Performance of the Unified Monte Carlo Method of Data Evaluation

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OVERVIEW

- Introduction: Monte Carlo method
- UMC formulation
- UMC sampling: Brute Force, Metropolis

- Toy models: Linear
- UMC convergence

- Toy models: Ratio data
- Log transformation

- Conclusions and outlook

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.

Merging of Model Calculated and Experimental Results … More

(a.k.a. "Auto Repair Shop" Solution)

$\bar{f}$ = 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"

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

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

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UNIFIED MONTE CARLO (UMC)

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

$$p(\boldsymbol{\sigma}) = \mathrm{C} \times \mathscr{L}(\mathbf{y}_E, \mathbf{V}_E \mid \boldsymbol{\sigma}) \times p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C, \mathbf{V}_C)$$

$$p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C, \mathbf{V}_C) \sim \exp\{-(½)[(\boldsymbol{\sigma}-\boldsymbol{\sigma}_C)^T \bullet (\mathbf{V}_C)^{-1} \bullet (\boldsymbol{\sigma}-\boldsymbol{\sigma}_C)]\}$$

$$\mathscr{L}(\mathbf{y}_E, \mathbf{V}_E \mid \boldsymbol{\sigma}) \sim \exp\{-(½)[(\mathbf{y}-\mathbf{y}_E)^T \bullet (\mathbf{V}_E)^{-1} \bullet (\mathbf{y}-\mathbf{y}_E)]\},\ \mathbf{y}=f(\boldsymbol{\sigma})$$

y_E, V_E: measured quantities with "n" elements

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

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

UMC sampling schemes

BF approach: A set of independent {**σ**}

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

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

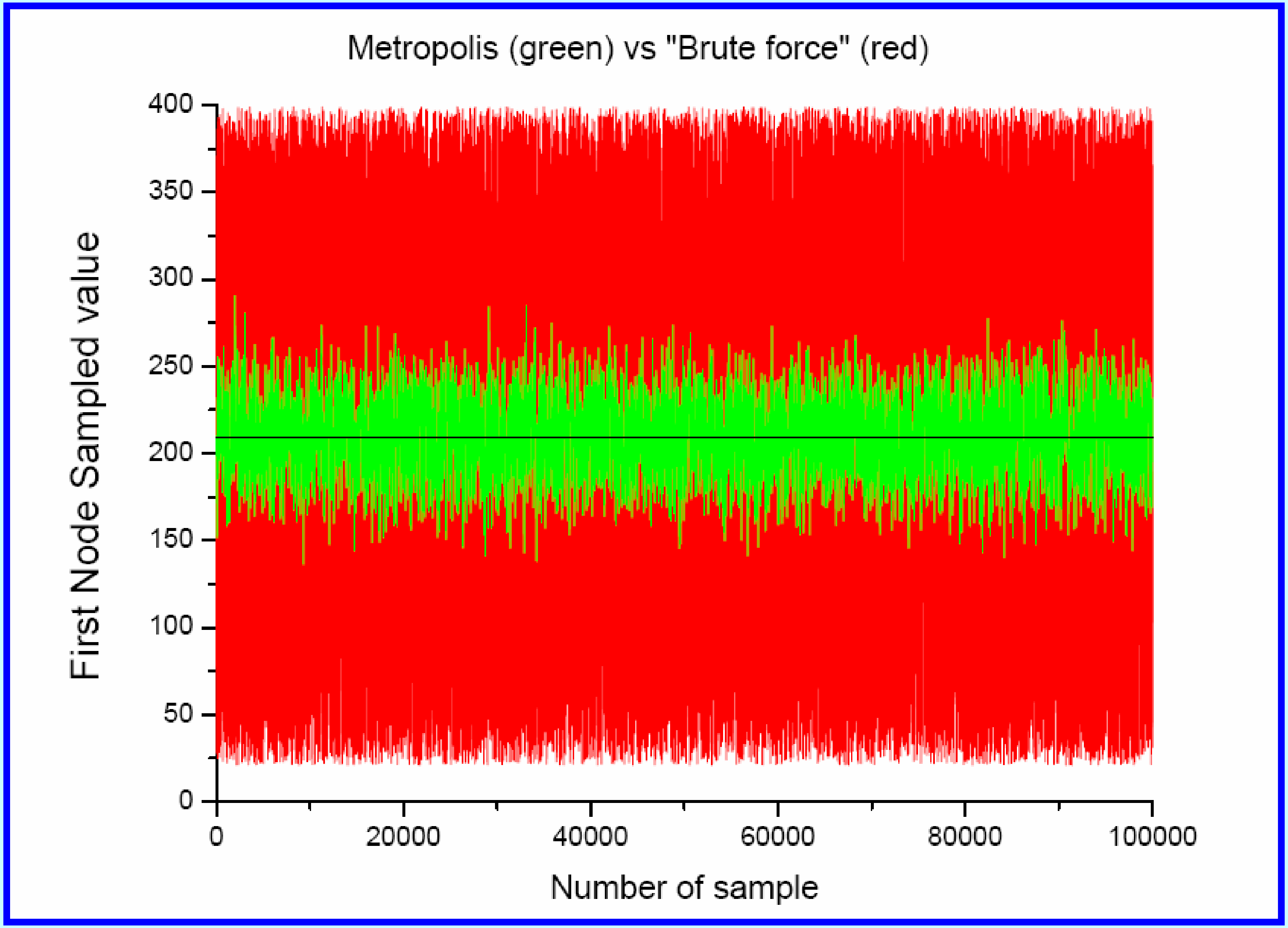
METROPOLIS approach: An stochastic Markov chain {**σ**} distributed following p(**σ**)

