, some of whose members may be highly non-linear, and if some of the variances in $\mathbf{V}_x$ are large, this "trash pail" may become stuffed with a considerable quantity of "**mathematical debris**" whose neglect could result in undesirable consequences in evaluations, including misleading biases and poor estimates of variances for the derived $\mathbf{V}_y$.



Linear uncertainty propagation generates approximate uncertainties and correlations

Experimental Data for Nuclear Reaction Evaluations

- Evaluators must rely on data provided by experimenters and experimental data compilers.
- Experimenters tend to do a rather "limited" job of estimating and reporting uncertainties for their experiments (and correlations are **in**frequently considered and reported).
- Data compilation efforts have improved considerably during the past 20 years (e.g., **EXFOR**), but compilers cannot document such information unless it is provided and approved by experimenters.
- For realistic evaluation exercises involving many reaction processes and large bodies of experimental data, it is necessary for evaluators to automatically acquire and manipulate experimental data information that is available from data centers in the form of compilations such as EXFOR.
- The available experimental data are frequently related indirectly to the variables that are to be evaluated (e.g., cross-section ratios, integral data, data at arbitrary energies and angles, etc.)
- To perform a "modern evaluation", an evaluator must assemble a collection of pertinent mean values and their covariance matrices from many origins, often reflecting widely variable reliability.

EXFOR (EXchange FORmat)

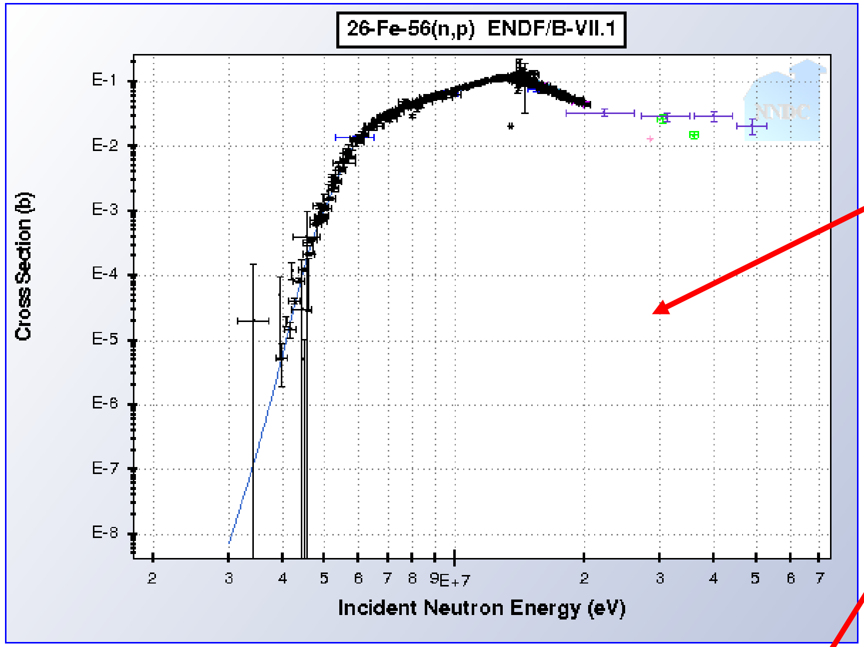
- An ongoing international collaboration with the mission of compiling experimental nuclear reaction data and making it readily available on-line in adopted standardized formats.
- Coordinated by IAEA Nuclear Data Section – Vienna, Austria.
- Website: https://www-nds.iaea.org/exfor/exfor.htm
- Provides numerical data plus information on data sources (reports, journal articles, author communications, etc.)
- Also, some descriptive information is usually available.
- Computer readable "computational" files are provided for automatic handling of large quantities of data.
- EXFOR data are also available from collaborating nuclear data centers (e.g., BNL-NNDC and NEA Data Bank - Paris).

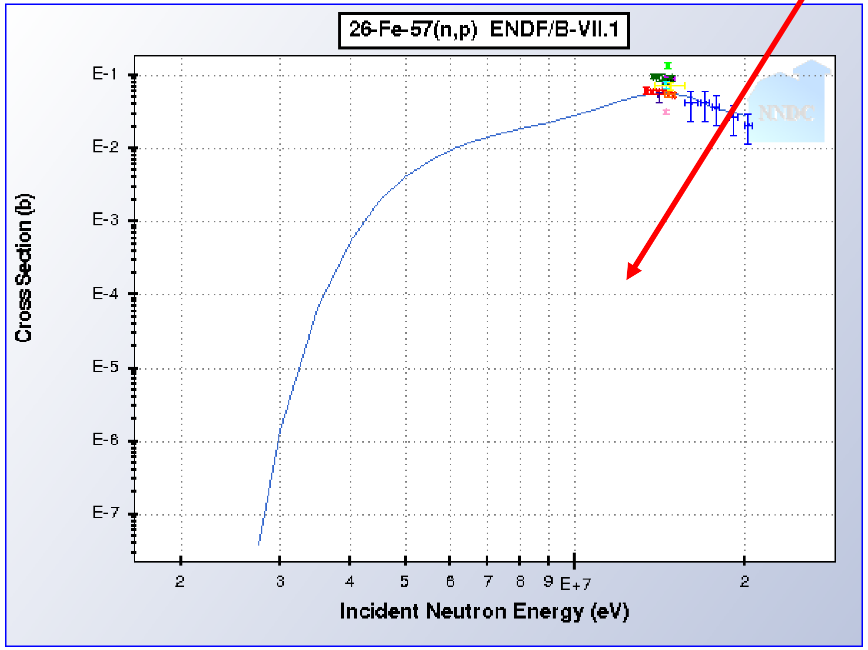
Example of an EXFOR File*

```
SUBENT        22282002   20080204
BIB                  5         20
REACTION    ((90-TH-232(N,F),,SIG)/(92-U-235(N,F),,SIG))
ERR-ANALYS  (ERR-T)        Total uncertainty
            (MONIT-ERR)    235U(n,f) monitor cross section (4%)
            (ERR-1)        Number of U-235 atoms          (1.47%)
            (ERR-2)        Number of Th-232 atoms         (1.64%)
            (ERR-3,,0.887) Fission rate ration           (<0.887%)
            (ERR-4,,0.276) Correction factor             (<0.276%)
COVARIANCE  (COR,ERR-T,PER-CENT) Macro correlation coefficients
             100
              87     100
              86      87     100
              87      87      87     100
ENDBIB                20
COMMON                 3          3
MONIT-ERR   ERR-1      ERR-2
PER-CENT    PER-CENT   PER-CENT
 4.          1.47       1.64
ENDCOMMON              3
DATA                   5          4
EN          EN-ERR     DATA       ERR-T
MEV         MEV        NO-DIM     PER-CENT
  13.47       0.18       0.150     2.41
  14.00       0.06       0.158     2.38
  14.46       0.16       0.166     2.37
  14.89       0.29       0.181     2.38
ENDDATA                6
ENDSUBENT             35
```

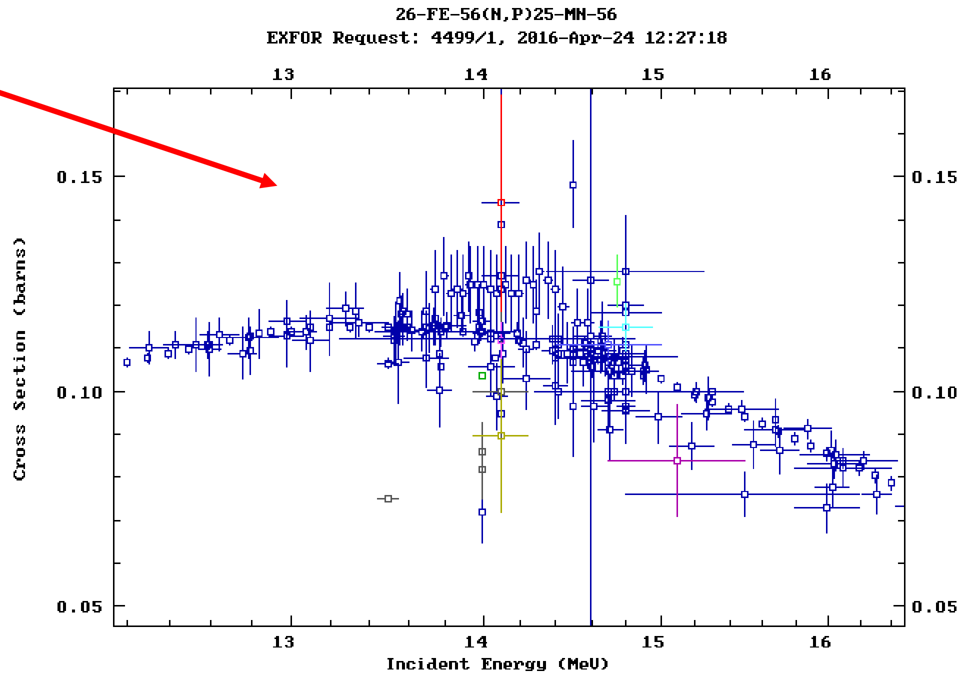
* 80-column ASCII format. Many EXFOR files are much longer and contain considerably more information than this one.

