The Abdus Salam
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International Atomic Energy Agency

**2141-34**

**Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies**

***3 - 14 May 2010***

# Monte Carlo Approaches for Model Evaluation of Cross Sections and Uncertainties

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*AUSTRIA*

# Monte Carlo approaches for Model evaluation of cross sections and uncertainties

Roberto Capote and Donald Smith (*)

International Atomic Energy Agency, NAPC - Nuclear Data Section

(*) Argonne National Laboratory

# OUTLINE

- Introduction: Monte Carlo method
- UMC formulation (normal distributions)
- UMC sampling: Brute Force, Metropolis
- Toy models: Linear
- UMC convergence
- Toy models: Ratio data
- Log transformation
- Non-normal PDFs (& examples):
  1) lognormal distribution;
  2) uniform interval distribution;
  3) exponential distribution.
- Results and discussions for each PDF


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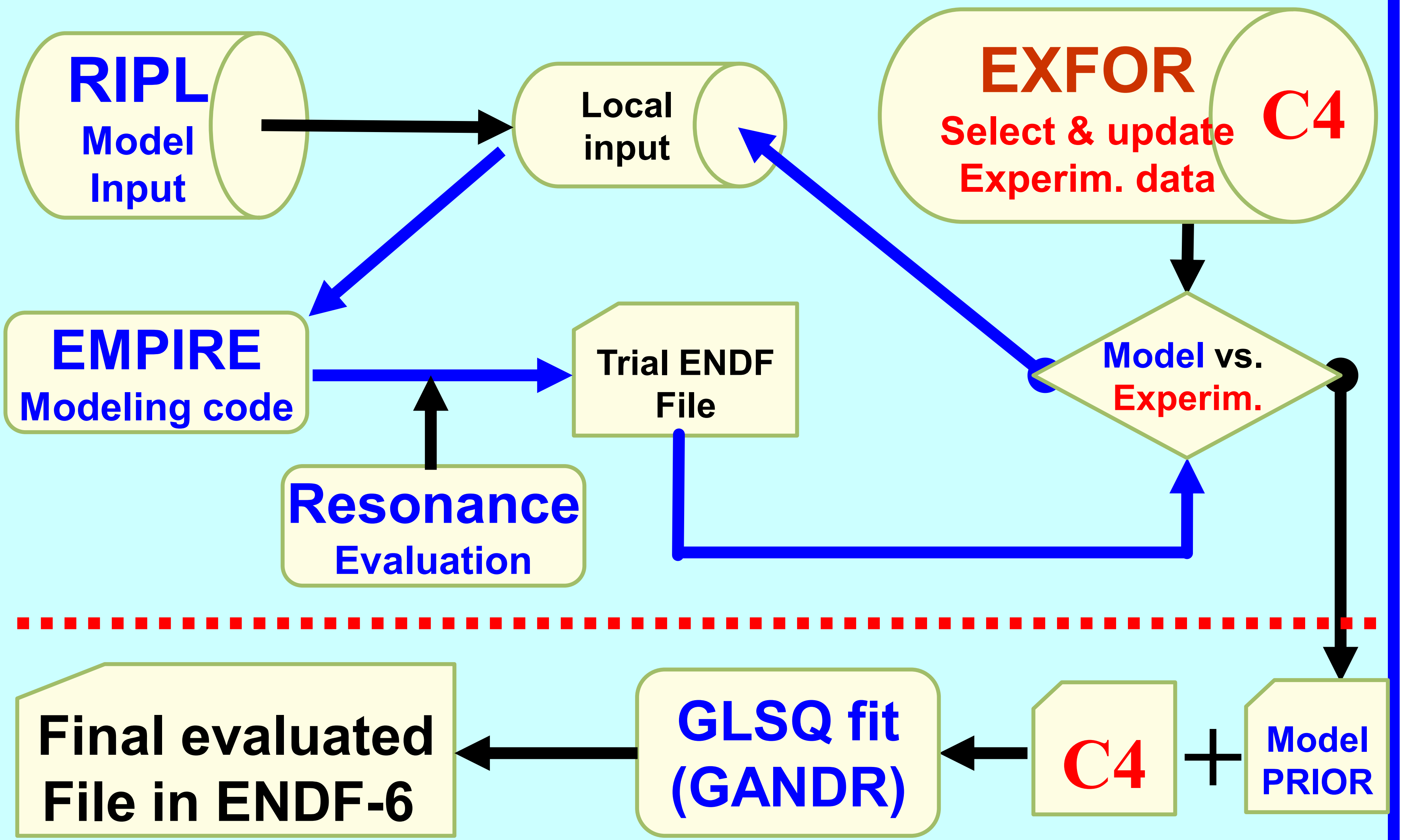
# Nuclear Data Evaluation process







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# 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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# Merging of Model Calculated and Experimental Results … More

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

1

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

$\bar{\sigma}_C$ = 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"

