Unified Monte Carlo evaluation method

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(Nuclear) Data Evaluation

Evaluated cross sections and covariance matrices

Experimental Input

Inter and -intra experiment correlations

Experimental cross sections

Prior Knowledge

Model Defects

Parameter Uncertainties

Model cross sections & correl

From D. Neudecker, S. Gundacker, H. Leeb *et al.*, ND2010, Jeju Isl., Korea

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Definition of (Nuclear) Data Evaluation

A properly weighted combination of selected experimental data (and modeling results if needed).

Bayesian approaches (may use prior knowledge):

- ❑ "Non-model" GLSQ fit (standards)
- ❑ Model prior + experimental data:
  - Deterministic: Model Prior (Sens) + GLSQ
  - Stochastic (MC): **UMC, TMC + UMC**
  - Hybrid: Model Prior (MC) + GLSQ

All stochastic methods may be used to produce samples for TMC

MONTE CARLO METHOD

D.L. Smith, "Covariance Matrices for Nuclear Cross-Sections Derived from Nuclear Model Calculations".
Report **ANL/NDM-159**, Argonne National Laboratory, 2005

$$\overline{\sigma}_i = \frac{1}{K}\sum_{k=1}^{K}\sigma_{ik} \qquad V_{ij} = \overline{\sigma_i\sigma_j} - \overline{\sigma}_i \times \overline{\sigma}_j$$

i, j - energy indexes

Monte Carlo calculation of covariance first tested by A. Koning

Monte Carlo prior
+
GANDR *(GLS)*

D.W. Muir, ***GANDR*** *project (IAEA)*, Online at www-nds.iaea.org/gandr/.

A. Trkov and R. Capote, "Cross-Section Covariance Data", Th-232 evaluation for ENDF/B-VII.0 (MAT=9040 MF=1 MT=451); Pa-231 and Pa-233 evaluations for ENDF/B-VII.0 (MAT=9133 and 9137 MF=1 MT=451), National Nuclear Data Center, BNL (http://www.nndc.bnl.gov), 15 December 2006.

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UMC-G a.k.a. "Garage" solution

UMC-B a.k.a. "Breakfast" solution

VS

D.L. Smith
San Diego 2007

R. Capote, A. Trkov
Port Jefferson 2008

UMC-G ("Garage" Solution)

$\bar{\sigma}$ = collection of evaluated cross sections

$\bar{y}_E$ = collection of experimental results. $\bar{V}_E$ = corresponding cov. matrix

$\bar{f}$ = collection of functions that relates $\bar{\sigma}$ to the data,
i.e., given $\bar{\sigma}$ we can calculate the equivalent to $\bar{y}$

(1)

$\bar{\sigma}_C$ = model calculated cross sections $\bar{V}_C$ = corresponding cov. matrix

$\therefore$ $p(\bar{\sigma}|E,C)$ = probability density function for $\bar{\sigma}$ given experimental data "E" and ~~calculated~~ model-calculated prior results "C"

$$p(\bar{\sigma}|E,C) = C \exp\left\{(-\tfrac{1}{2})[\bar{y}_E - \bar{f}(\bar{\sigma})]^{+} \bar{V}_E^{-1} [\bar{y}_E - \bar{f}(\bar{\sigma})] + (-\tfrac{1}{2})(\bar{\sigma} - \bar{\sigma}_c)^{+} \bar{V}_c^{-1} (\bar{\sigma} - \bar{\sigma}_c)\right\}$$

$\bar{\sigma} = \sigma_1, \sigma_2, \ldots, \sigma_i, \ldots, \sigma_N$

Donald L. Smith, ANL
Argonne National Laboratory
WPEC 2007 – SG24

UNIFIED MONTE CARLO (UMC-G)

D.L. Smith, "A Unified Monte Carlo Approach to Fast Neutron Cross Section Data Evaluation," *Proceedings of the 8th International Topical Meeting on Nuclear Applications and Utilization of Accelerators*, Pocatello, July 29 – August 2, 2007, p. 736.