Experimental data can be "uncooperative" …





- **Too much experimental data**, even if consistent, can result in unrealistically small evaluated uncertainties if the data are treated as uncorrelated … and estimating correlations can be difficult.
- **Too little experimental data** places a heavy demand on modeling.
- **Discrepant experimental data** Forces an evaluator to make hard choices: estimate corrections, keep or discard, down-weight, etc.



Least-squares Data Evaluation in a Linear(ized) World [~ mid 1970]

- The Generalized Least-Squares Method (GLS) is the "workhorse" of contemporary nuclear reaction data evaluation activities. It has been used to produce many of the evaluations included in ENDF/B.
- GLS is based on the **assumptions** that the data being evaluated are **normally (Gaussian) distributed**, that **linear relationships** exist between the various involved variables (both primary and derived), and that the model and experimental data are **uncorrelated**.
- There are two distinct approaches to applying GLS:
  1) Essentially **averaging (merging)** theoretical model-calculated and experimental information.
  2) Employing experimental data to adjust assumed prior values of model parameters and then using the **adjusted models** to derive mean values and covariances that constitute the evaluations.
- Both variants are **conceptually Bayesian** although probability functions are not considered explicitly.
- The equations used are relatively simple, but assembling the required information and performing the analyses for large-scale evaluations is very challenging, both administratively and computationally:

$$[y-y_a-A(p-p_a)]^+V_y^{-1}[y-y_a-A(p-p_a)] + (p-p_a)^+V_a^{-1}(p-p_a) = \text{minimum}$$

$$p = p_a + V_aA^+(Q+V_y)^{-1}(y-y_a),$$

$$Q = AV_aA^+,$$

$$V_p = V_a - V_aA^+(Q+V_y)^{-1}AV_a,$$

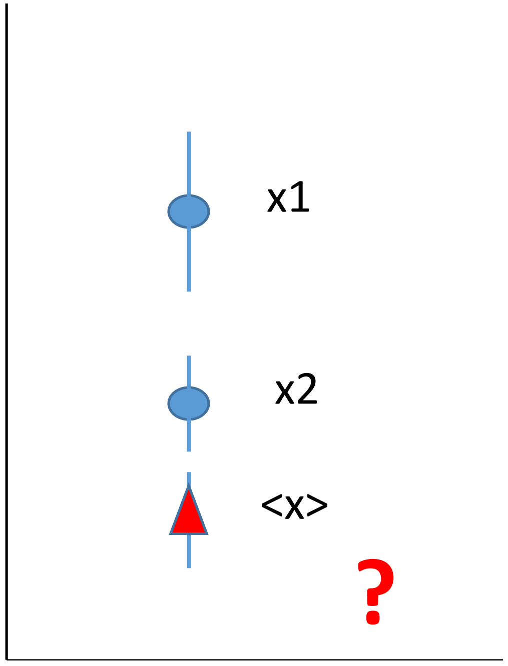
$$(\chi^2)_{min} = (y-y_a)^+(Q+V_y)^{-1}(y-y_a)$$

These equations* show the least-square condition in linear form as well as the solution mean values and covariance matrix. The subscript "a" refers to prior information that usually is generated from nuclear model calculations.

* D.L. Smith, Report ANL/NDM-128, Argonne National Laboratory (1993).

A Celebrated Problem Encountered with GLS: “Peelle’s Pertinent Puzzle” (PPP)

- By ≈1987 it was clearly evident that some evaluations produced by the least squares method (GLS) yielded **unreasonable solutions** (e.g., “too low” mean values). This effect was first described by Robert Peelle ,ORNL.
- Discovery of the PPP phenomenon challenged the previously assumed **invincibility** of the GLS evaluation method.
- PPP was eventually attributed to improperly constructed covariance matrices, nonlinearities, discrepancies, large uncertainties, and strong correlations (usually the consequence of “hidden” variables).
- “Fixes” (approximations) to deal with the PPP effect have been suggested (and used) to “minimize” its impact in practical evaluations.
- A better solution would be to avoid “hidden” variables as much as possible by including them in the evaluation process. (Kenneth Hanson, LANL).



Comment: PPP may be mitigated by these “fixes” but the effect never goes away completely as long as GLS is strictly applied.

UNIFIED MONTE CARLO: GOING BEYOND LINEARITY

Desired Features of an Advanced Data Evaluation Method

- Able to deal with nonlinear theoretical models without the need to linearize them.
- Able to handle model and experimental data that are not necessarily normally distributed (Gaussian) w/o the need to reject useful information.
- Able to include accurate integral data in a way that reduces uncertainties while avoiding introducing biases (QUESTION: Any ideas how to do this?).
- Consistent with Bayesian statistical concepts.
- Evaluated results converge to the Generalized Least-Squares (GLS) solution when the conditions for GLS are adequately satisfied.
- Computationally "manageable".
- Offer the possibility for seamless progression from (models + experiments) ➔ evaluated results ➔ derived results for system variables.

Variable Transformation and Stochastic Uncertainty Propagation [~ 2004]

- Model parameters **x** (vector dimension "n") are governed by a normalized probability density function *r*(**x**). If all that is known about these parameters are mean values <**x**> and covariance matrix $\mathbf{V}_x$, then we assume *r* is a multi-variable normal distribution (according to Jaynes' Principle of Maximum Entropy).

- Generate a collection of values $\{\mathbf{x}_k\} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k, \ldots \mathbf{x}_K\}$ through random sampling in a manner consistent with the probability function *r*. Note that K will need to be a rather large number (as large as necessary to achieve statistical convergence in computational applications that employ these values).

- Derived variables **y** (vector dimension "m") are then calculated using a model $\mathfrak{M}$ such that $\mathbf{y} = \mathfrak{M}(\mathbf{x})$.

- Generate a corresponding collection of random values $\{\mathbf{y}_k\}$ by applying the relation $\mathbf{y}_k = \mathfrak{M}(\mathbf{x}_k)$, (k=1,K).

- The $\mathbf{y}_k$ will be distributed according to an inherent prior probability function p_0, which is unlikely to be expressible analytically but can be characterized by its moments that can be calculated from the collection $\{\mathbf{y}_k\}$, e.g., mean values <**y**>, covariance matrix $\mathbf{V}_y$, skewness, kurtosis, etc.

Information of potential value is not explicitly discarded by this stochastic approach.

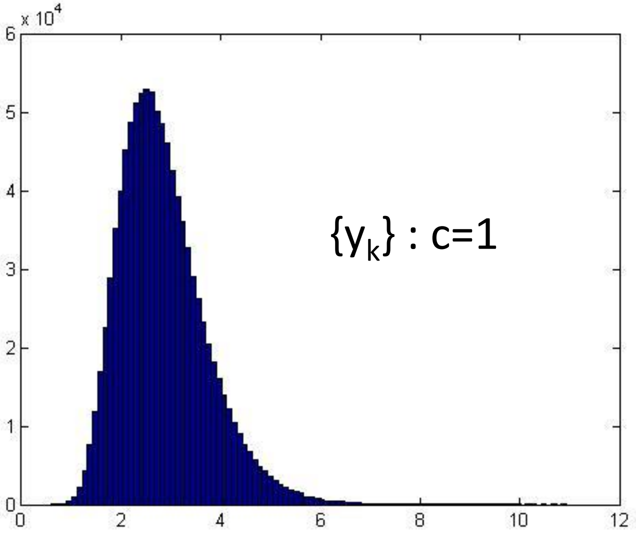
Mean Values: $\langle y_i \rangle = y_{i0} \approx (1/K) \times \Sigma_{k=1,K}\, y_{ik}$ for i = 1,m

Covariances: $V_{yij} \approx (1/K) \times \Sigma_{k=1,K}\, (y_{ik}-y_{i0})(y_{jk}-y_{j0})$ for i,j = 1,m

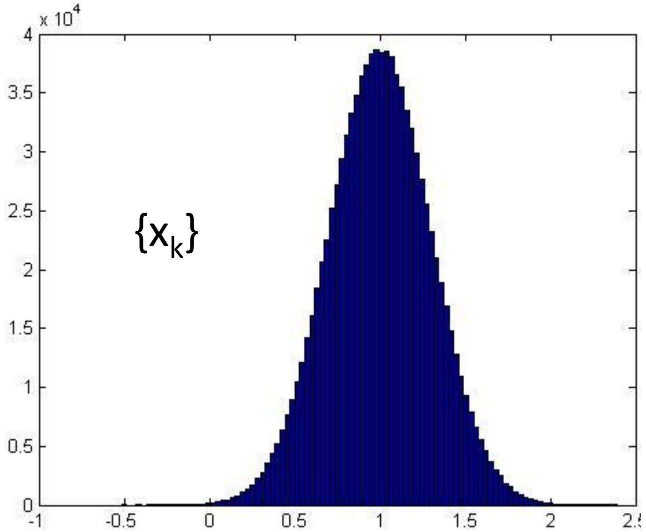
Moments of any order can be calculated in principle, but the higher the order, the bigger K must be to achieve statistical convergence, e.g., mean values ($K>10^3$), covariances ($K>10^4$), skewness ($K>10^5$), etc.