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

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

$$p_0(\sigma \mid \sigma_C, V_C) \sim \exp\{-(1/2)[(\sigma - \sigma_C)^T \bullet (V_C)^{-1} \bullet (\sigma - \sigma_C)]\}$$

SPREAD OF SAMPLED VALUES



LINEAR MODEL: $y = \sigma$

Node	Model	Expt	$\sigma_E(\%)$	Expt / Model	Comments
1	210	205.6	30.0%	0.979	within error
2	40	39.3	2.0%	0.983	within error
3	20	26	30.0%	1.300	marginal
4	10	14	5.0%	1.400	discrepant
5	7	6.7	3.0%	0.957	marginal
6	6	8.5	50.0%	1.417	within BIG error
7	6				No exp.data

covexp(3,1) = covexp(1,3) = 0.2 $\sigma_E(1)\,\sigma_E(3)$ - weak correlation

covexp(5,2) = covexp(2,5) = 0.8 $\sigma_E(2)\,\sigma_E(5)$ - strong correlation

MODEL DATA & CORRELATION

```
   ***** MODEL DATA
 Pmod(  1)= 210.0000 +/-   63.0000 ( 30.0% )          Ymod(  1)= 210.0000
 Pmod(  2)=  40.0000 +/-   12.0000 ( 30.0% )          Ymod(  2)=  40.0000
 Pmod(  3)=  20.0000 +/-    6.0000 ( 30.0% )          Ymod(  3)=  20.0000
 Pmod(  4)=  10.0000 +/-    3.0000 ( 30.0% )          Ymod(  4)=  10.0000
 Pmod(  5)=   7.0000 +/-    2.1000 ( 30.0% )          Ymod(  5)=   7.0000
 Pmod(  6)=   6.0000 +/-    1.8000 ( 30.0% )          Ymod(  6)=   6.0000
 Pmod(  7)=   6.0000 +/-    1.8000 ( 30.0% )          Ymod(  7)=   6.0000

 MODEL CORRELATION MATRIX (PRIOR):
0.1000000E+01
0.9500000E+00 0.1000000E+01
0.9000000E+00 0.9500000E+00 0.1000000E+01
0.8500000E+00 0.9000000E+00 0.9500000E+00 0.1000000E+01
0.8000000E+00 0.8500000E+00 0.9000000E+00 0.9500000E+00 0.1000000E+01
0.7500000E+00 0.8000000E+00 0.8500000E+00 0.9000000E+00 0.9500000E+00 0.1000000E+01
0.7000000E+00 0.7500000E+00 0.8000000E+00 0.8500000E+00 0.9000000E+00 0.9500000E+00 0.1000000E+01
```

~ 95% correlation

LINEAR MODEL: RESULTS

BF Calculations $0.5\,\sigma_C < \psi < 3.5\,\sigma_C$ **Mean Values**

30% Strong Correlations

Maximum Deviations from GLS For All Nodes (%)

