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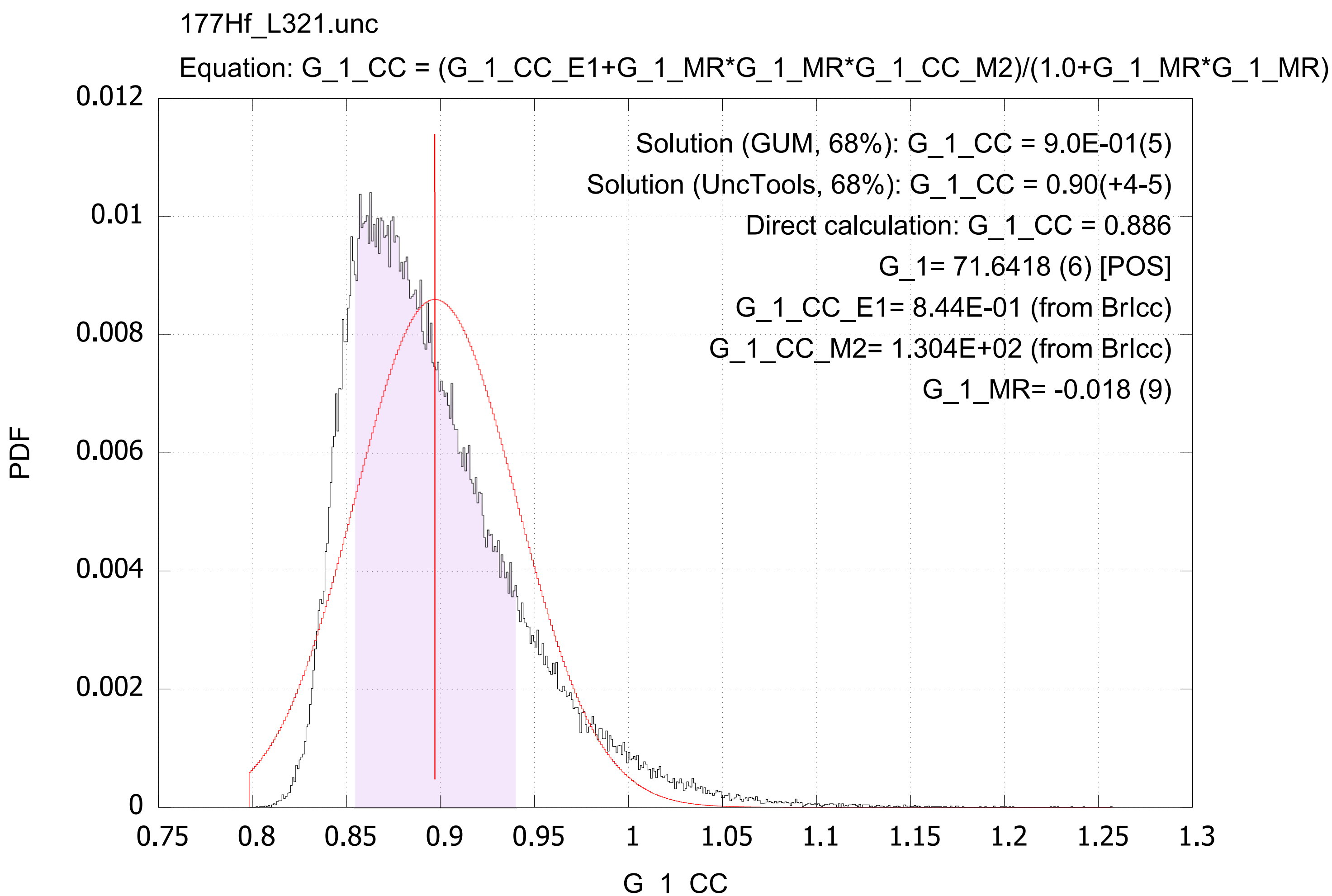
UncTools (NS_Lib) – treatment of uncertainties using Monte Carlo

T. Kibèdi (ANU)

Experimental quantitates in ENSDF



Experimental quantitates in ENSDF

2001TuZZ J.K. Tuli, *A Manual for Preparation of Data Sets*

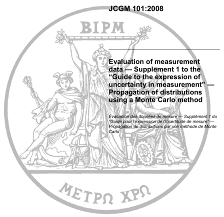
- Single unsigned number: BR, CC, HF, LOGFT, NB, NP, NR, NT, QP
- Single signed number: MR, Q-, QA, SN, SP
- Standard symmetric uncertainty; two character field (ENSDF Manual V.11):
  - an up to two digits integer, up to 99, preferable less than 25
  - LT, GT, LE, GE, AP, CA, S

    DBR, DCC, DE, DHF, DIA, DIB, DIE, DIP, DNB, DNR, DNP, DNT, DQP, DQ-, DS, DSP, DTI
- Standard asymmetric uncertainty; two signed integers (ENSDF Manual V.12):
  - DFT, DMR, DT, DNB, DQA
- Special rules for E, M, J, S, L fields

Uncertainty propagation in ENSDF codes:

- Gaussian (analytical) method, only valid for small DX/X values
- For multi-variant functions (Ruler, Gabs, Gtol) difficult / impossible to manage