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

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


**Donald L. Smith**
*Argonne National Laboratory*
WPEC 2007 – SG24

# 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

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

$$p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C, \mathbf{V}_C) \sim \exp\{-(1/2)[(\boldsymbol{\sigma}-\boldsymbol{\sigma}_C)^T \bullet (\mathbf{V}_C)^{-1} \bullet (\boldsymbol{\sigma}-\boldsymbol{\sigma}_C)]\}$$

$$\mathscr{L}(\mathbf{y}_E, \mathbf{V}_E \mid \boldsymbol{\sigma}) \sim \exp\{-(1/2)[(\mathbf{y}-\mathbf{y}_E)^T \bullet (\mathbf{V}_E)^{-1} \bullet (\mathbf{y}-\mathbf{y}_E)]\}, \ \mathbf{y}=f(\boldsymbol{\sigma})$$

$y_E$, $V_E$: 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**



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# UMC sampling schemes

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

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

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

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

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

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

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



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# Central Limit Theorem

```
do MCsteps=1,naccept,K
   rnorm=-6
   do i=1,12
    CALL RANDOM(rnd)
    rnorm=rnorm+rnd
   enddo
   rnorm are normally distributed
   RANDOMS1(MCSTEPS)=rnorm
enddo
```



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# Metropolis algorithm

```
naccept=0
do MCsteps=1,NEVENTS
   CALL RANDOM(rnd)
   xt=xn+(2*rnd-1)*3
   wt=f(xt)
   CALL RANDOM(rnd)
   if(wt.GT.(rnd*wn)) then
       xn=xt
       wn=wt
       naccept=naccept+1
   endif
   xn are normally distributed
   RANDOMS(MCSTEPS)=xn
enddo
```


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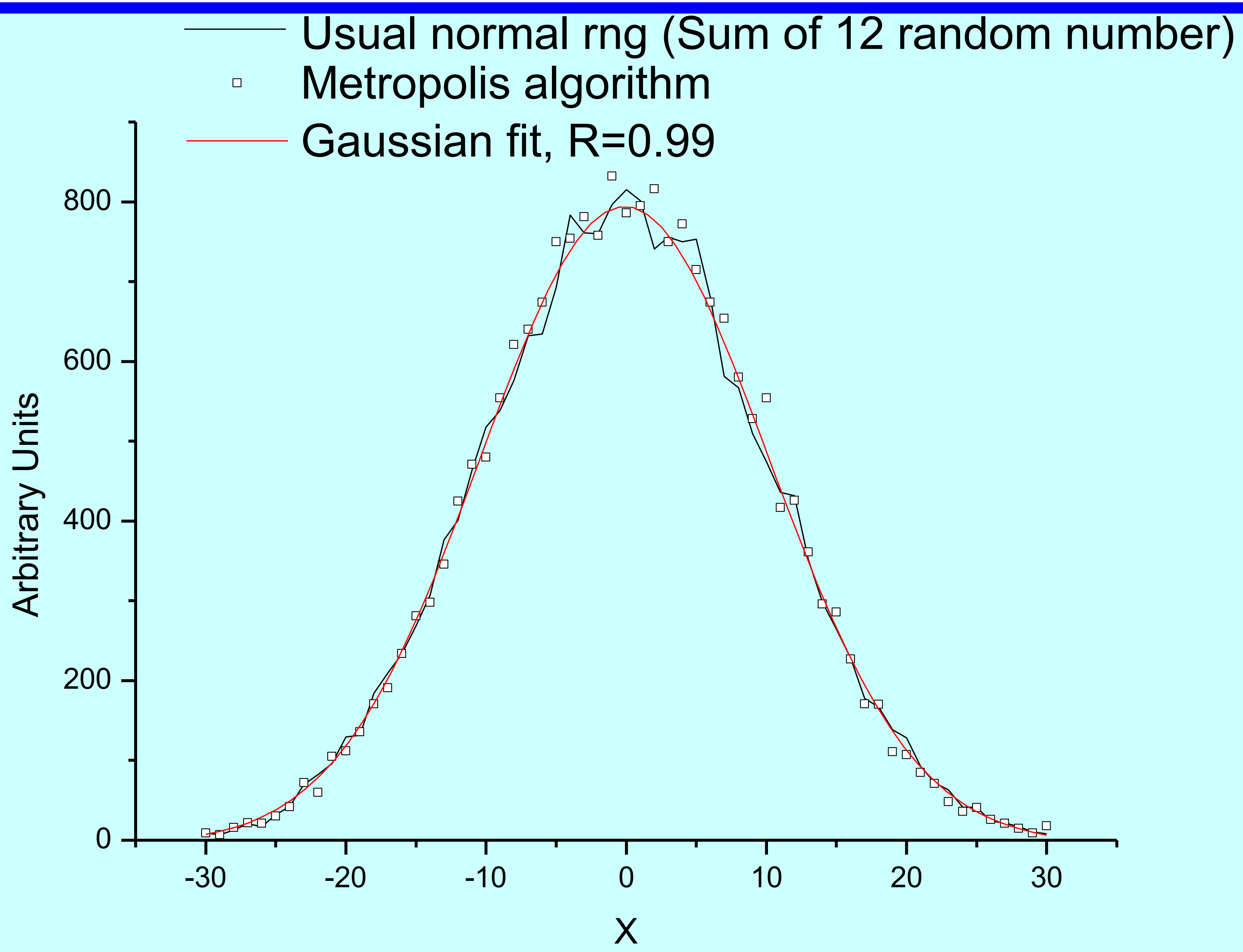