30% Strong Correl	0.50/GLS	0.75/GLS	1.00/GLS	1.50/GLS	1.75/GLS	2.00/GLS	2.50/GLS	3.00/GLS	3.50/GLS
BF Mean Values	<7.7%	<3.2%	<0.55%	<0.45%	<1.1%	<0.77%	<1.5%	<8.5%	<7.9%

30% Zero Correlations

Maximum Deviations from GLS for All Nodes (%)

30% Zero Correl	0.50/GLS	0.75/GLS	1.00/GLS	1.50/GLS	1.75/GLS	2.00/GLS	2.50/GLS	3.00/GLS	3.50/GLS
BF Mean Values	<18%	<13%	<8.2%	<2.8%	<2.0%	<1.2%	<1.6%	<1.7%	<2.6%

5% Strong Correlations

Maximum Deviations from GLS for All Nodes (%)

5% Strong Correl	0.50/GLS	0.75/GLS	1.00/GLS	1.50/GLS	1.75/GLS	2.00/GLS	2.50/GLS	3.00/GLS	3.50/GLS
BF Mean Values	<1.7%	<1.2%	<0.68%	<0.21%	<0.07%	<0.05%	<0.10%	<0.37%	<0.34%

METR Calculations $0.02\,\sigma_C < \delta < 1.25\,\sigma_C$ **Mean Values**

30% Strong Correlations

Maximum Deviations from GLS For All Nodes (%)

30% Strong Correl	0.02/GLS	0.05/GLS	0.10/GLS	0.15/GLS	0.25/GLS	0.50/GLS	0.75/GLS	1.00/GLS	1.25/GLS
MET Mean Values	<0.28%	<0.07%	<0.39%	<0.15%	<0.22%	<1.3%	<0.14%	<1.2%	<3.7%

30% Zero Correlations

Maximum Deviations from GLS for All Nodes (%)

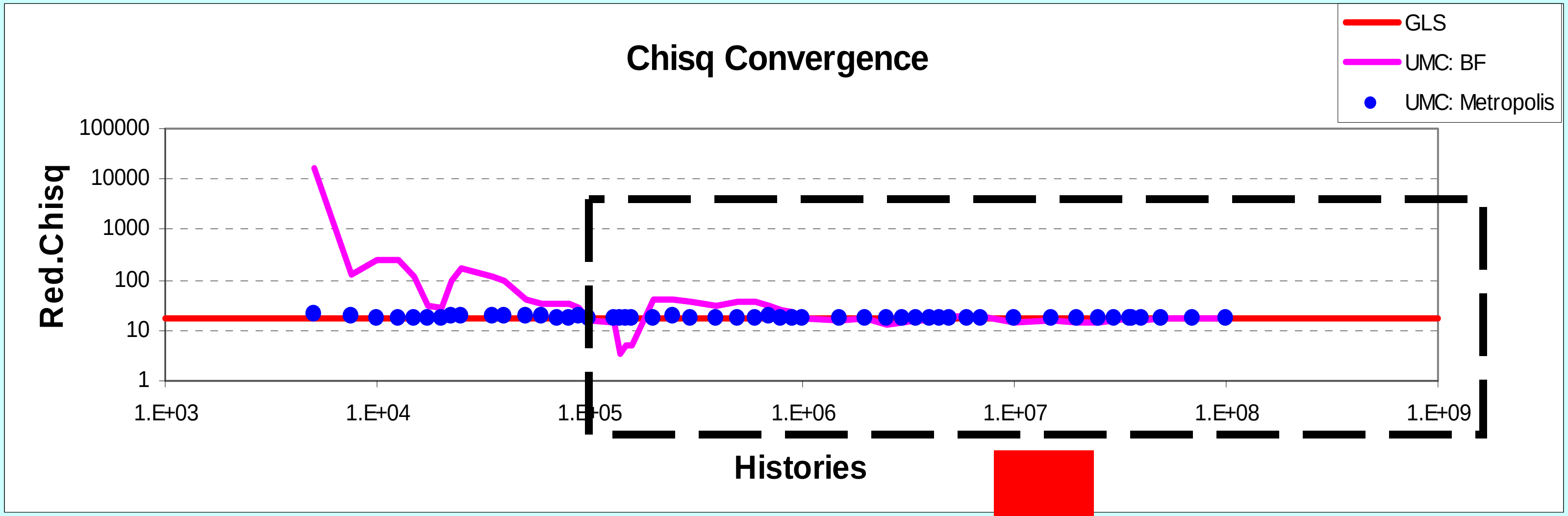
30% Zero Correl	0.02/GLS	0.05/GLS	0.10/GLS	0.15/GLS	0.25/GLS	0.50/GLS	0.75/GLS	1.00/GLS	1.25/GLS
MET Mean Values	<1.5%	<3.6%	<1.5%	<2.0%	<0.75%	<1.4%	<0.42%	<0.86%	<1.5%