BAYES THEOREM & PRINCIPLE OF MAXIMUM ENTROPY

$$p(\boldsymbol{\sigma}) = \mathrm{C} \times \mathscr{L}(\mathbf{y_E}, \mathbf{V_E} \mid \boldsymbol{\sigma}) \times p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma_C}, \mathbf{V_C})$$

$$p_0(\sigma \mid \sigma_C, V_C) \sim \exp\{-(½)[(\sigma-\sigma_C)^T \bullet (V_C)^{-1} \bullet (\sigma-\sigma_C)]\}$$

$$\mathscr{L}(y_E, V_E \mid \sigma) \sim \exp\{-(½)[(y-y_E)^T \bullet (V_E)^{-1} \bullet (y-y_E)]\}, \; y=f(\sigma)$$

y_E, V_E: measured quantities with "n" elements

y_C, V_C: calculated using models with "m" elements

UMC based on p(σ), GLS on the peak of the distribution

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Unified Monte Carlo (UMC-B)

1) MC modeling (EMPIRE, TALYS, CCONE, CoH,…) $\{\boldsymbol{\sigma}_\mathbf{i}\}$

2) For each random set $\{\boldsymbol{\sigma}_\mathbf{i}\}$ we calculate $w^{\exp}(\vec{\sigma}_i) = \mathcal{L}(\mathbf{y_E}, \mathbf{V_E} \mid \boldsymbol{\sigma}_\mathbf{i})$

$$\mathcal{L}(\mathbf{y_E}, V_E \mid \boldsymbol{\sigma}_\mathbf{i}) = \exp\{-(½)[(f(\boldsymbol{\sigma}_\mathbf{i}) - \mathbf{y_E})^T \bullet (V_E)^{-1} \bullet (f(\boldsymbol{\sigma}_\mathbf{i}) - \mathbf{y_E})]\}$$

$$\langle \vec{\sigma} \rangle = \frac{\sum_{i=1}^{N} w^{\exp}(\vec{\sigma}_i) \quad \vec{\sigma}_i}{\sum_{i=1}^{N} w^{\exp}(\vec{\sigma}_i)}, \qquad \mathrm{cov}(\vec{\sigma}_i, \vec{\sigma}_j) = \langle \vec{\sigma}_i \vec{\sigma}_j \rangle$$

OUTPUT: 1) $\langle \vec{\sigma} \rangle, \quad \mathrm{cov}(\vec{\sigma}_i, \vec{\sigma}_j) = \langle \vec{\sigma}_i \vec{\sigma}_j \rangle$

2) Stochastic set $\{\boldsymbol{\sigma}_\mathbf{i}\}$

RC, D. L. Smith, A. Trkov, M. Meghzifene, A New Formulation of the Unified Monte Carlo Approach (UMC-B) and Cross-Section Evaluation for …, *J. ASTM International* **9**, JAI104115 (2012)

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Two variable toy model: ratio experimental data