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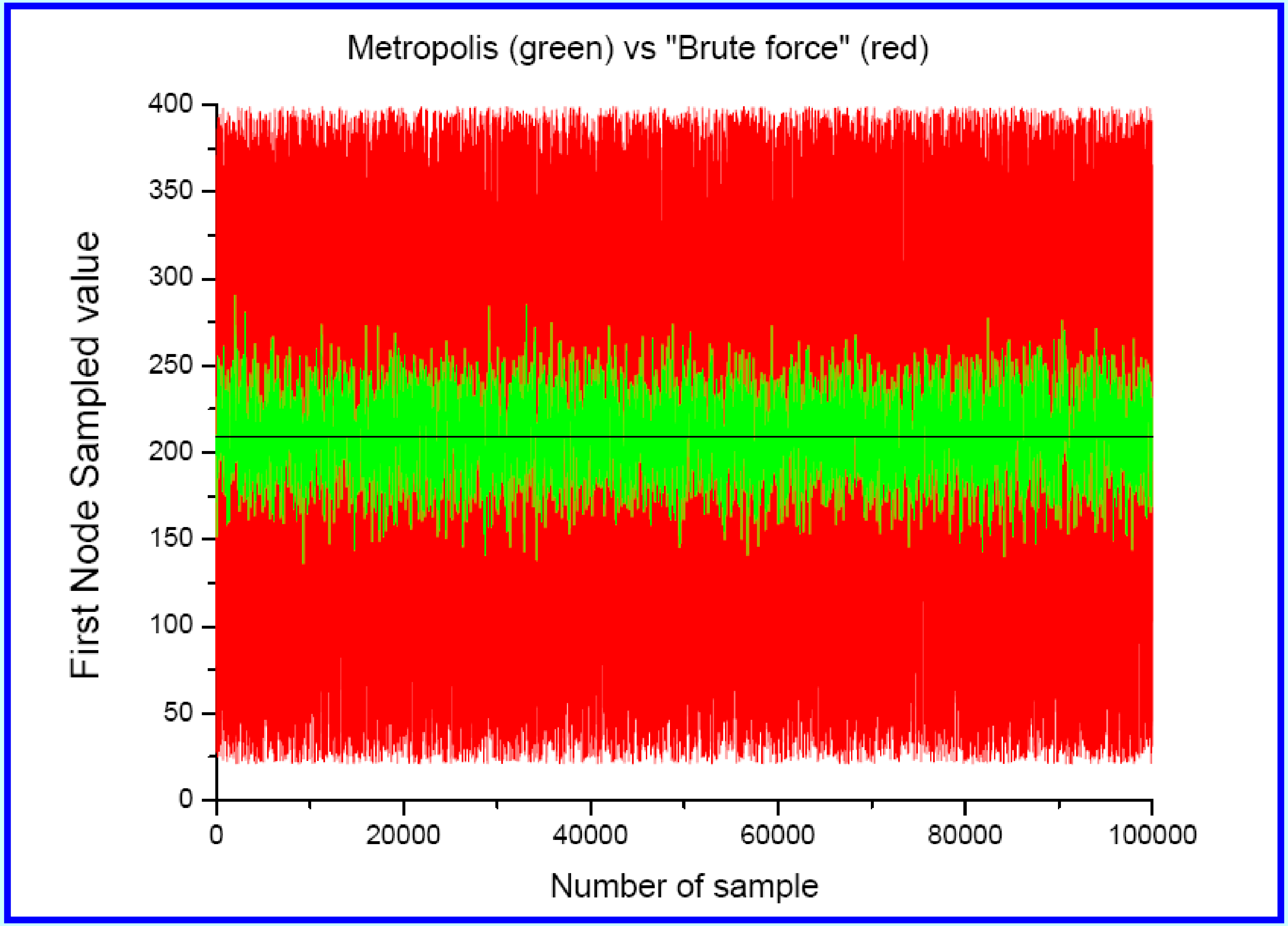
# SPREAD OF SAMPLED VALUES







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# 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


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# 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**