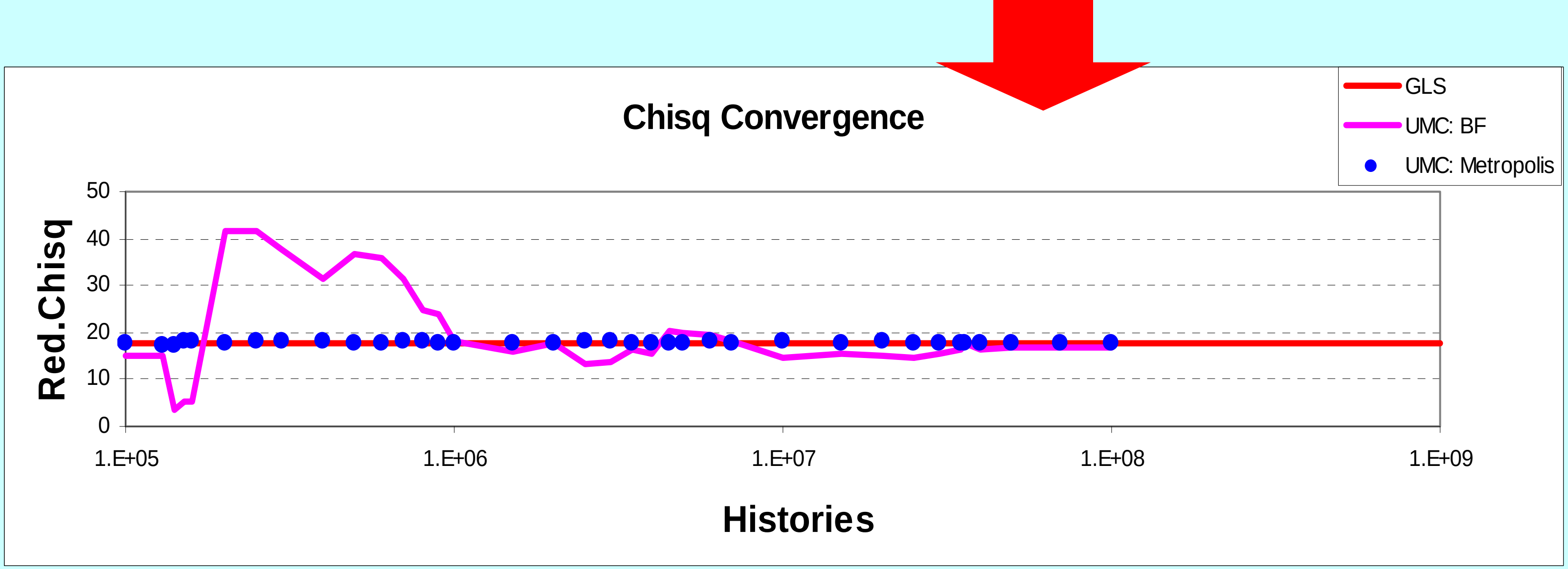
5% Strong Correlations

Maximum Deviations from GLS for All Nodes (%)