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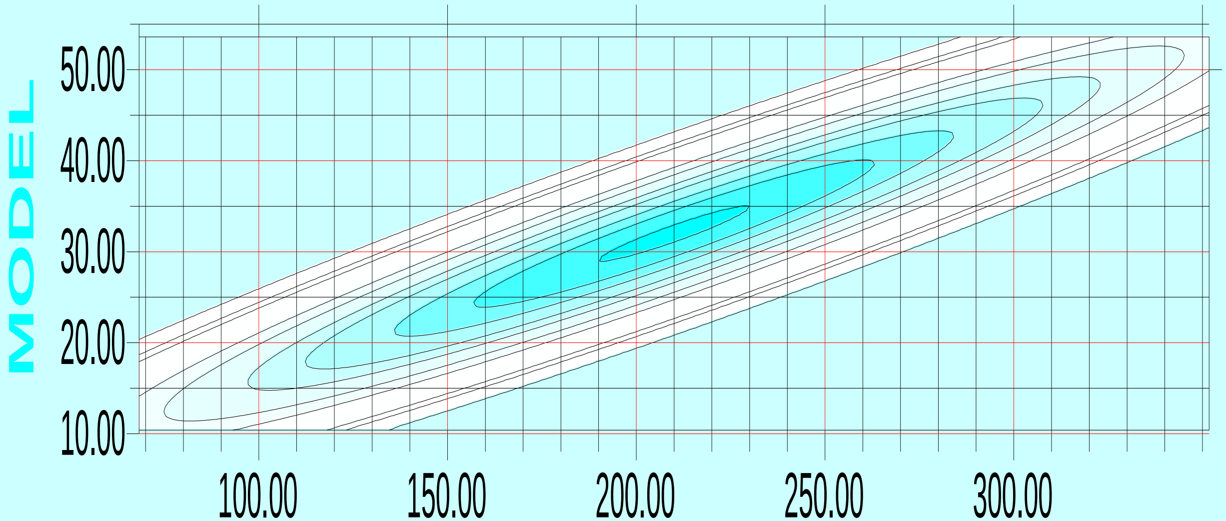
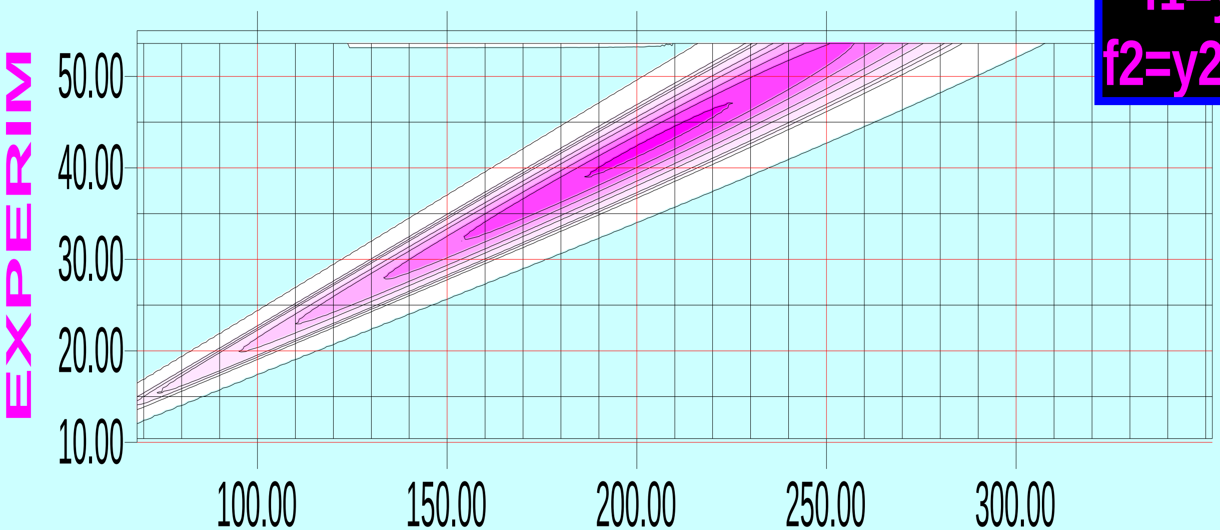
RATIO CASE



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

Cov(1,2) = 0.95



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

Cov(1,2) = 0.