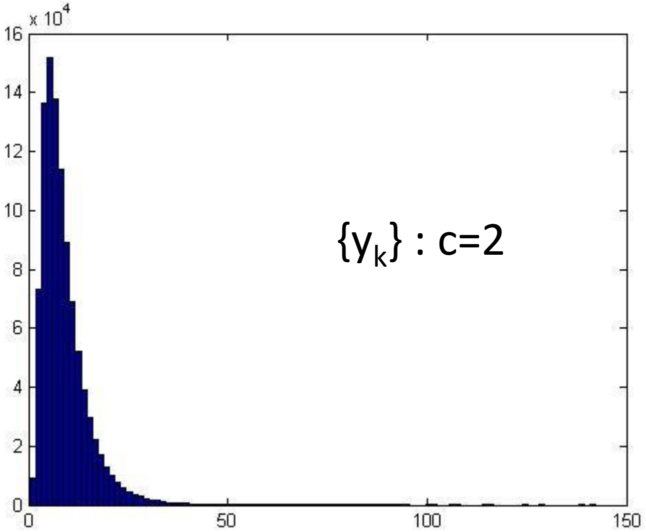
Non-linear transformations change the shape of PDF's …

- **Exercise**: Stochastic analyses with K = 1,000,000 histories (MATLAB).
- Random collection **$\{x_k\}$** generated from a **normal distribution** with mean value = 1, standard deviation = 0.3, skewness = 0, and kurtosis = 3.
- M.C. results for $\{x_k\}$ collected into 100 bins and plotted as a histogram.
- Calculate mean value, standard deviation, skewness, and kurtosis for $\{x_k\}$.
- Transformation: **$y = \mathfrak{M}(x) = \exp(c\,x)$ with c = constant**.
- Generate 1,000,000 corresponding samples of **$\{y_k\}$** for both **c = 1** and **c = 2**.
- M.C. results for the $\{y_k\}$ collected into 100 bins and plotted as histograms.
- Calculate mean value, standard deviation, skewness, and kurtosis for the $\{y_k\}$ sets corresponding to both c = 1 and c = 2.



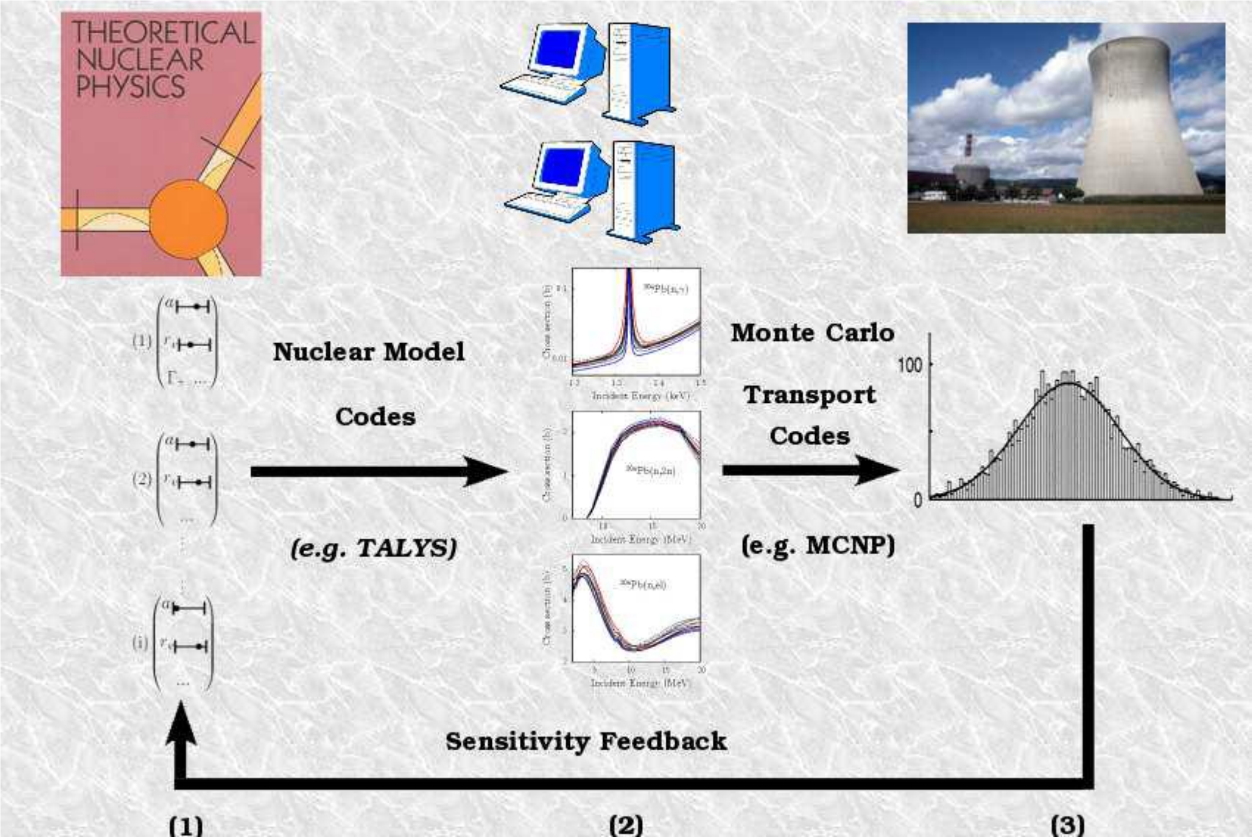
Moments	$\{x_k\}$	$\{y_k\}$: c=1	$\{y_k\}$: c=2
Mean Value	1.0003	2.8426	8.8526
Standard Deviation	0.3001 (30.0%)	0.8720 (30.7%)	5.8380 (66.0%)
Skewness	≈0 (varies)	0.9518	2.2910
Kurtosis	3.0036	4.6592	13.7593

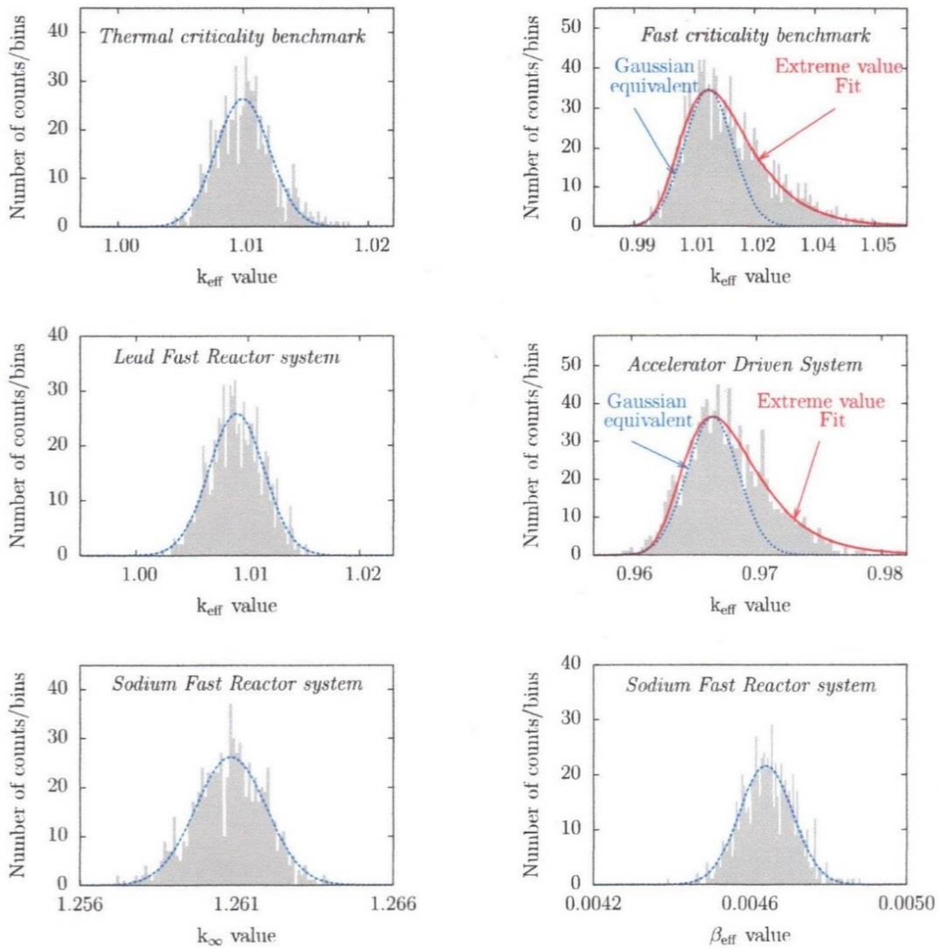




Note: The $\{y_k\}$ PDF's are actually **lognormal**!