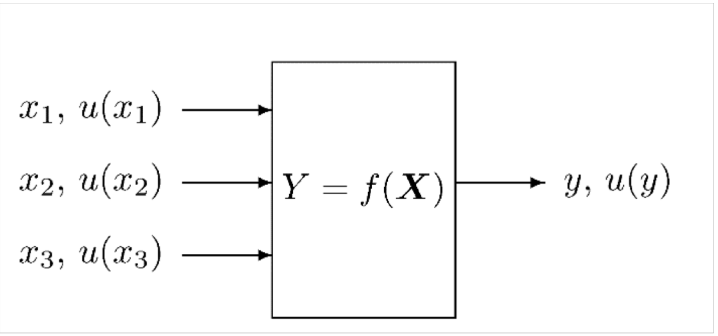
GUM framework

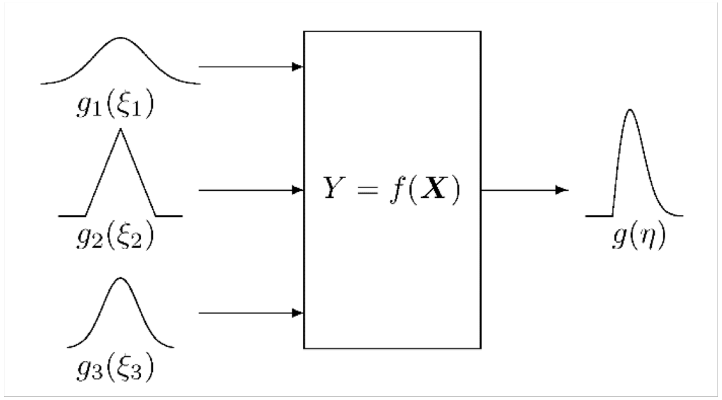


Joint Committee for Guides in Metrology (JCGM, 1993)
Guide to the Expression of Uncertainty in Measurement

Concept

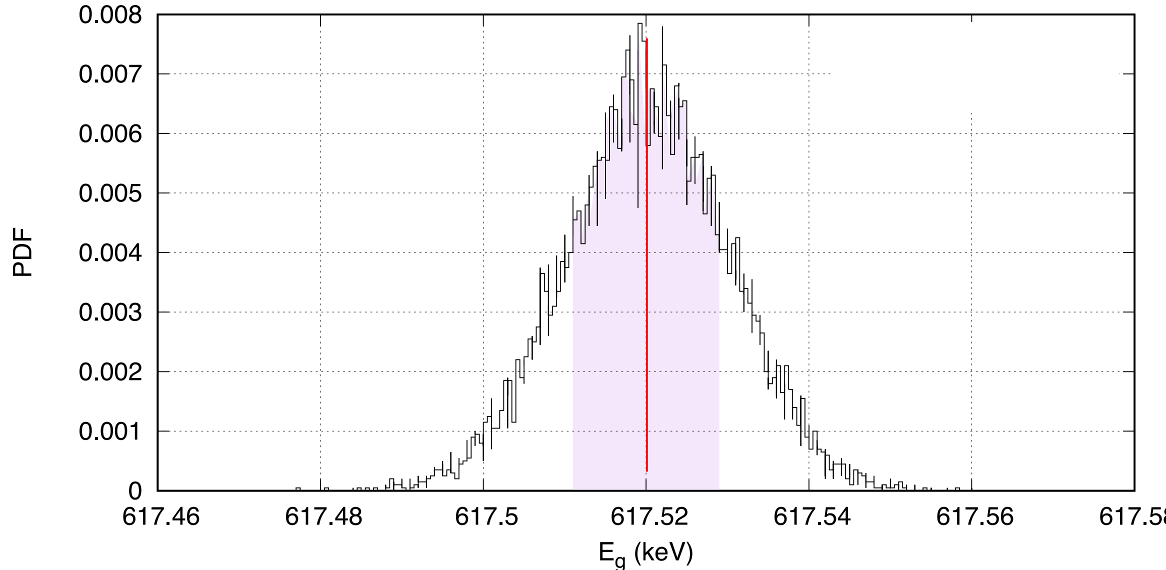
- Define the output quantity, the quantity required to be measured.
- Decide the input quantities upon which the output quantity depends.
- Develop a model relating the output quantity to these input quantities.
- On the basis of available knowledge assign probability density - Gaussian normal), rectangular (uniform), etc. - to the values of the input quantities.