"y2"=43+/-2

vs 32+/- 9

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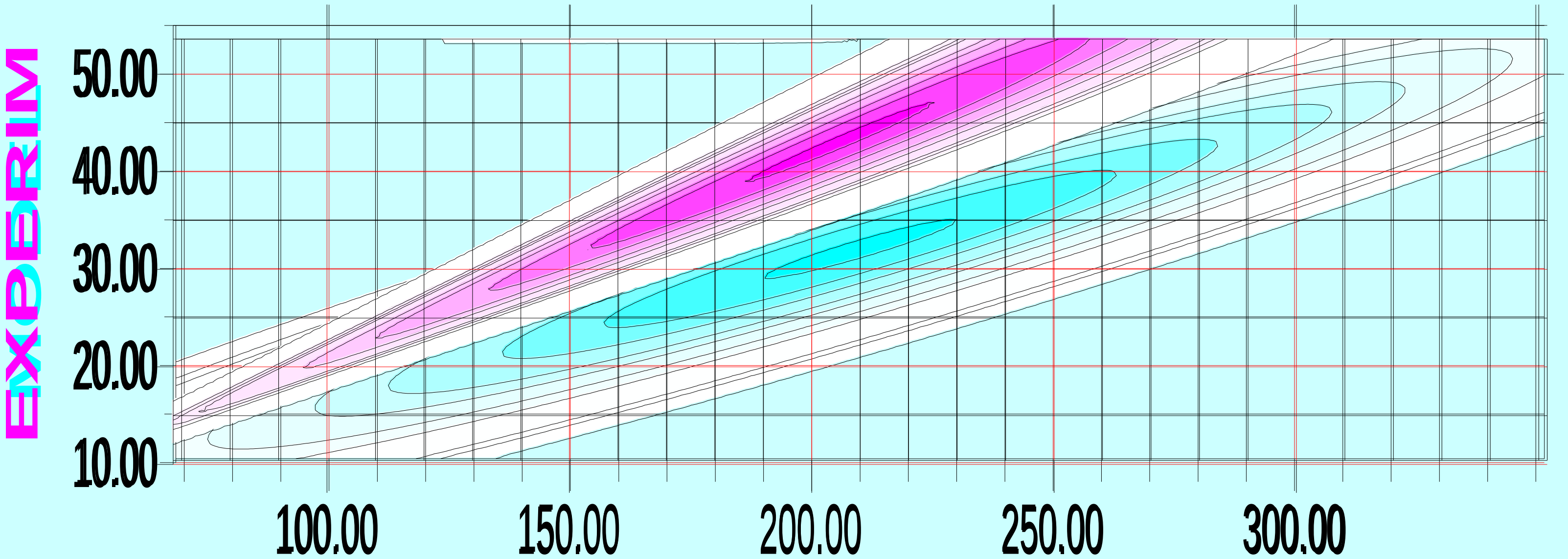
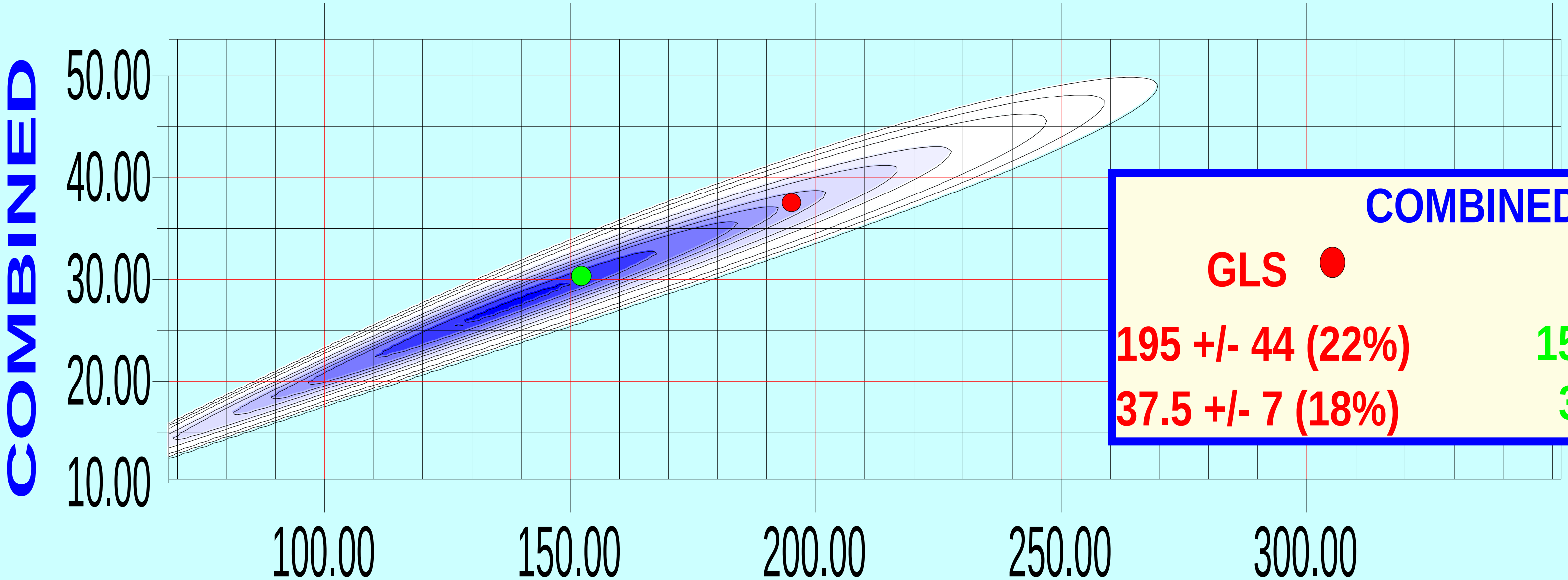
5% exp. ratio unc., 95% model correl.





COMBINED

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

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GLS FAILURE: ANALYSIS

5% exp. ratio unc.
95% model correlation
(discrepant model vs data)

Quantity	Node 1	Node 2	Ratio
BF/GLS	0.7767	0.7929	1.0209
METR/GLS	0.7728	0.7891	1.0210
METR/BF	0.9950	0.9951	1.0001

5% exp. ratio unc.
no model correlation

Quantity	Node 1	Node 2	Ratio
BF/GLS	1.0180	0.9795	0.9622
METR/GLS	1.0232	0.9850	0.9626
METR/BF	1.0051	1.0056	1.0004

30% exp. ratio unc.
95% model correlation

Quantity	Node 1	Node 2	Ratio
BF/GLS	1.0002	1.0007	1.0005
METR/GLS	0.9995	0.9998	1.0004
METR/BF	0.9992	0.9991	0.9999

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Evaluation of $^{55}Mn(n,\gamma)$ cross section