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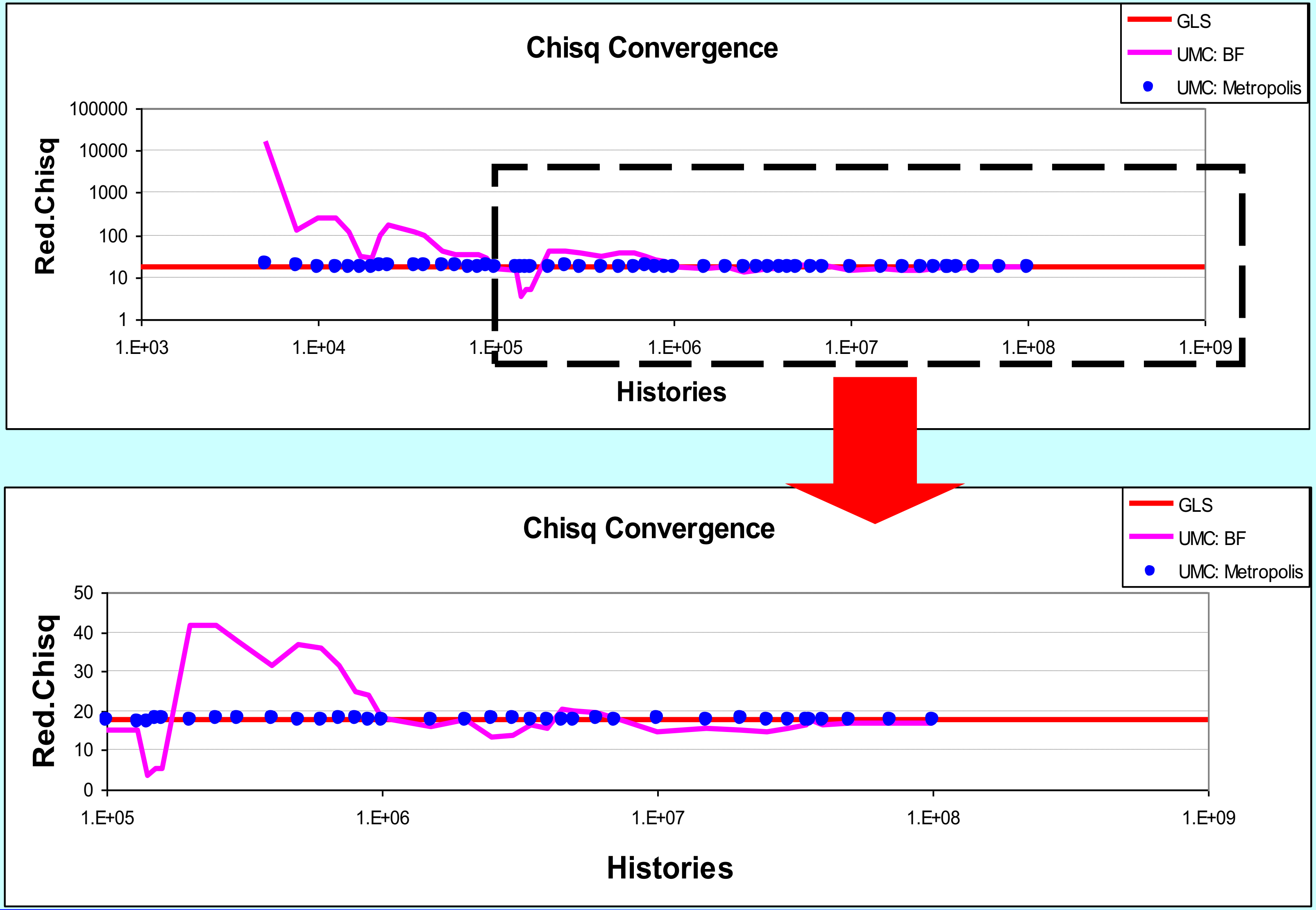
# UMC convergence







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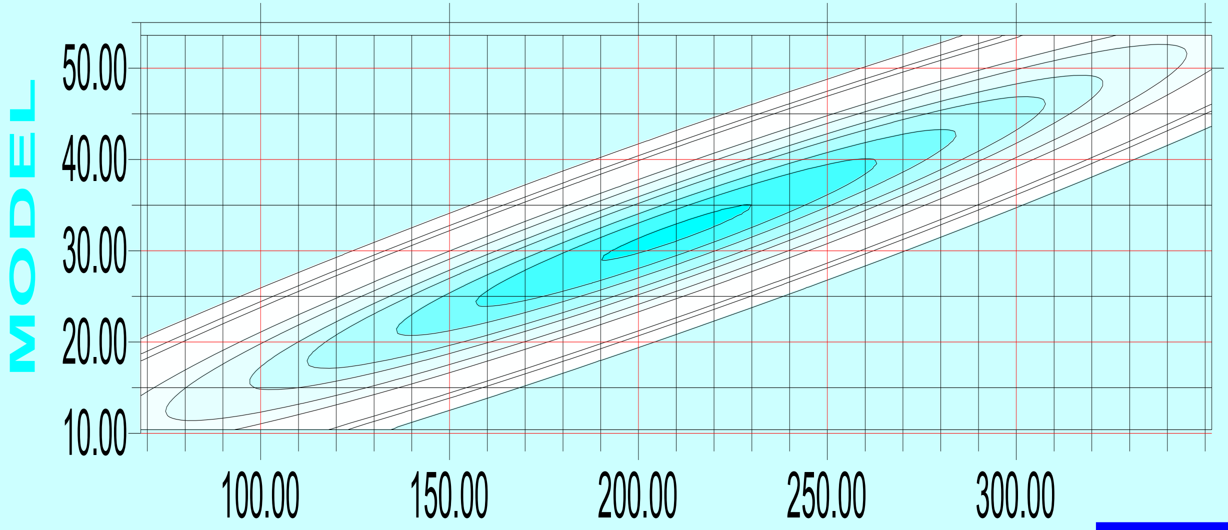
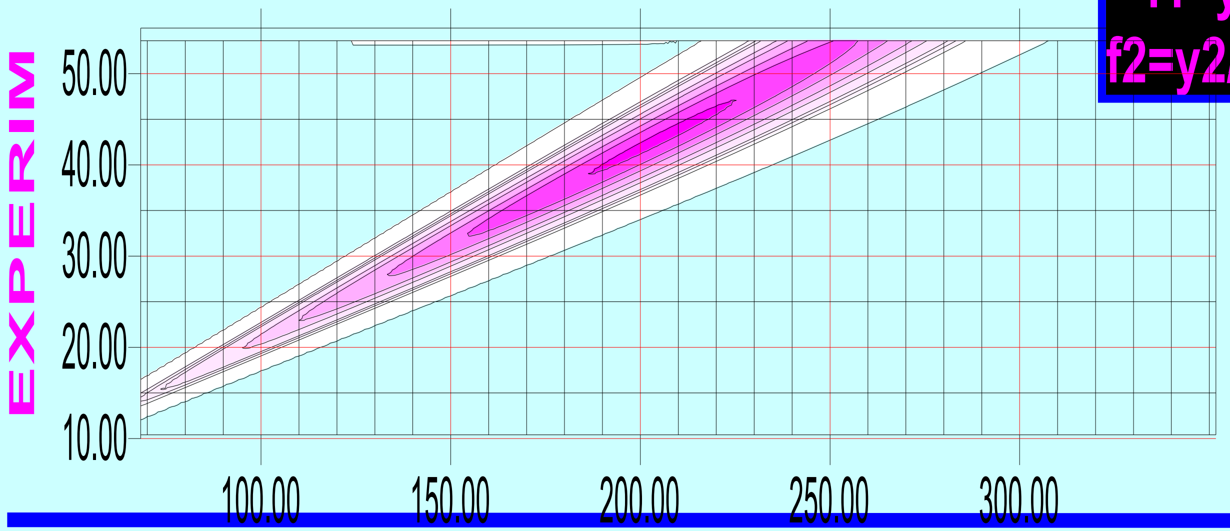
# RATIO CASE