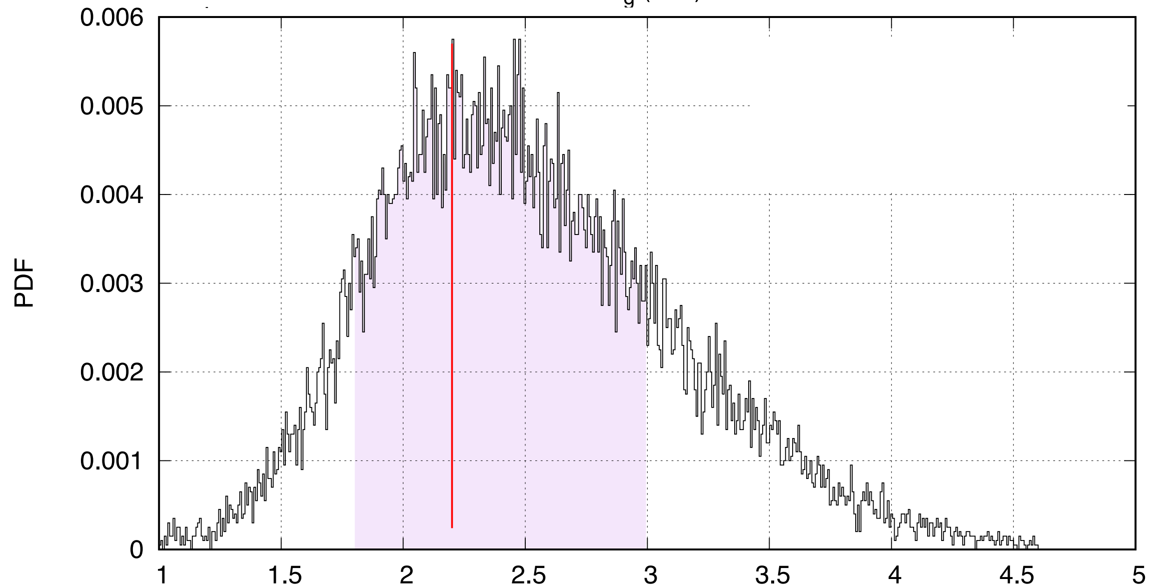


Probability Density Function (PDF)

Symmetric Normal Distribution:
E_γ=617.520(10) keV



Asymmetric normal distribution:
MR=+2.2(+8-4)



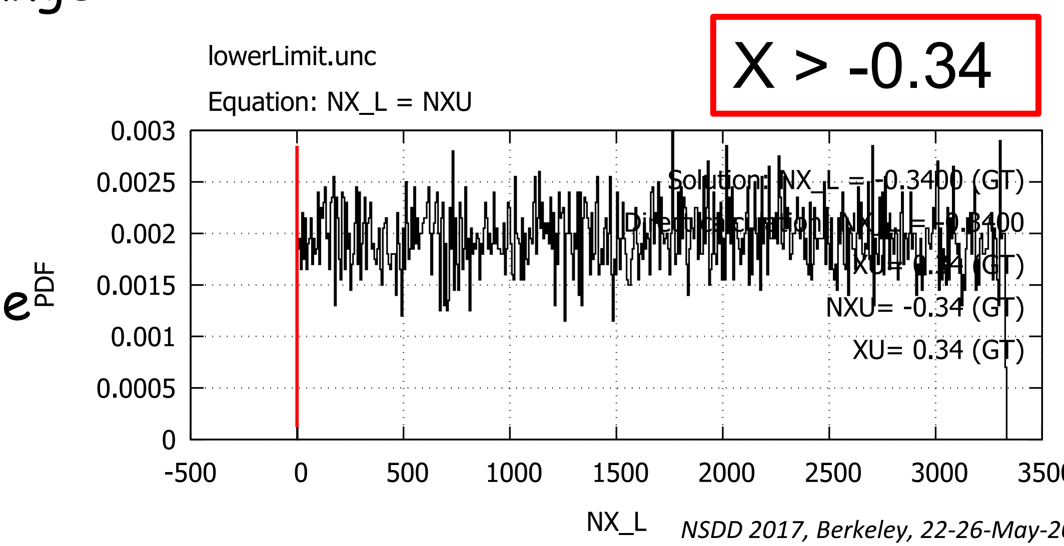
Probability Density Function (PDF)

Limits

	Limit	Range	Range Used in MC
UPPER	<0.5	[0 : +0.5]	[0 : +0.5]
	<+0.5	[-infinity : +0.5]	[-4999.5:+0.5]
	<-0.5	[-infinity : -0.5]	[-5000.5:-0.5]
LOWER	>0.5	[+0.5:+infinity]	[+0.5:+5000.5]
	>+0.5	[+0.5:+infinity]	[+0.5:+5000.5]
	>-0.5	[-0.5:+infinity]	[-0.5:+4999.5]

PDF uniform over the entire range

- Infinite range: PDF = Zero
- Replace infinity with a sufficiently large range: Infinity ~ 10000 Limit value