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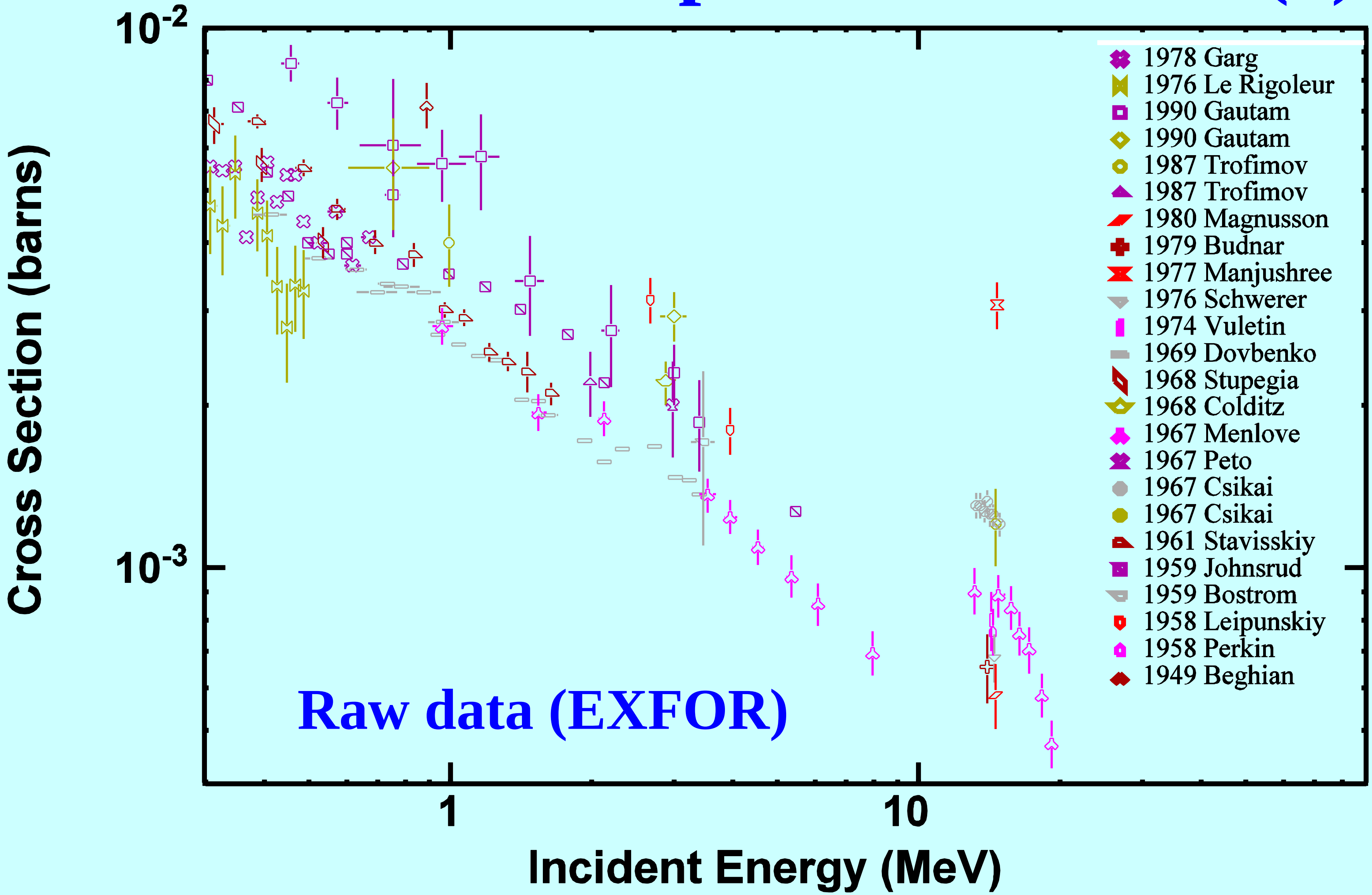