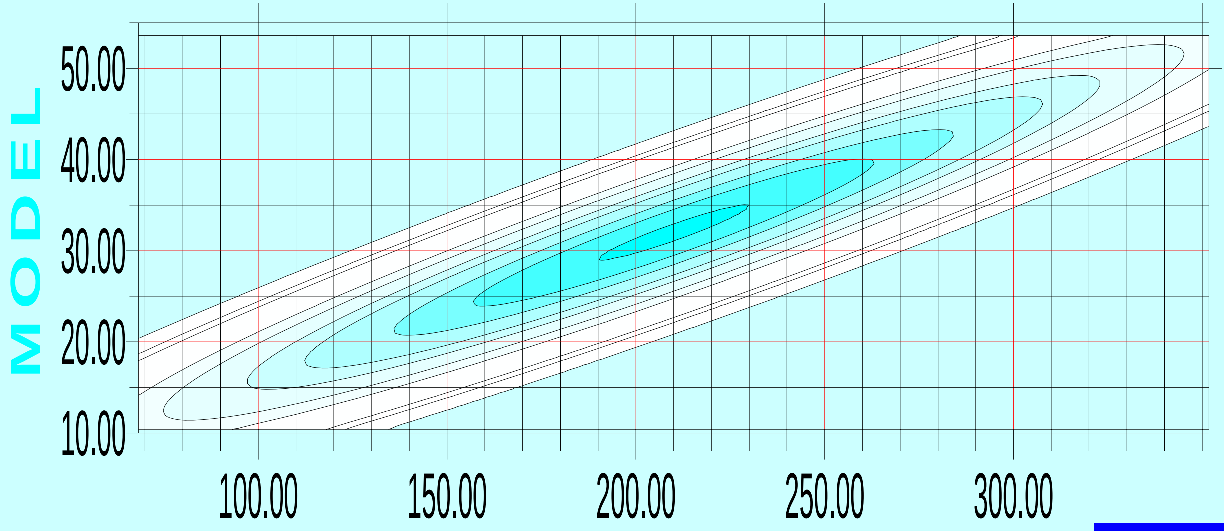
5% Strong Correl	0.02/GLS	0.05/GLS	0.10/GLS	0.15/GLS	0.25/GLS	0.50/GLS	0.75/GLS	1.00/GLS	1.25/GLS
MET Mean Values	<0.16%	<0.11%	<0.04%	<0.08%	<0.03%	<0.02%	<0.04%	<0.11%	<0.11%

UMC convergence





RATIO CASE

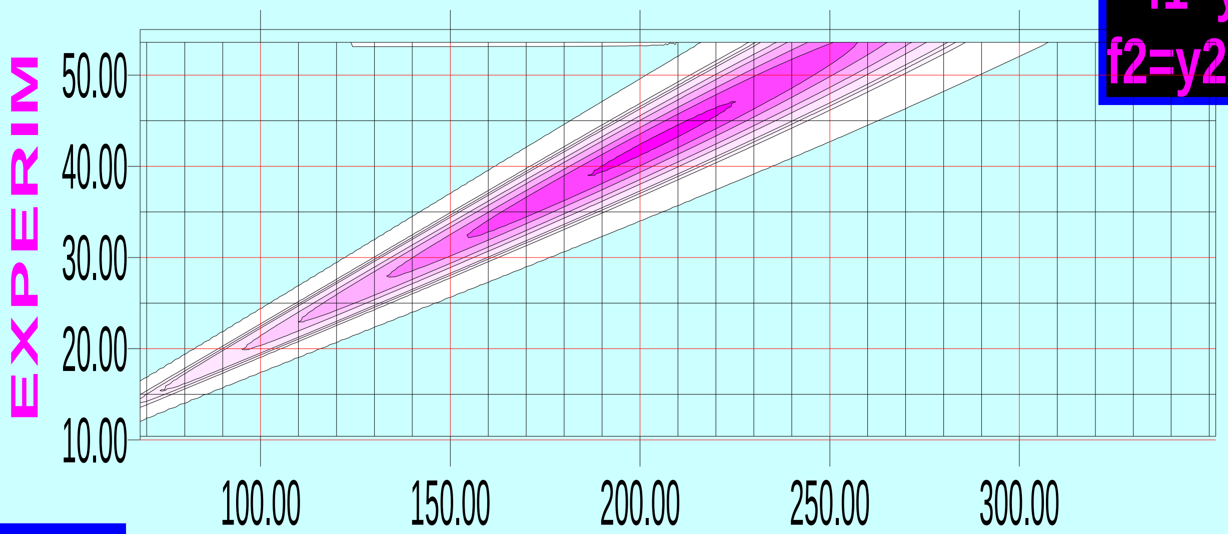


MODEL

y1=210 +/- 63 (30%)

y2=32 +/- 9.6 (30%)