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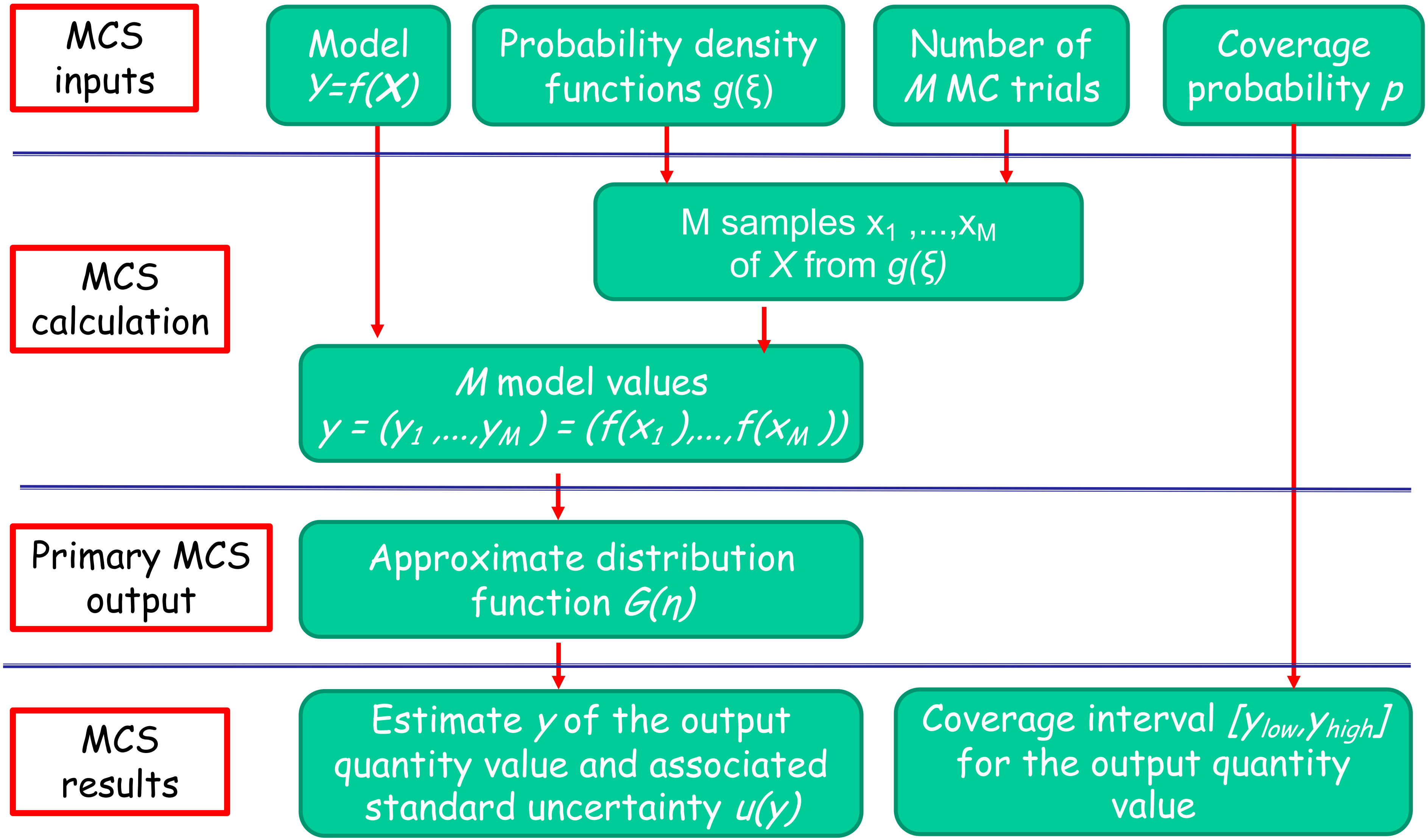
Monte Carlo simulations to obtain the output quantity



Estimate of the output quantity

After *M* draws model values obtained as (JCGM 101:2008 7.6)

$Y_r = f(X_r)$, $r = 1, 2, \ldots M$

Average:

$$\tilde{y} = \frac{1}{M}\sum_{r=1}^{M} y_r$$

Standard deviation:

GUM solution

$$u^2(\tilde{y}) = \frac{1}{M-1}\sum_{r=1}^{M}(y_r - \tilde{y})^2$$

NOTE: $\tilde{y}$ may not agree f(X), where X is the best parameter values!c

Pure ICC

Balraj Singh (26-May-2012)

One question: ^{211}Po: 34(5) keV gamma: I am now assigning (E4) based on model considerations. When I run interactive BrIcc, total CC=4.E6 (8). Does it mean 4(8)E-6 or 4.0(8)E6? Seems former is the case since when I run BrIcc on 29, 34 and 39 keV, I get values from 1.4E6 to 14E6, but I think the nomenclature needs some clarification. When researchers quote numbers in papers like 4.(8), they generally imply 4.0(8).

BrIcc ^{211}*Po* 34(5) keV E4 CC=4.E6 DCC=8.E6

DICC=ICC(E), ICC(E-DE), ICC(E+DE)

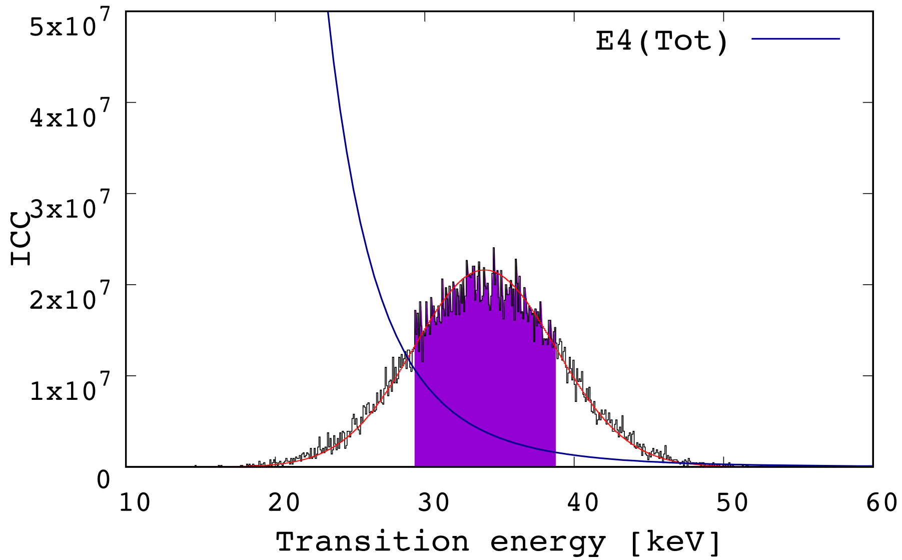
3.9E+6, 1.2E+7, 1.5E+6

Pure ICC

BrIcc ^{211}*Po* 34(5) keV E4

DICC=ICC(E), ICC(E-DE), ICC(E+DE)