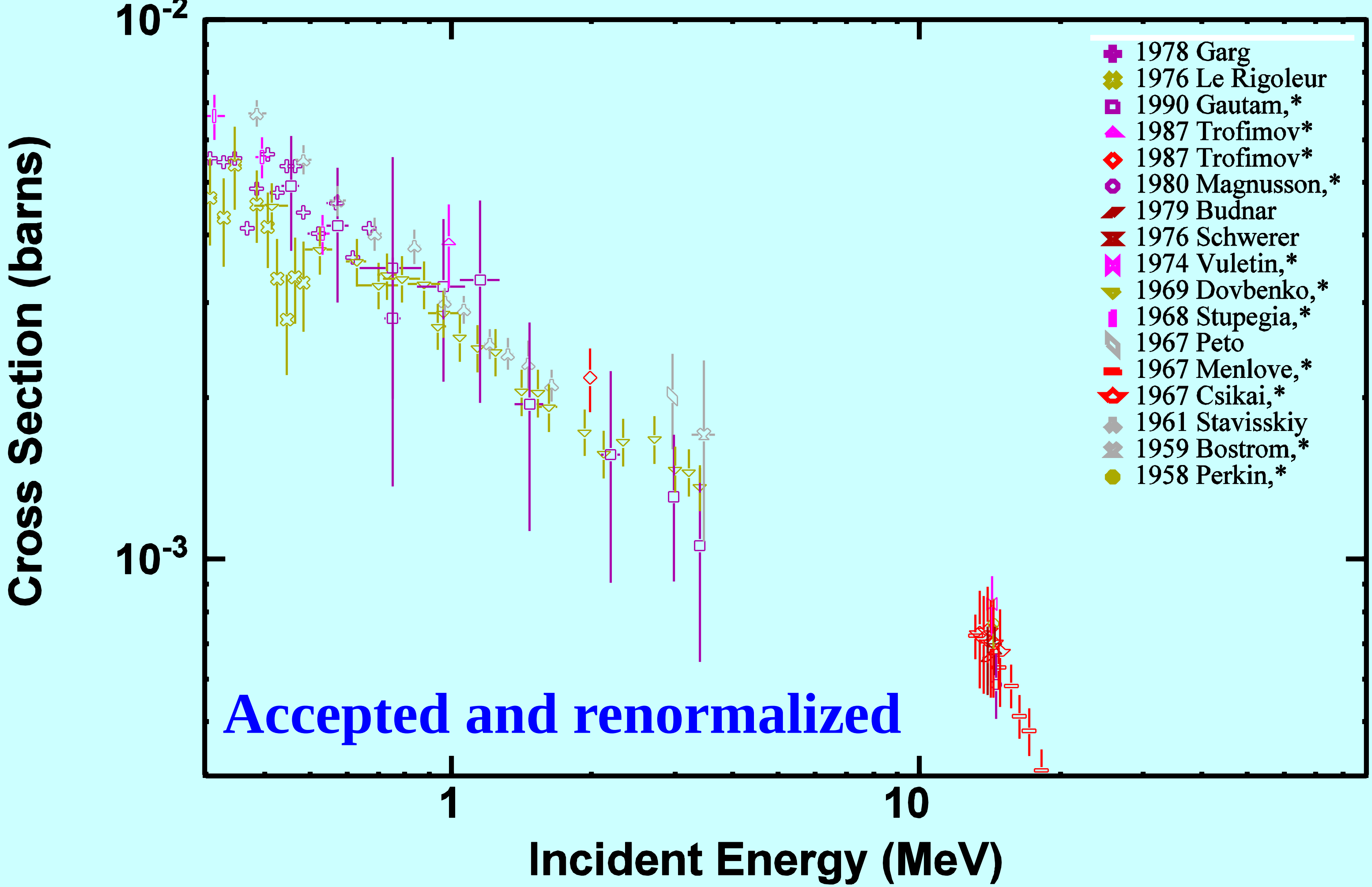
Selection of experimental data (1)