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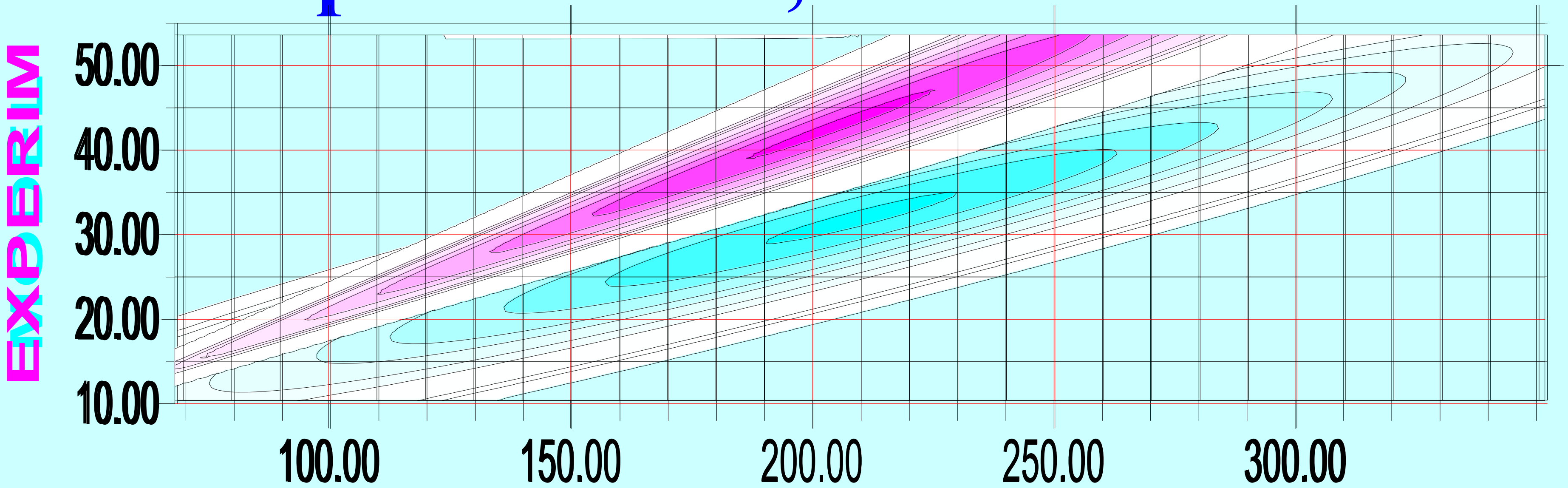
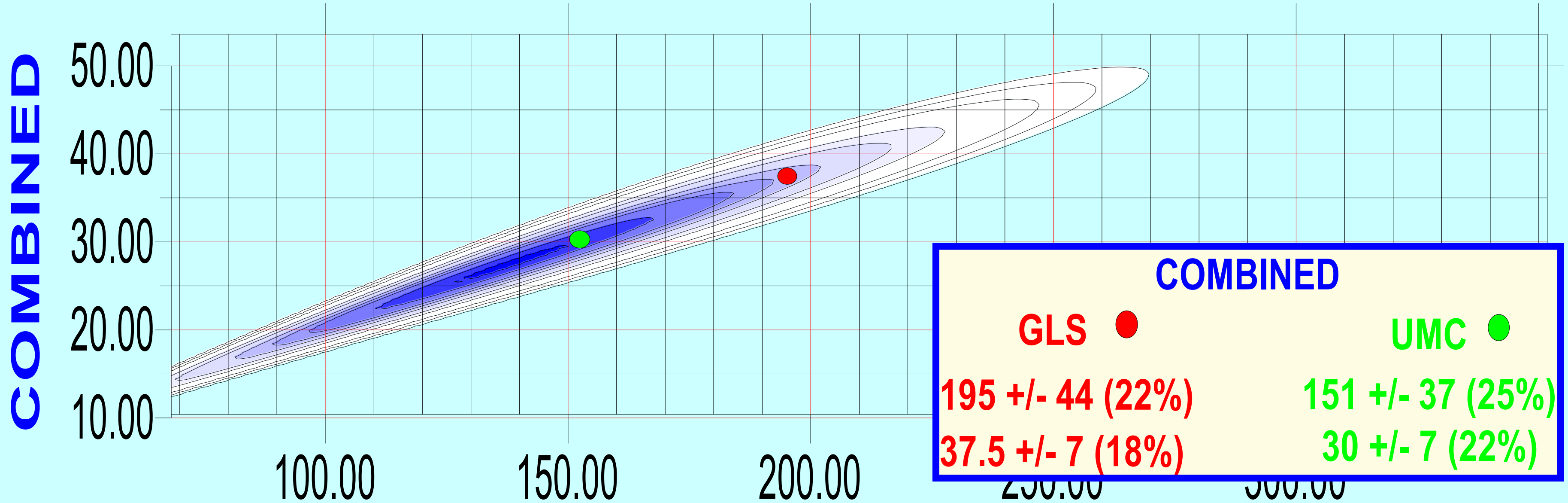
# 5% exp. ratio unc., 95% model correl.