Total Monte Carlo (TMC) [~ 2007]





A.J. Koning* and D. Rochman, *Annals of Nuclear Energy*, Volume **35**, Issue 11, November 2008, Pages 2024–2030.
*Preprint with figures shown in this slide obtained from A.J.K. prior to publication.

- The **TMC** concept demonstrated the potential for performing seamless Monte Carlo analyses progressing from estimated nuclear model parameters ➔ calculated nuclear reaction data ➔ nuclear system performance (including uncertainties).
- As originally proposed, the influence of experimental nuclear data was not treated explicitly in this approach. Also, TMC is not truly Bayesian.
- More recent studies by Koning and Rochman, as well as by Helgesson and Sjoestrand, have been investigating ways to remedy these deficiencies.

Unified Monte Carlo – Variant "G" (**UMC-G**) [~ 2007]

- The concept is based on a direct application of Bayes Theorem: $p(\mathbf{y}) = C \times p_0(\mathbf{y}|\mathbf{y}_C,\mathbf{V}_C) \times \mathscr{L}(\mathbf{q}|\mathbf{q}_E,\mathbf{V}_E)$. The prior probability p_0 and likelihood $\mathscr{L}$ are independent probability density functions, while C is a normalization constant. It is assumed here that the analytical forms of both p_0 and $\mathscr{L}$ are known explicitly. Note that **q** = **f**(**y**) since the evaluated (and model-calculated) variables **y** and experimental variables **q** need not be related one-to-one, but only through functions **f**.

- The mean values $\mathbf{y}_C$ and covariance matrix $\mathbf{V}_C$ are derived from model parameters **x** with mean values $\mathbf{x}_0$ and covariance matrix $\mathbf{V}_x$ through the model transformation $\mathfrak{M}$, i.e., $\mathbf{y} = \mathfrak{M}(\mathbf{x})$. The stochastic method is used to determine these mean values $\mathbf{y}_C$ and the covariance matrix $\mathbf{V}_C$ in this approach. The **higher moments are ignored**.

- The analytical form of p_0 associated with the stochastically generated collection $\{\mathbf{y}_k\}$ is unknown so it is **approximated** by a normal (Gaussian) probability function by invoking the Principle of Maximum Entropy (**erroneously**, as it happens, since more information **IS** actually known!). Thus:

$$p_0(\mathbf{y}|\mathbf{y}_C,\mathbf{V}_C) \sim \exp\{-(½)[(\mathbf{y} - \mathbf{y}_C)^+ \bullet \mathbf{V}_C^{-1} \bullet (\mathbf{y} - \mathbf{y}_C)]\}$$

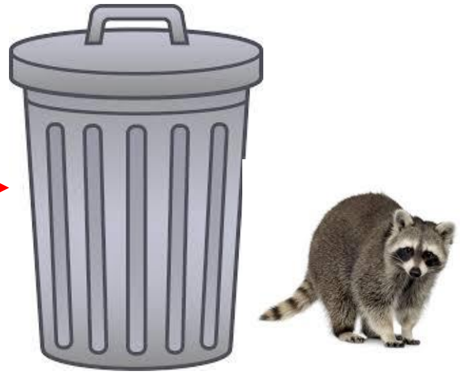
("+" signifies "transpose")

- We then assume that the mean values $\mathbf{q}_E$ and covariance matrix $\mathbf{V}_E$ for the experimental data are known so that, by the same reasoning as applied to the prior, we have a normal function $\mathscr{L}$:

$$\mathscr{L}(\mathbf{q}|\mathbf{q}_E,\mathbf{V}_E) \sim \exp\{-(½)[(\mathbf{q} - \mathbf{q}_E)^+ \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{q} - \mathbf{q}_E)]\} .$$

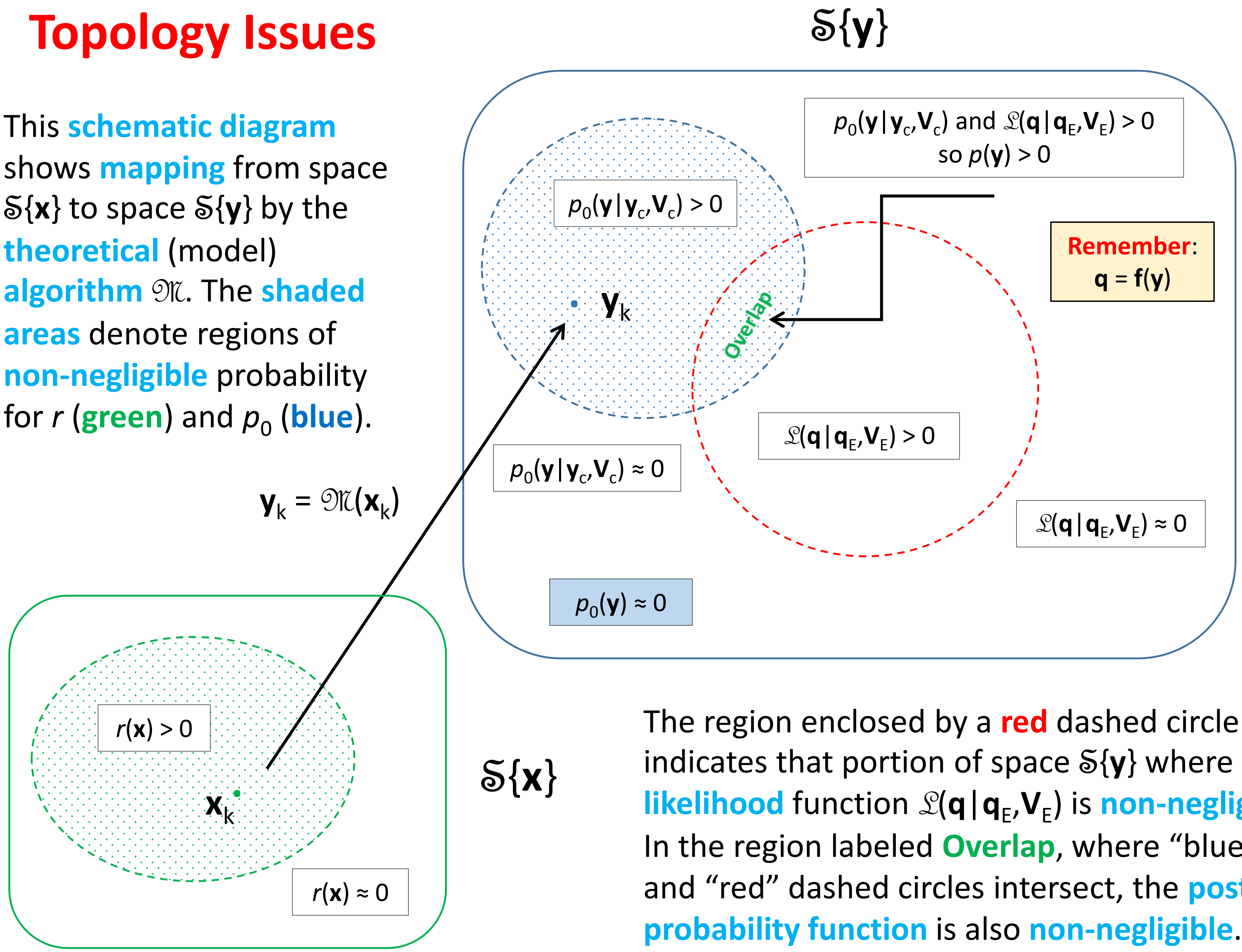
- A stochastic analysis of the posterior probability function $p(\mathbf{y})$ yields the evaluated results.