Selection of experimental data (2)



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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

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Nuclear Data Sheets

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

www.elsevier.com/locate/nds

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

EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

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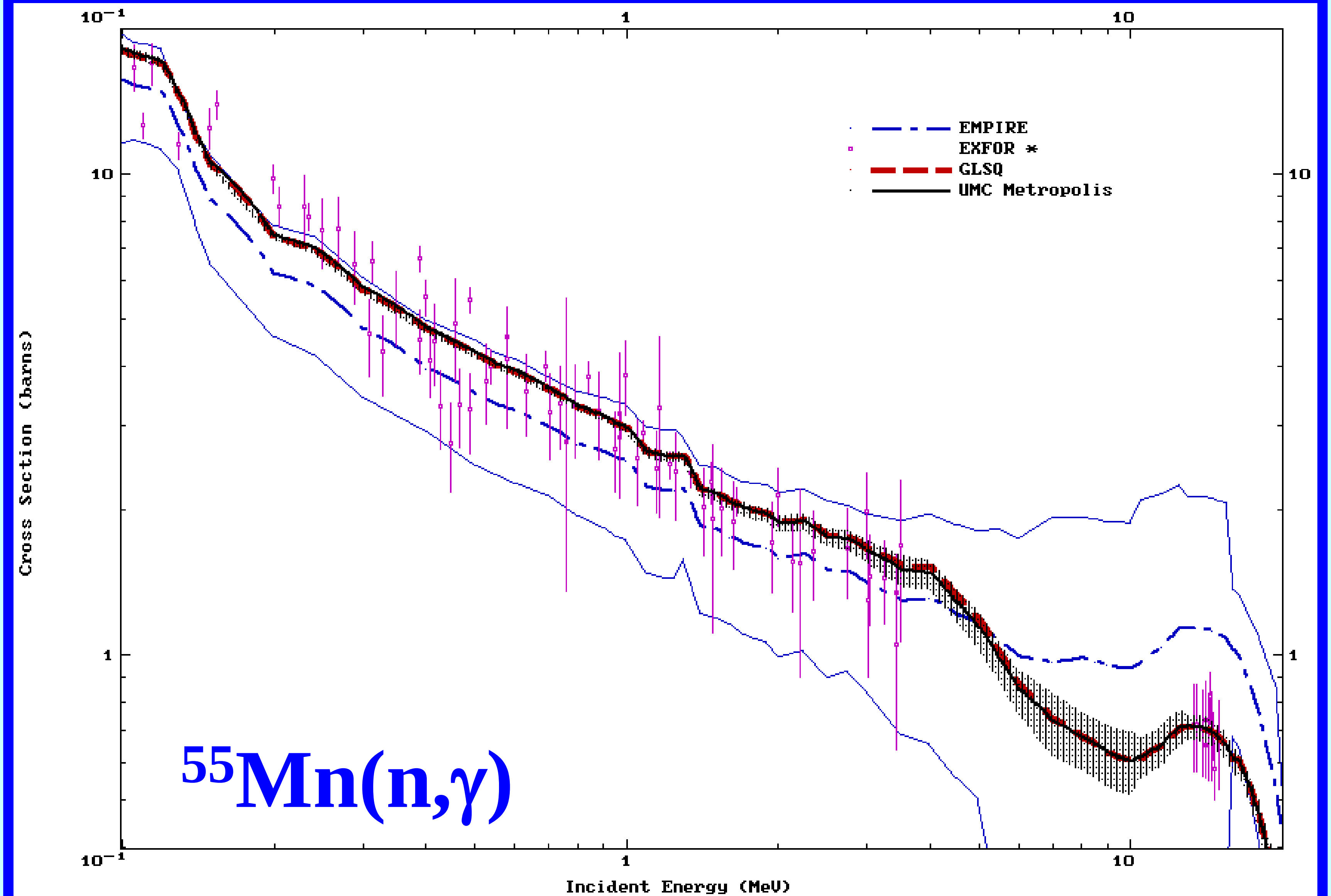
UMC vs GLSQ: a real evaluation



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Concluding remarks

- A careful selection and adjustment of raw experimental data is a critical step to achieve a consistent (non discrepant) database for the evaluation

- Linear case studied (no ratio data) : UMC-G and GLSQ are in excellent agreement

- Non-gaussian case studied (ratio data): GLSQ fails, UMC (Metr) solution obtained

- UMC-G (Metr), UMC-B and GLSQ applied to ^{55}Mn(n,γ) case (energy range 100 keV to 20 MeV)

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UMC sampling schemes

Brute Force approach: A set of independent {**σ**}

$$\overline{\sigma}_{Ck} - \psi\, [(\mathbf{V}_C)_{ii}]^{1/2} \leq \sigma_{ik} \leq \overline{\sigma}_{Ck} + \psi\, [(\mathrm{V}_C)_{ii}]^{1/2}$$

$$\sigma_{ik} = \overline{\sigma}_{Ck} + (2\,\gamma - 1)\, \psi\, [(\mathbf{V}_C)_{ii}]^{1/2}$$

METROPOLIS[1] approach: An stochastic Markov chain {**σ**} distributed following p(**σ**)