3.9E+6, 1.2E+7, 1.5E+6

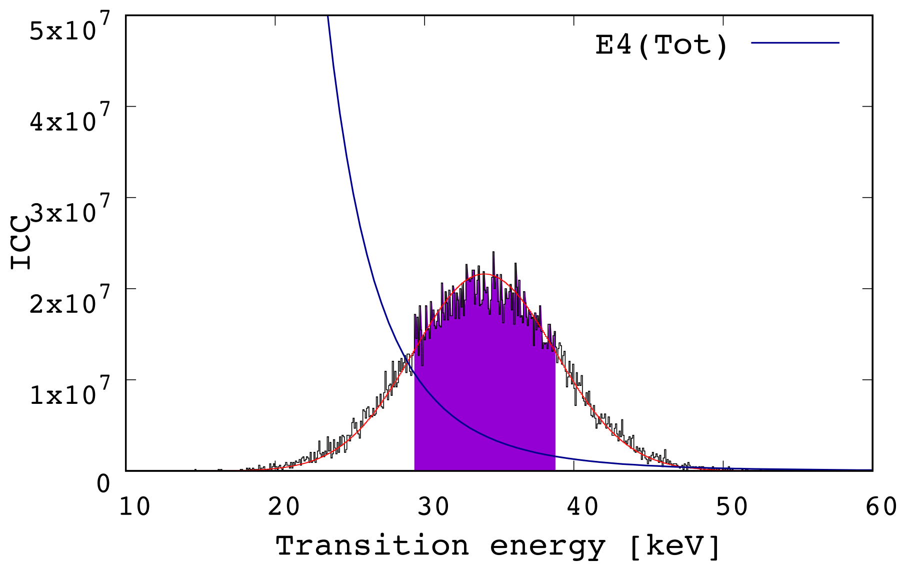


Pure ICC

BrIcc ^{211}*Po* 34(5) keV E4

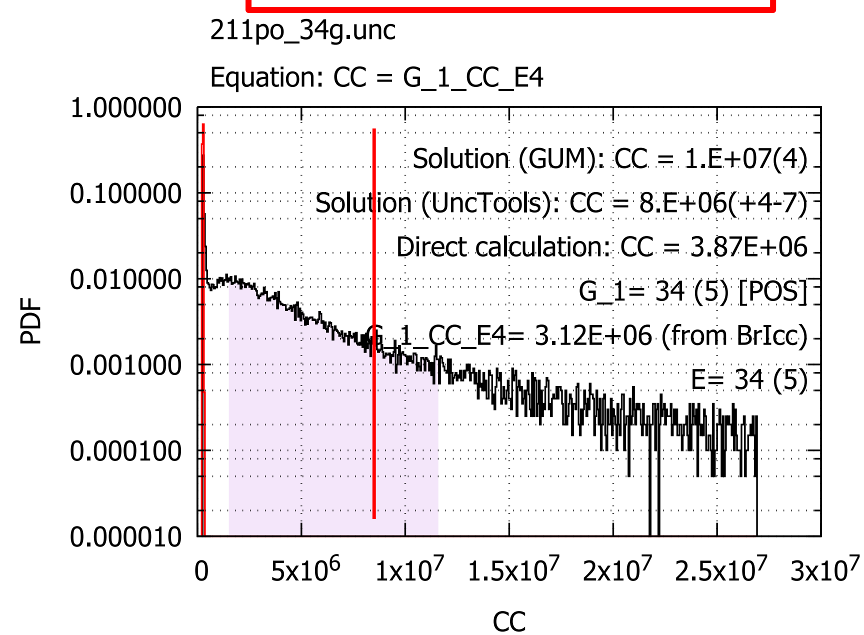
DICC=ICC(E), ICC(E-DE), ICC(E+DE)

3.9E+6, 1.2E+7, 1.5E+6



BrIcc:
CC=4.E6 (8)

GUM (68%):
CC=1.E7(4)



UncTools:
CC=8.(+4-7)E+6

Same uncertainty propagation used across the ENSDF codes!

Mixed ICC with limit on MR

BrIcc ^{111}AG 70.44(5) keV M1+E2, MR: 0.12 LE

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==============================================================================================
BrIcc v2.3b (16-Dec-2014)  Z= 47 Egamma= 70.44 5 keV        Multipolarity= M1+E2       22:42:05 24-May-2017
                                             M1+E2        Mixing ratio= 0.12 LE
                                    M1+E2 Mixed
Shell     M1         E2                  Icc        dIcc        dIccDMRL    dIccDMRH
        ---------- ----------          ---------- ---------- ----------- ----------
K       9.869E-01 3.445E+00           1.004E+00 2.250E-02  1.745E-02  1.745E-02

L-tot   1.233E-01 1.298E+00           1.317E-01 8.546E-03  8.340E-03  8.340E-03
K/L     8.002E+00 2.654E+00           7.628E+00 5.237E-01

M-tot   2.349E-02 2.565E-01           2.514E-02 1.691E-03  1.654E-03  1.654E-03
L/M     5.251E+00 5.062E+00           5.237E+00 4.896E-01

N-tot   4.058E-03 4.069E-02           4.318E-03 2.671E-04  2.600E-04  2.600E-04
L/N     3.039E+01 3.191E+01           3.049E+01 2.734E+00

O-tot   1.860E-04 4.678E-04           1.880E-04 3.328E-06  2.000E-06  2.000E-06
L/O     6.631E+02 2.776E+03           7.004E+02 4.712E+01