The concept of UMC-**G** stemmed from boredom experienced while waiting for auto repairs to be performed at a **garage**.



Topology Issues

This **schematic diagram** shows **mapping** from space $\mathbb{S}\{\mathbf{x}\}$ to space $\mathbb{S}\{\mathbf{y}\}$ by the **theoretical** (model) **algorithm** $\mathfrak{M}$. The **shaded areas** denote regions of **non-negligible** probability for r (**green**) and p_0 (**blue**).

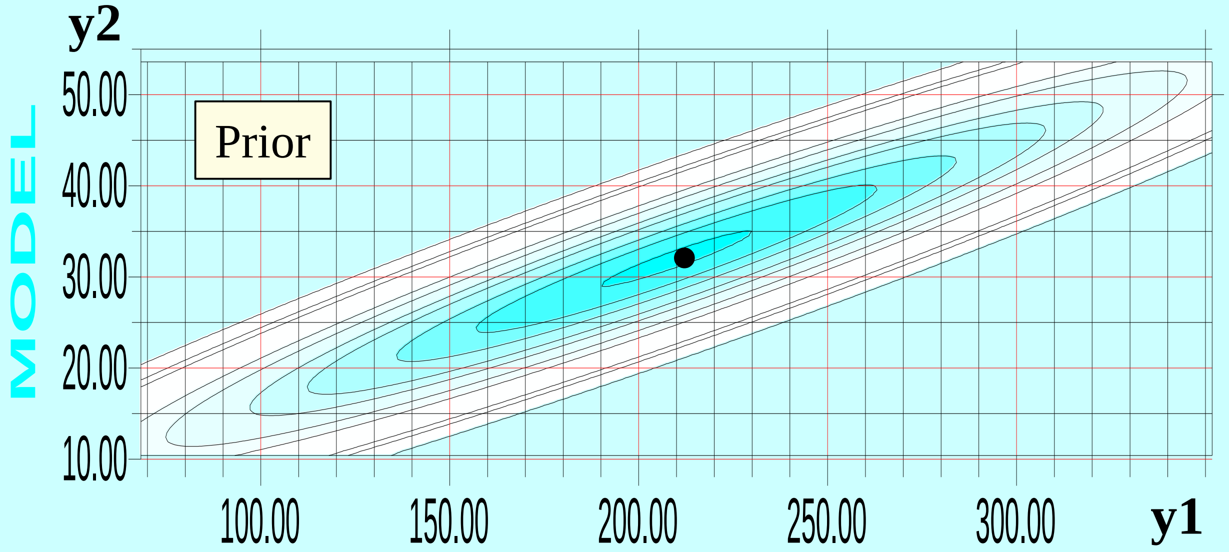


The region enclosed by a **red** dashed circle indicates that portion of space $\mathbb{S}\{\mathbf{y}\}$ where the **likelihood** function $\mathscr{L}(\mathbf{q}|\mathbf{q}_E,\mathbf{V}_E)$ is **non-negligible**. In the region labeled **Overlap**, where "blue" and "red" dashed circles intersect, the **posterior probability function** is also **non-negligible**.

RATIO CASE

"Toy" Example

In this example, q1 = f1 = y1 and q2 = f2 = y2/y1. Consistency of the experimental ratio data and model calculated values for the variables is poor.

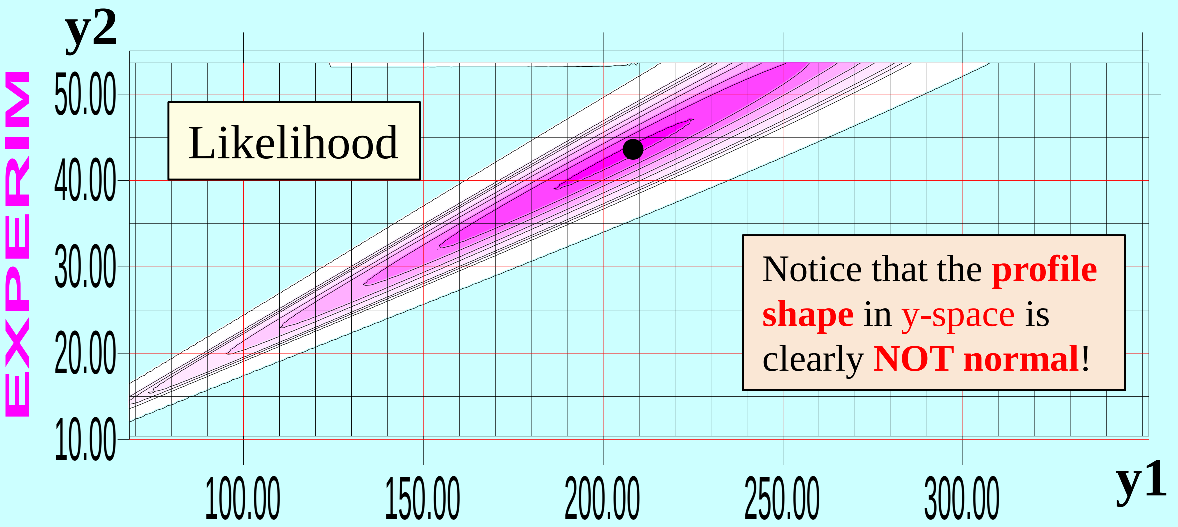


MODEL
y1=210 +/- 63 (30%)
y2=32 +/- 9.6 (30%)

Cov(1,2) = 0.95

"y2"= 43+/-2
vs 32+/- 9

This profile shows the region in y-space where the normal probability distribution for experimental data in q-space appears to be concentrated.



EXPERIM
f1=y1=205.6 +/- 61.7 (30%)
f2=y2/y1=0.209 +/- 0.010 (5%) ~ 43

Cov(1,2) = 0.