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# 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 |


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# 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 |





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# 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



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# PDF 1. Lognormal distribution

There is a problem associated with utilizing normal distributions if the uncertainties in the variables are large (e.g., typically > 30%).

$$q(z) = (C/z)\,\exp[-(ln\ z - \nu)^2/(2\sigma^2)] \quad \text{where } 0 < z < +\infty ,$$

$$\text{mean value} = \langle z \rangle = \exp[\nu + (\sigma^2/2)] ,$$
$$\text{variance} = V_z = \exp(2\nu + 2\sigma^2) - \exp(2\nu + \sigma^2) .$$

Best approach: $x = ln\ z$

Lognormal PDF in **z** → a normal PDF in **x**.

If the variable z has an uncertainty $E_z$, then the uncertainty in $E_x = E_z/z$ = relative error in **z**.

See paper by Capote R and Smith D in NDST2010 (Korea)


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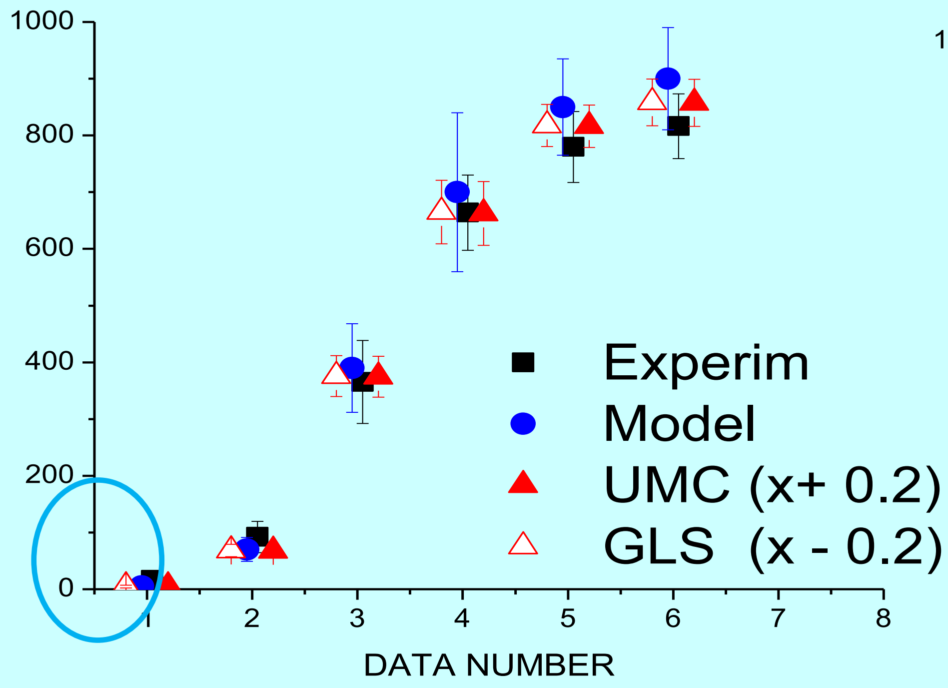