Cov(1,2) = 0.95



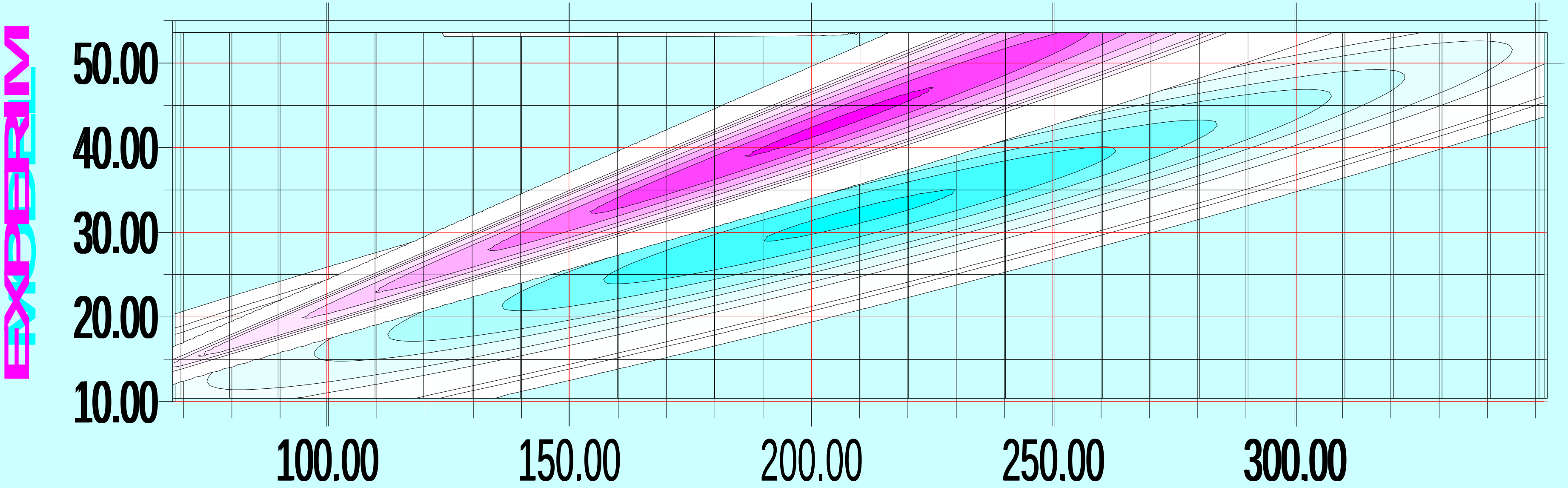
EXPERIM

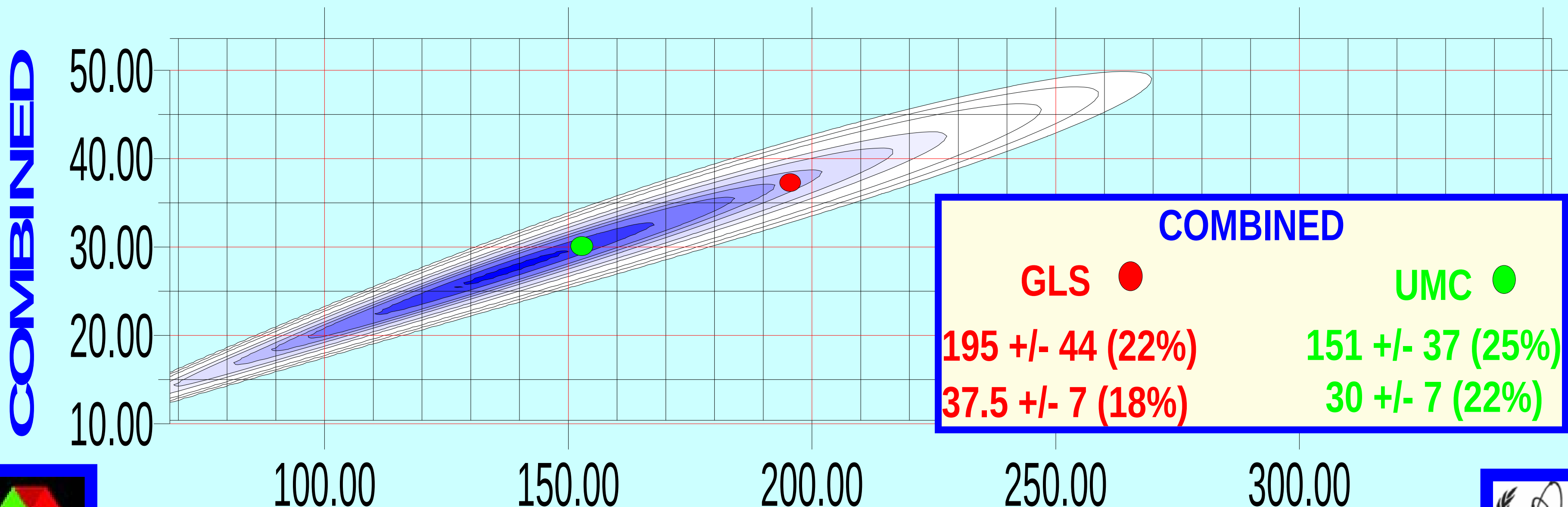
f1=y1=205.6 +/- 61.7 (30%)