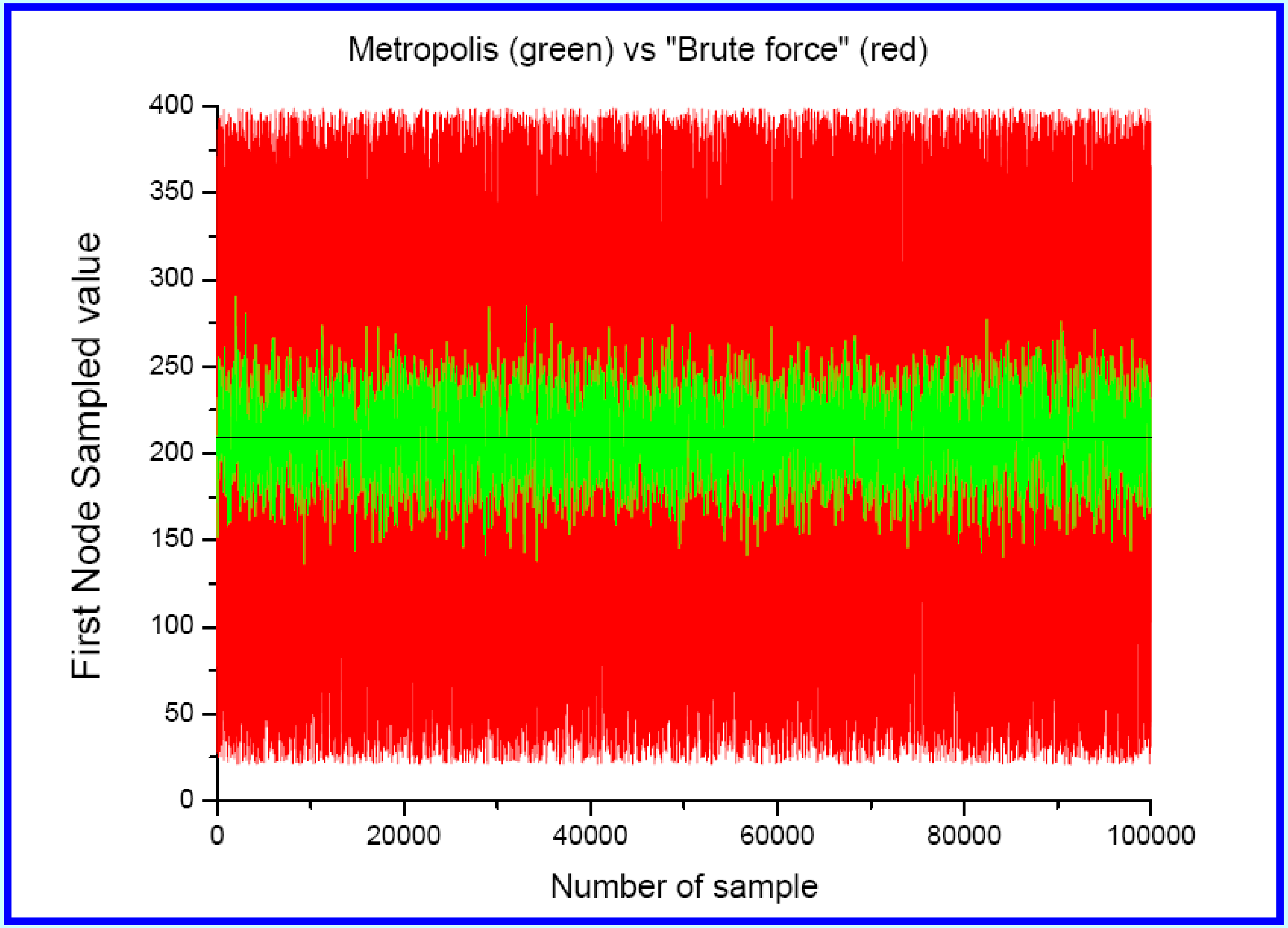
$$\boldsymbol{\sigma}' = \boldsymbol{\sigma}(t) + (2\,\gamma - 1)\, \delta\, [(\mathbf{V}_C)_{ii}]^{1/2}, \text{ being } \boldsymbol{\sigma}(t=0) = \overline{\sigma}_C$$

If $p(\boldsymbol{\sigma}') > \gamma\, p(\boldsymbol{\sigma}(t))$ then $\boldsymbol{\sigma}(t+1)=\boldsymbol{\sigma}'$; else $\boldsymbol{\sigma}(t+1)=\boldsymbol{\sigma}(t)$

RC and D.L. Smith, *Nucl. Data Sheets* **109**, 2768 (2008)
(1)N. Metropolis *et al.*, *J. Chem. Phys.* **21**, 1087 (1953)

UMC-G: BF vs Metropolis

Nuclear Data Sheets **109** (2008) 2768
An Investigation of the Performance of the Unified Monte Carlo Method of Neutron Cross Section Data Evaluation



UMC convergence