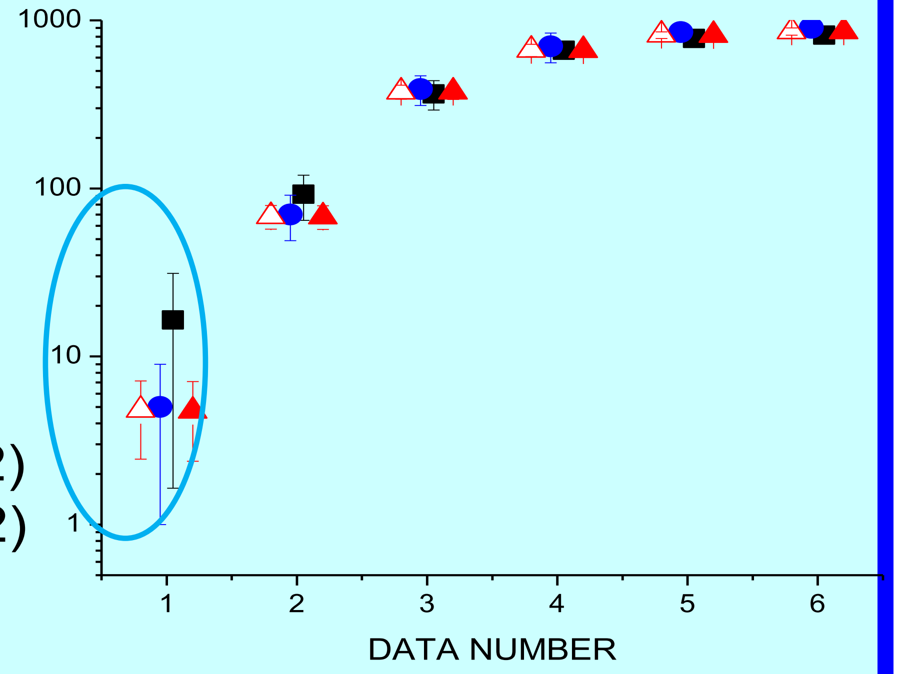
# Normal – Lognormal CASE




```
 ***** MODEL DATA              MODEL CORRELATION MATRIX (PRIOR):
Pmod(  1)=   5 +/-  4 ( 80.0% ) .1000000E+01
Pmod(  2)=  70 +/- 21 ( 30.0% ) .9500000E+00  .1000000E+01
Pmod(  3)= 390 +/- 78 ( 20.0% ) .9000000E+00  .9500000E+00  .1000000E+01
Pmod(  4)= 700 +/-140 ( 20.0% ) .8500000E+00  .9000000E+00  .9500000E+00  .1000000E+01
Pmod(  5)= 850 +/- 85 ( 10.0% ) .8000000E+00  .8500000E+00  .9000000E+00  .9500000E+00  .1000000E+01
Pmod(  6)= 900 +/- 90 ( 10.0% ) .7500000E+00  .8000000E+00  .8500000E+00  .9000000E+00  .9500000E+00  .1000000E+01
```

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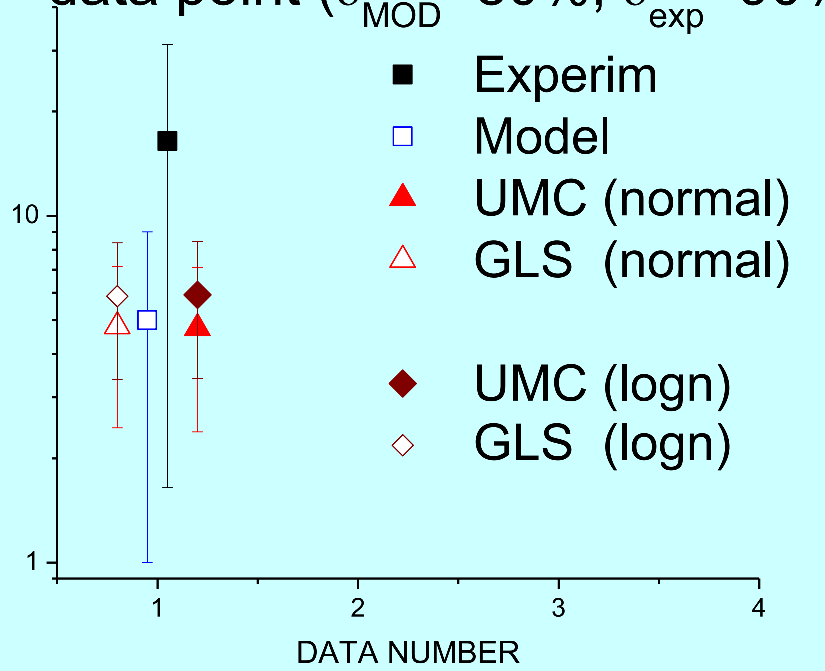
# RESULTS

1st data point ($\delta_{MOD}$=80%, $\delta_{exp}$=90%




| GLS (normal) | GLS(logn) | Diff(%) |
|---|---|---|
| 4.80017 | 5.87065 | **22.30102** |
| 68.22307 | 72.07464 | **5.64556** |
| 375.88501 | 385.8047 | **2.63902** |
| 664.97919 | 675.7487 | **1.61953** |
| 817.72153 | 822.9619 | **0.64085** |
| 858.30519 | 862.9309 | **0.53894** |