f2=y2/y1=0.209 +/- 0.010 (5%) ~ 43

Cov(1,2) = 0.

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





GLS FAILURE: ANALYSIS

5% exp. ratio unc.
95% model correlation

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

LOG TRANSFORMATION

```
   ***** LOG(MODEL DATA)
 Pmod(  1)=    5.3471 +/-     .6000 ( 11.2% )
 Pmod(  2)=    3.4657 +/-     .6000 ( 17.3% )

   ***** LOG(MODEL FUNCTION)
 Ymod(  1)=    5.3471
 Ymod(  2)=   -1.8814

 MODEL CORRELATION MATRIX (PRIOR):
.1000000E+01
.9500000E+00  .1000000E+01

   ***** LOG(EXPERIMENTAL DATA)
 Yexp(  1)=    5.3259 +/-     .3000 (  5.6% )
 Yexp(  2)=   -1.5654 +/-     .0100 (  -.6% )
```

```
   ***** ORIGINAL MODEL DATA
 Pmod(  1)= 210.0000 +/-   126.0000 ( 60.0% )
 Pmod(  2)=  32.0000 +/-    19.2000 ( 60.0% )

   ***** ORIGINAL MODEL FUNCTION
 Ymod(  1)= 210.0000
 Ymod(  2)=     .1524

  EXPERIMENTAL CORRELATION MATRIX:
.1000000E+01
.0000000E+00  .1000000E+01

   ***** ORIGINAL EXPERIMENTAL DATA
 Yexp(  1)= 205.6000 +/-    61.6800 ( 30.0% )
 Yexp(  2)=     .2090 +/-      .0021 (  1.0% )
```

RESULTS FOR GLS METHOD (LOG TRANSFORMATION):

Mean	Sigma[%]	Red.Chisq
1.999575E+02	2.676447E+01	-1.261845E-02
4.175392E+01	2.677929E+01	1.020535E+02

RESULTS FOR UMC Metropolis (model + exp)

Mean	Sigma[%]	Red.Chisq
1.999971E+02	2.665413E+01	-1.266861E-02
4.176194E+01	2.666949E+01	1.029021E+02

RESULTS FOR GLS METHOD (DIRECT):

Mean	Sigma[%]	Red.Chisq
1.988118E+02	2.779634E+01	2.383451E+03
4.212220E+01	2.001335E+01	-1.662790E+01

RESULTS FOR UMC Metropolis (DIRECT):

Mean	Sigma[%]	Red.Chisq
1.859502E+02	2.391304E+01	5.271764E+01
3.881475E+01	2.387615E+01	-3.378792E-03

SUMMARY

- ❑ UMC is a viable tool for cross-section data evaluation

- ❑ Metropolis sampling scheme is recommended for UMC calculations

- ❑ When data values are cross sections or cross sections and integral (spectrum-averaged) cross sections, GLS and UMC are equivalent so GLS is recommended

- ❑ If ratio or other explicitly non-linear data are introduced UMC may be preferable to GLS