Tot     1.138E+00 5.041E+00           1.166E+00 3.224E-02  2.770E-02  2.770E-02
```

CC=1.17(4)

$$\alpha = \left[\frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1+\delta^2} + \alpha(\pi L)\right] \times 0.5\,,$$

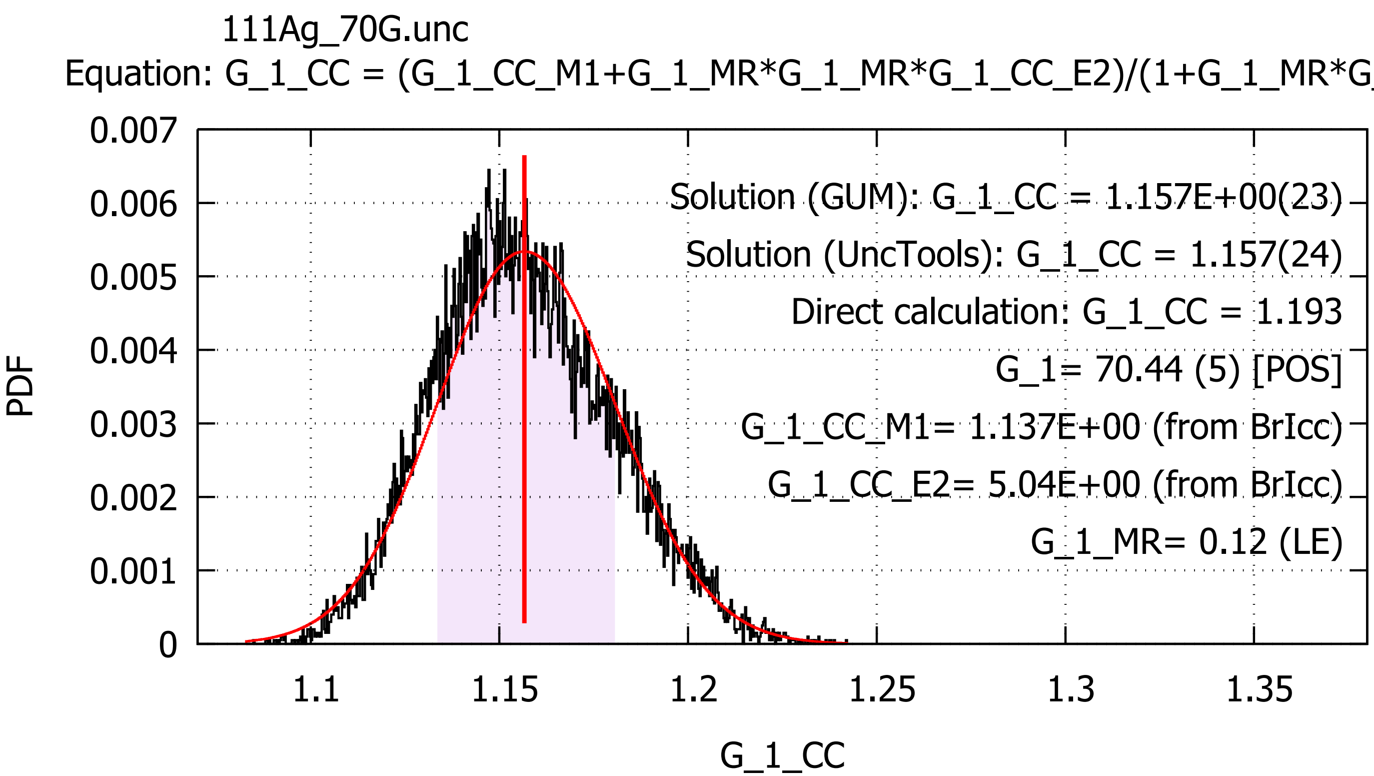
$$\Delta\alpha_{DMR\_H} = \Delta\alpha_{DMR\_L} = \left|\frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1+\delta^2} - \alpha(\pi L)\right| \times 0.5\,.$$

$$\Delta\alpha_{DE\_H} = \alpha(E_\gamma + \Delta E_H) - \alpha(E_\gamma)\,,$$
$$\Delta\alpha_{DE\_L} = \alpha(E_\gamma - \Delta E_L) - \alpha(E_\gamma)\,.$$

Mixed ICC with limit on MR

BrIcc ^{111}AG 70.44(5) keV M1+E2, MR: 0.12 LE