UMC method

| Mean | Sigma[%] |
|---|---|
| 5.9143153E+00 | 4.2513903E+01 |
| 7.2285629E+01 | 1.4169891E+01 |
| 3.8663715E+02 | 8.9229268E+00 |
| 6.7760062E+02 | 8.1024980E+00 |
| 8.2389039E+02 | 4.4594776E+00 |
| 8.6352086E+02 | 4.7502835E+00 |

GLS method

| Mean | Sigma[%] |
|---|---|
| 5.870653E+00 | 4.248953E+01 |
| 7.207464E+01 | 1.419907E+01 |
| 3.858047E+02 | 8.931793E+00 |
| 6.757487E+02 | 8.114550E+00 |
| 8.229619E+02 | 4.460754E+00 |
| 8.629309E+02 | 4.751476E+00 |





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# PDF 2. Uniform distribution

$a,b \geq 0$ (cross sections)

---

**Uniform distribution**

$$q(z) = \begin{cases} [1/(b-a)] & \text{if } a < z < b, \\ 0 & \text{otherwise.} \end{cases}$$

---

Mean value $\langle z \rangle = (a+b)/2$;

Variance $E_z^2 = [(b-a)^2/12]$

Rel. Error = $(b-a)/(a+b)/\sqrt{3}$

If $a=0$ => Rel. Error = $1/\sqrt{3}$ = 57.7% !!!



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# Uniform – normal (no correlations)

$$<z> = (a+b)/2$$

**1st point – uniform**
**2nd point – normal**

<u>Case 1</u> (identical intervals):
**$a_{C1}$ = 10, $b_{C1}$ = 40**, $\sigma_{C2}$ = 100 (20%)
**$a_{E1}$ = 10, $b_{E1}$ = 40**, $\sigma_{E2}$ = 85 (15%)

SOLUTION: $a_{S1}$ = 10 and $b_{S1}$ = 40.
UMC analysis $<\sigma_1>$ = 25.00 **(34.6%)**
$<\sigma_2>$ = 89.33 (12.0%)
GLS analysis $<\sigma_1>$ = 25.00 **(24.5%)**
$<\sigma_2>$ = 89.33 (12.0%)

<u>Case 2</u> (strong overlap):
**$a_{C1}$ = 2, $b_{C1}$ = 40**
**$a_{E1}$ = 5, $b_{E1}$ = 60**

SOLUTION: $a_{S1}$ = 5 and $b_{S1}$ = 40.
UMC analysis $<\sigma_1>$ = 22.50 **(44.9%)**
GLS analysis $<\sigma_1>$ = 24.72 **(36.5%)**

<u>Case 3</u> (weak overlap):
**$a_{C1}$ = 10, $b_{C1}$ = 20**
**$a_{E1}$ = 16, $b_{E1}$ = 40**

SOLUTION: $a_{S1}$ = 16 and $b_{S1}$ = 20.
UMC analysis $<\sigma_1>$ = 18.00 **(6.4%)**
GLS analysis $<\sigma_1>$ = 16.92 **(15.7%)**


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# PDF 3. exponential– normal (no correl)

**A cross section estimate is provided but no uncertainty is given**

**Exponential distribution**

$$q(z) = C \exp(-z/\langle z \rangle) \quad \text{where } 0 < z < \infty \text{ and } \langle z \rangle > 0 ;$$

**Mean value =** $\langle z \rangle$ **, Variance** $V_z = \langle z^2 \rangle - \langle z \rangle^2 = E_z^{\,2} = \langle z \rangle^2$.

| Case 1: | UMC | GLS |
|---|---|---|
| $\sigma_{C1}$ = 210 .0 (30.00%), $\sigma_{C2}$ = 22 | (no uncert) | **(100%)** |
| $\sigma_{E1}$ = 205.6 (61.68%), $\sigma_{E2}$ = 34 | (no uncert) | **(100%)** |

**SOLUTION:**

UMC analysis $\langle\sigma_1\rangle$ = 208.1 (21.1%); $\langle\sigma_2\rangle$ = **14.90 ( 9.9%)**

GLS analysis $\langle\sigma_1\rangle$ = 207.8 (21.1%) ; $\langle\sigma_2\rangle$ = **25.54 (72.3%)**

**The posterior function *p* includes the product of two simple exponentials. This product equals the exponential factor** $\exp(-\sigma_2/\sigma_{m2})$**, where** $(1/\sigma_{m2}) = (1/\sigma_{C2}) + (1/\sigma_{E2})$**. Thus, for the input values given, one obtains** $\sigma_{m2} = 13.4$





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# CONCLUDING REMARKS

**Covariance Workshop, Port Jefferson 2008**

- UMC is a viable tool for cross-section data evaluation.
- UMC Metropolis sampling scheme is recommended.
- 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.**

- GLS is equivalent to UMC for PDFs closely resembling symmetric normal distributions with small to modest uncertainties.
- UMC results are more reliable for broad or strongly asymmetric distributions.
- The lognormal distribution can be used to good advantage in certain situations involving large uncertainties.
- Use of the uniform and exponential distributions discouraged.