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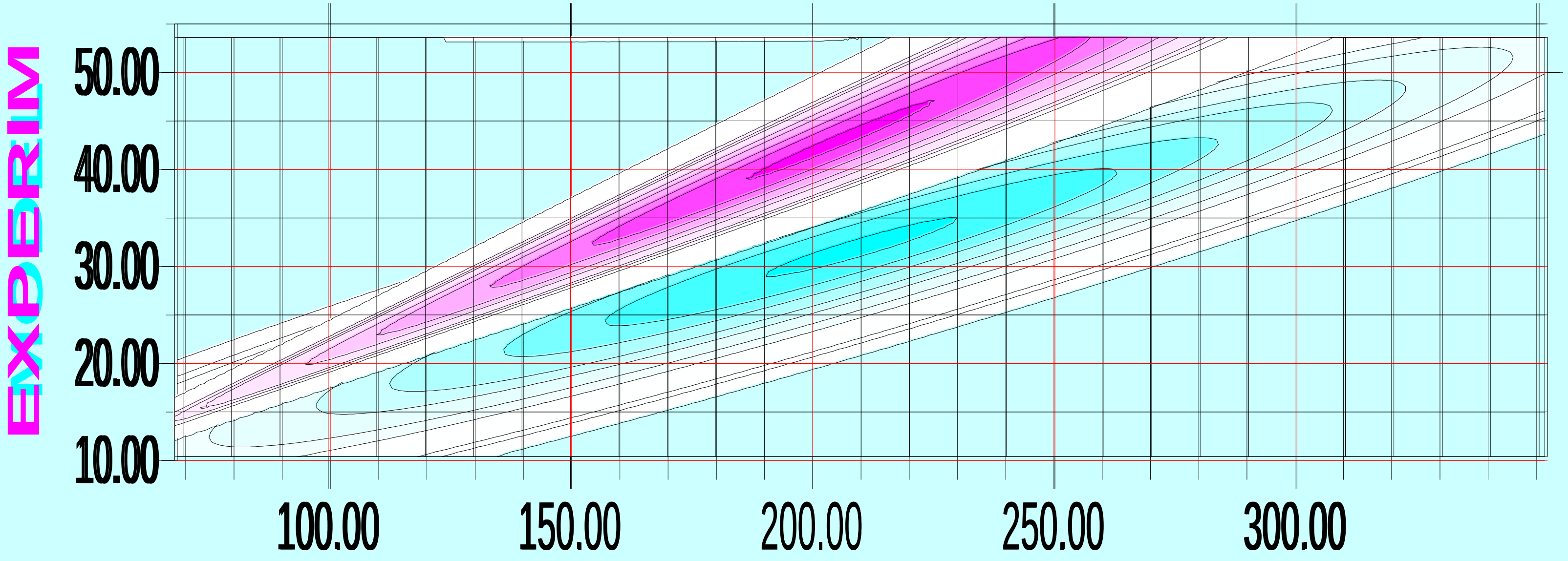
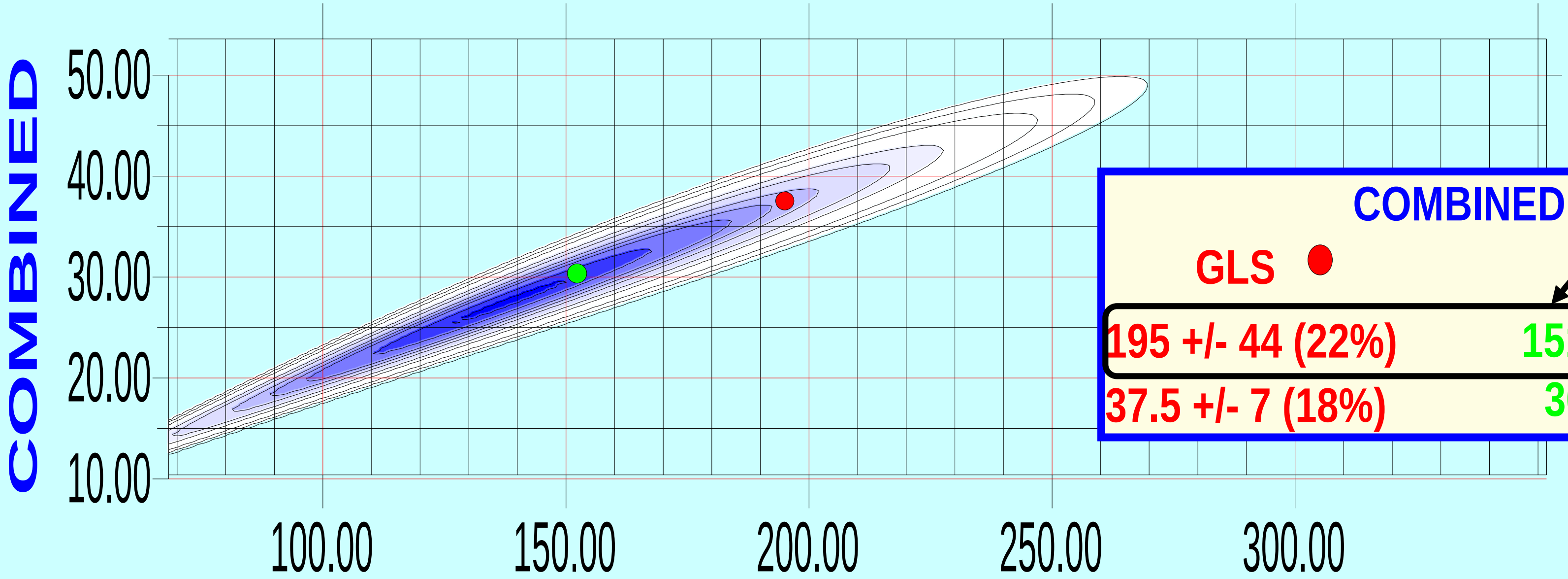
R. Capote, IAEA Nuclear Data Section
R.CapoteNoy@iaea.org

Extreme Case: 5% exp. ratio unc., 95% model correl.





GLS evaluated Mean Value <**y1**> is **29% larger** than for **UMC**!

COMBINED

GLS	UMC
195 +/- 44 (22%)	151 +/- 37 (25%)
37.5 +/- 7 (18%)	30 +/- 7 (22%)

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Nuclear Data Sheets **110** (2009) 3107

RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

R. Capote,[1] M. Herman,[1,2] P. Obložinský,[1,2] P.G. Young,[3] S. Goriely,[4] T. Belgya,[5] A.V. Ignatyuk,[6] A.J. Koning,[7] S. Hilaire,[8] V.A. Plujko,[9] M. Avrigeanu,[10] O. Bersillon,[8] M.B. Chadwick,[3] T. Fukahori,[11] Zhigang Ge,[12] Yinlu Han,[12] S. Kailas,[13] J. Kopecky,[14] V.M. Maslov,[15] G. Reffo,[16] M. Sin,[17] E.Sh. Soukhovitskii,[15] and P. Talou[3]

Available online at www.sciencedirect.com

ScienceDirect

Nuclear Data Sheets

Nuclear Data Sheets **108** (2009) 2655

www.elsevier.com/locate/nds

$$\rightarrow p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C, \mathbf{V}_C)$$

EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

M. Herman[1,*], R. Capote[2], B.V. Carlson[3], P. Obložinský[1], M. Sin[4], A. Trkov[5], H. Wienke[6], and V. Zerkin[2]

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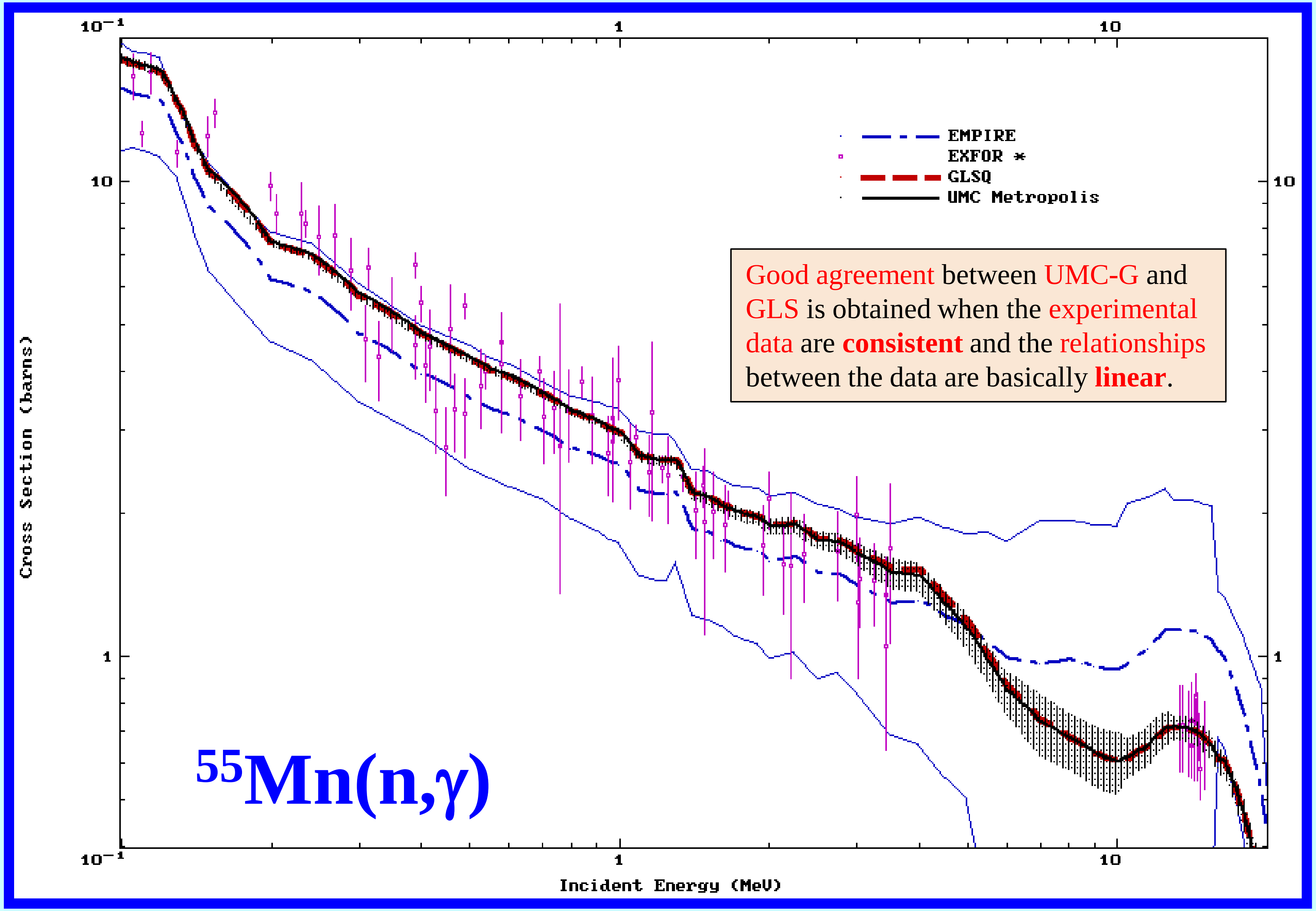
[4] *Nuclear Physics Department, Bucharest University, P.O. Box MG-11, Bucharest-Magurele, Romania*

[5] *Jozef Stefan Institute, Reactor Physics Division R-1, Jamova 39, 1000 Ljubljana, Slovenia and*

[6] *Belgonucleaire, Dessel, B2480, Belgium*

UMC vs GLS: a real evaluation



4th IAEA TM of the International A&M Code Centre Network, Vienna, Austria, July 29-31, 2015

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Additional Comments on UMC-G

Some Strengths of UMC-G:

- It is explicitly a Bayesian approach that works directly with probability functions.
- It does not require either the prior or likelihood probability functions to be normal in order to generate an acceptable posterior probability function.
- Efficient Monte Carlo sampling techniques, such as the Metropolis-Hastings method, can be used to generate a collection of variable vectors that represent the posterior probability function. They can then be used to calculate estimates of the moments such as mean values, covariance matrix, skewness, etc.
- UMC-G will yield the same results as GLS provided that the prior, likelihood, and thus the posterior, are explicitly normal probability functions w.r.t. the variables to be evaluated (no ratio data).
- UMC-G will yield the same results as GLS when the relationships between the various data are linear.
- UMC-G results converge to GLS results when the data are consistent and uncertainties are small.

Some Weaknesses of UMC-G:

- Analytical expressions for both the prior and likelihood functions must be known to generate an analytical posterior function that can be sampled by Monte Carlo.
- While in most instances the likelihood function will be explicitly normal because of limited knowledge of the moments of experimental data probability distributions, it is unlikely that the prior probability function from modeling will be normal or even known analytically. Thus, it must be approximated by an analytic function (resulting in lost information) to be able to employ UMC-G.
- It is computationally intensive (as is the case for ALL the Monte Carlo approaches).

Unified Monte Carlo – Variant "B" (**UMC-B**) [~ 2011]

- It was recognized early-on that the requirement in UMC-G for the prior, likelihood, and posterior probability functions to be expressible analytically was a serious limitation of this approach. In order to apply UMC-G it is necessary, in most cases, to discard potentially useful information about the prior function p_0 in order to approximate it by a normal distribution.

- To overcome this limitation, UMC-B uses a distinct Bayesian approach in which each individual transformed k[th] sample value from variable space $\mathbb{S}(\mathbf{x})$ to variable space $\mathbb{S}(\mathbf{y})$ - in accordance with $r(\mathbf{x})$ and model $\mathfrak{M}$ - is ultimately weighted by a corresponding scalar likelihood factor ω_k.

$$\{\mathbf{x}_k\} \Rightarrow \mathfrak{M}(\mathbf{x}_k) \Rightarrow \{\mathbf{y}_{Ck}\} \Rightarrow \{\mathbf{q}_k\} \Rightarrow \{\omega_k\}$$

Note: Subscript "C" signifies "calculated" using model $\mathfrak{M}$.

Remember: $\mathbf{q} = \mathbf{f}(\mathbf{y})$

The concept of **UMC-B** emerged while Roberto Capote and Andrej Trkov were having **breakfast** one morning before a daily session of the covariance workshop being held at Port Jefferson, New York.

- The collection $\{\mathbf{y}_{Ck}\}$ is distributed according to a prior probability function p_0 that is not explicitly analytical but can be incorporated in a Bayesian analysis by employing as likelihood factors the collection of scaler weighting factors $\{\omega_k\}$ that are defined by experimental data and given by:

$$\omega_k = \exp\{-(½)[(\mathbf{q}_k - \mathbf{q}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{q}_k - \mathbf{q}_E)]\ .$$

No information is discarded in UMC-B

- While an analytical expression for the posterior probability function $p(\mathbf{y})$ is not provided, it is possible to calculate the moments of p by employing the collection of pairs of quantities $\{\mathbf{y}_{Ck},\omega_k\}$. For example, the "solution" mean values and covariance matrix are given by:

$$\langle y_i \rangle \approx [\Sigma_{k=1,K}\ \omega_k\ y_{Cik}] \,/\, [\Sigma_{k=1,K}\ \omega_k]\ , \quad (i=1,m)$$

$$(\mathbf{V}_y)_{ij} = [\Sigma_{k=1,K}\ \omega_k\ y_{Cik}\ y_{Cjk}] \,/\, [\Sigma_{k=1,K}\ \omega_k] - \langle y_i \rangle \langle y_j \rangle\ . \quad (i,j=1,m).$$

UMC-B offers a way to incorporate experimental information in TMC.

Comments on UMC-B

Some Strengths of UMC-B*:

- UMC-B shares several favorable attributes with UMC-G, e.g., it does not demand linearity.
- UMC-B overcomes a major limitation of UMC-G since it does not require an explicit analytical representation of the prior probability function.
- It is conceptually very easy to understand and implement.

Some Weaknesses of UMC-B*:

- A disadvantage of UMC-B is encountered if the region of **y**-space where **both** the prior and posterior probability functions have non-negligible probability is very small. In order that this region be adequately sampled, a very large number of Monte Carlo sampling histories, and a wide space of sampling variable values, may be required to minimize the chance of introducing bias and to yield adequate statistical precision for the derived moments.
- All sample values considered by this approach are based on calculations involving the theoretical model $\mathfrak{M}$ (i.e., sampling p_0) rather than on sampling the actual posterior probability function p that treats the calculated and experimental results on an equal footing. So, UMC-B is quite sensitive to the possible existence of model defects.
- **Summarizing**: While both GLS and UMC-G can be symmetric w.r.t. the handling of experimental and model data, UMC-B is not symmetric. Depending on one's perspective, this may be an advantage or a disadvantage.
- The analysis can be very computationally intensive, especially if the model and experimental data disagree.

*NOTE: In her talk at this workshop, **Denise Neudecker** will discuss recent investigations of these issues, and she will also show comparisons of results from GLS, UMC-G, and UMC-B analyses for some specially designed "toy examples".

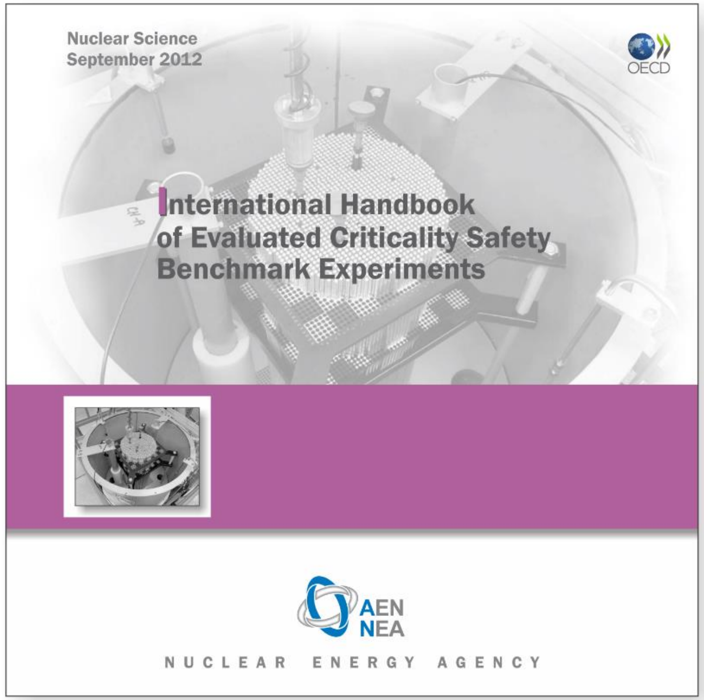
EVALUATED DATA VALIDATION

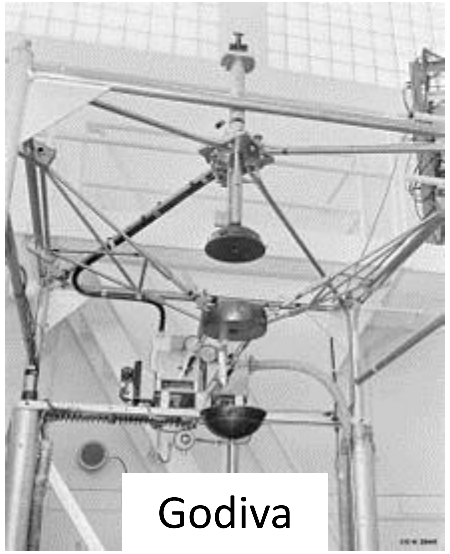
“Proof of the Pudding” is in the eating …

- Before a comprehensive evaluated nuclear data library such as ENDF/B-VII.1 is formally released it is subjected to extensive C/E testing of its performance for thousands of well-defined nuclear-application benchmarks* (mostly critical and sub-critical reactors).

- Before a new library can be licensed for use by various governmental agencies (e.g., NRC or NNSA) it must be established that it yields C/E values that are deemed by experts from the data user groups to be within acceptable limits (i.e., C/E ≈ 1), considering all the estimated uncertainties. Achieving this goal always involves many iterations and compromises.

- Inclusion of covariance (i.e., uncertainty) data is quite important for contemporary data libraries owing to a growing emphasis on **Uncertainty Quantification**. Covariances are also employed to produce “adjusted” evaluated data libraries for specific applications. These adjusted libraries may be used to seek approval from authorities (e.g., for reactor licensing).




Godiva

*The **International Handbook of Evaluated Criticality Safety Benchmark Experiments** was prepared by a working group comprised of experienced criticality safety personnel from the United States, the United Kingdom, Japan, the Russian Federation, France, Hungary, Republic of Korea, Slovenia, Serbia, Kazakhstan, Israel, Spain, Brazil, Czech Republic, Poland, India, Canada, China, Sweden, and Argentina. The handbook contains criticality safety benchmark specifications that have been derived from experiments that were performed at various nuclear critical facilities around the world. The benchmark specifications are intended for use by criticality safety engineers to validate calculational techniques used to establish minimum subcritical margins for operations with fissile material. The example calculations presented do not constitute a validation of the codes or cross section data. The **handbook** contains 549 evaluations with benchmark specifications for 4708 critical, near-critical, or subcritical configurations and 24 criticality alarm placement/shielding configurations with multiple dose points for each, and 200 configurations that have been categorized as fundamental physics measurements that are relevant to criticality safety applications.

WRAP-UP

It's important to re-emphasize that combinations of data from theory and experiment are generally needed to produce an acceptable evaluation …

- Contemporary theoretical models are usually approximations due to incomplete knowledge about nuclear processes. As a consequence there are defects (some known and many likely unknown) in these models.
- Many nuclear models involve semi-empirical parameters that must be adjusted to yield qualitative agreement with the available experimental data:
  - Normalization issues.
  - Shape variations with energy.
- Data from good-quality experiments can provide useful information that is pertinent to both the normalization and shape of cross-section excitation functions, but often this occurs only in certain energy regions that were (are) accessible with former (contemporary) experimental facilities and techniques.
- Many archival experimental data were acquired and analyzed with inadequate understanding of the existing experimental conditions (backgrounds, calibrations, etc.)
- While either models or experiments alone are usually insufficient when performing an evaluation, they tend to complement each other so that a **combination of model data and experimental data**, implemented in a Bayesian context, can go a long way toward fulfilling evaluated data needs for applications.

Many of the difficulties encountered in performing nuclear data evaluations tend to **vanish** when there is good agreement between "defect-free" model-calculated data (**C**) and comparable accurate experimental data (**E**), with modest-to-small uncertainties, regardless of the evaluation method used …

$C \neq E$

(Conflict)

"The Truth"

$C \approx E$

(Harmony)

But … it's a bit idealistic to think that in most cases this could happen anytime soon …

Fulfillment of the **goal** of achieving complete RIGOR continues to be **elusive**. So … contemporary practices in nuclear data evaluation still involve a considerable degree of **SORCERY** ... Nevertheless, meaningful progress is being made toward improving both the data available to be evaluated as well as the evaluation methods used.

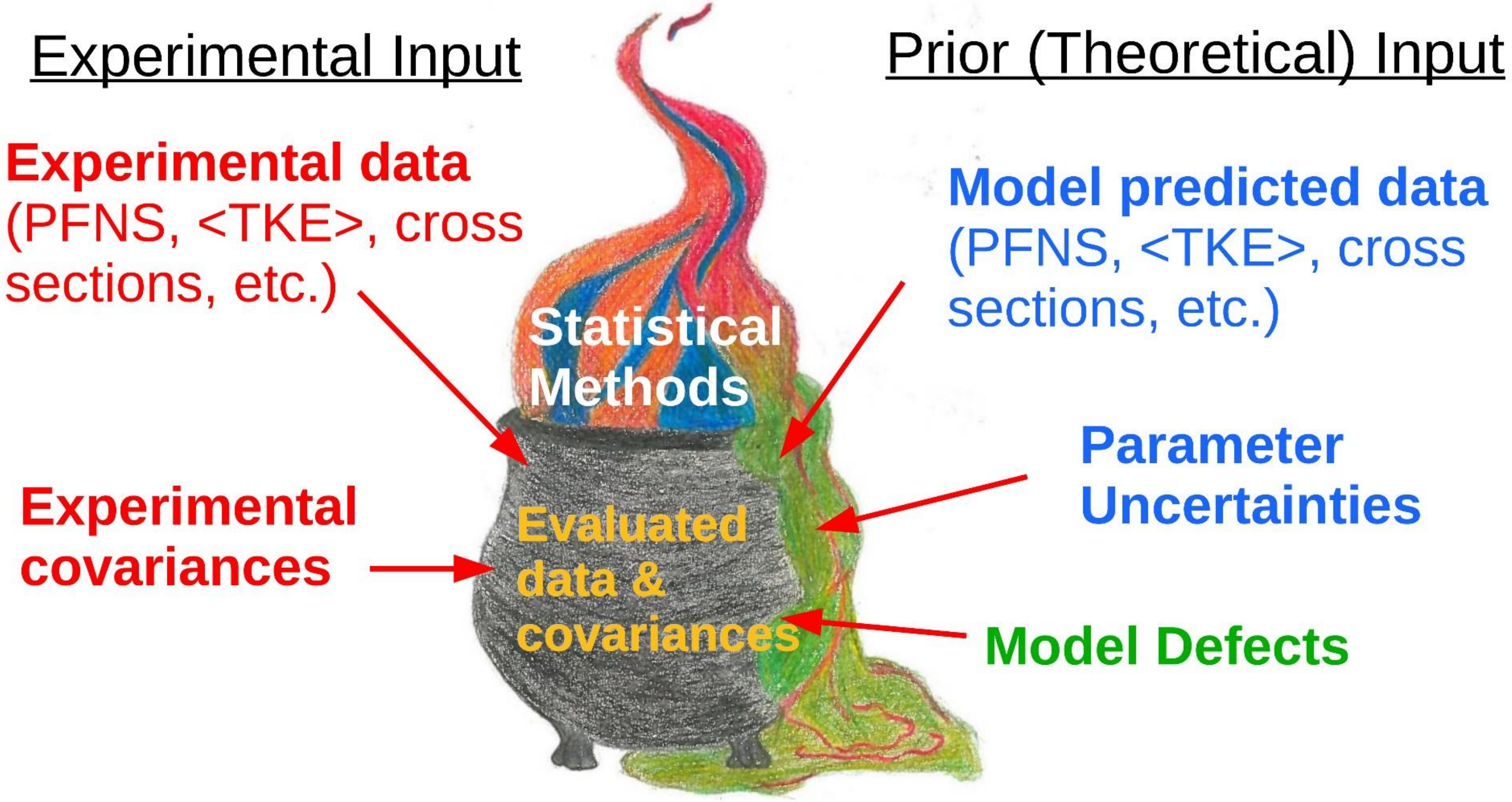


Image provided by Denise Neudecker (May 2016)

Is UMC a “Silver Bullet” solution for every evaluation situation?

- Obviously (from the preceding discussions) it is not.

- But … one or another variant of UMC (and there are others besides UMC-G and UMC-B that are now being explored by the nuclear data community) can be useful in situations where non-linear effects are significant and non-normal data probability distributions are involved.

- For many situations, GLS has been shown to be a viable evaluation tool that can provide reasonable results which adequately incorporate the underlying theoretical and experimental data employed in these evaluations.

- For the foreseeable future it is likely that a combination of GLS and UMC-type techniques will be employed, especially considering the large volumes of information that need be handled in producing most evaluations.

This is an allusion to a mythical “**miraculous fix**”, sometimes also portrayed as “waving a magic wand”. This figurative use derives from the use of actual **silver bullets** and the widespread folk belief that they were the only way of killing werewolves or other supernatural beings.

Erma Bombeck

Born: February 21, 1927
Died: April 22, 1996

Erma Louise Bombeck, born Erma Fiste, was an American humorist who achieved great popularity for a newspaper column that depicted suburban home life humorously, in the second half of the 20th century.

For 31 years since 1965, Erma Bombeck published 4,000 newspaper articles. Already in the 1970s, her witty columns were read, twice weekly, by thirty million readers of 900 newspapers of USA and Canada. Besides, the majority of her 15 books became instant best sellers.

"Housework can kill you if done right."

… That may also be true with nuclear data evaluation!!!

The End