BrIcc
CC=1.17(4)

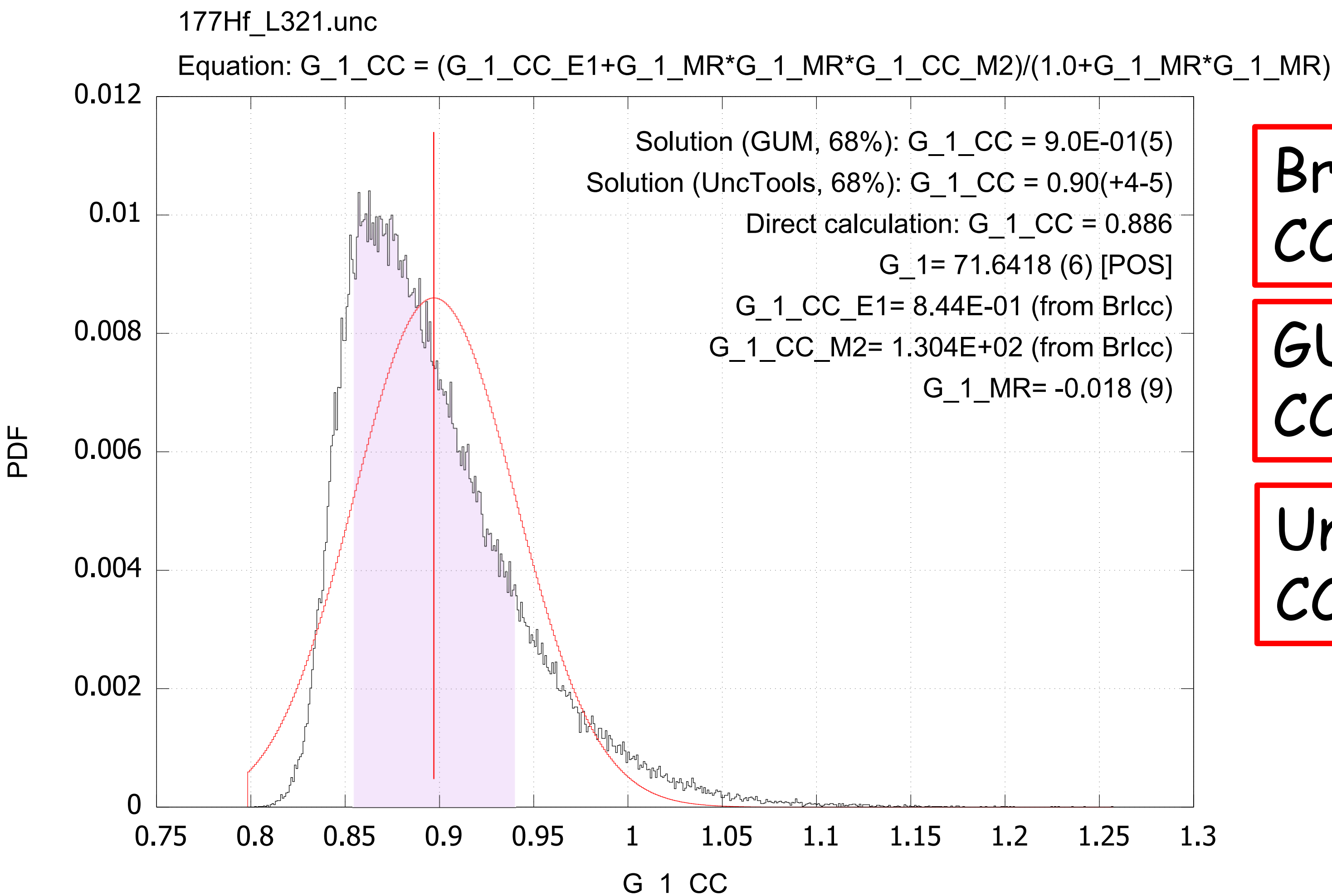


GUM
CC=1.157(23)

UncTools
CC=1.157(24)

Mixed ICC with limit on MR

BrIcc ^{177}Hf 71.6418(6) keV E1+M2, MR: -0.018(9)



BrIcc
CC=0.89(6)

GUM
CC=0.90(5)

UncTools
CC=0.90(+4-5)

Mixed ICC - MR unknown

BrIcc: MR=1.00 FOR E2/M1, MR=1.00 FOR E3/M2 AND MR=0.10 FOR THE OTHER MULTIPOLARITIES

MC uncertainty propagation: What is the uncertainty on the assumed values?

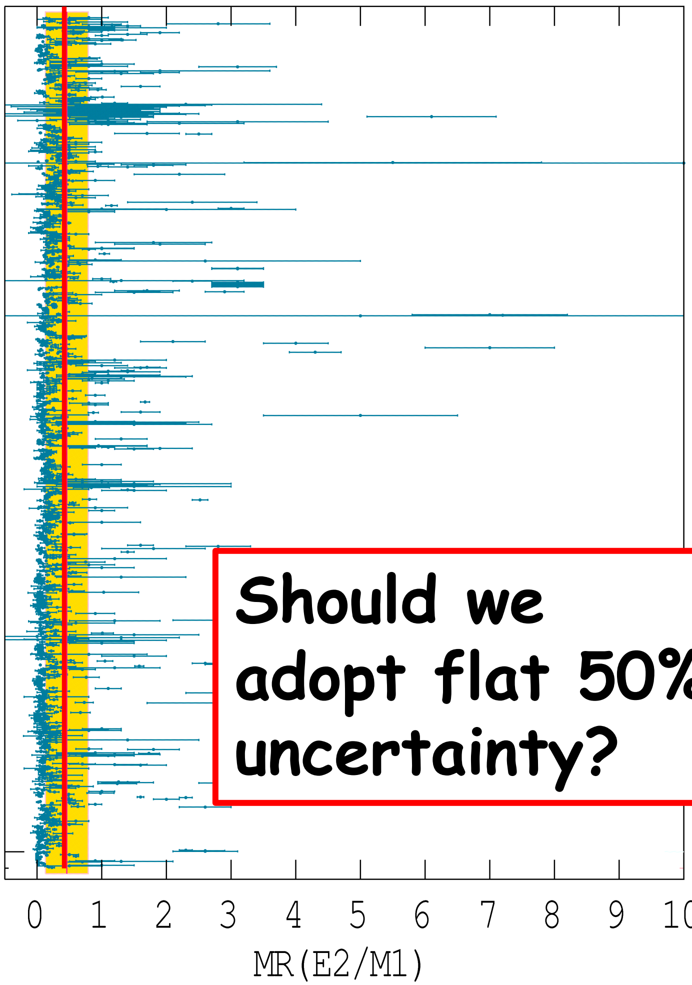
E2/M1

MR(E2/M1): N=4894; LWM=0.80(80)

Should we use PDF of the existing data?

~A, ~N, ~Z
Nuclear Structure effects?

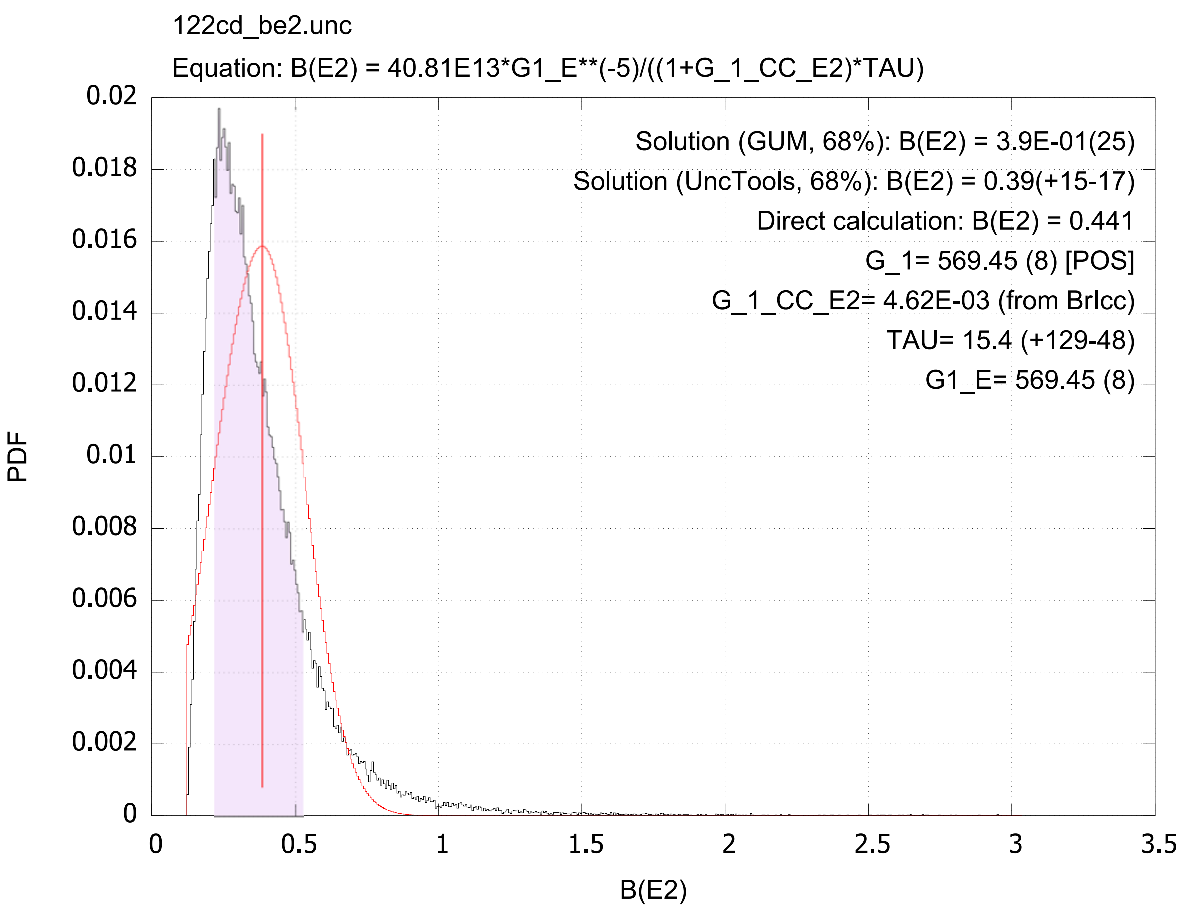
MR(E2/M1): N=1530; LWM=0.46(33)



Should we adopt flat 50% uncertainty?

B(E2)

^{122}Cd τ=15.4(+129-48) ps; 569.45(8) keV E2 (2016Pr01)



2016Pr01
B(E2)=0.44(20) e^2b^2

GUM
B(E2)=0.38(24)

UncTools
B(E2)=0.38(+15-17)

Directly calculated
B(E2)=0.441

TRuler - transition strength

86 F.G. Kondev et al. / Atomic Data and Nuclear Data Tables 103–104 (2015) 50–105

Table 1 (*continued*)

E_i [keV]	$T_{1/2}^{exp}$	K_i^{π} [$\hbar$]	J_f^{π} [$\hbar$]	K_f^{π} [$\hbar$]	$\sigma\lambda$	E_γ [keV]	I_γ	α_T	Γ_γ [eV]	F_w	ν	f_ν
^{244}Cm ($Z = 96$, $N = 148$)												
1040.188 (12)	34 (2) ms	6^+	8^+	0^+	E2	538.400 (16)	1.0 (3)	4.95E−02	9 (3)E−17	3.8 (12)E+10	4	440 (30)
			6^+	0^+	M1 + E2	743.971 (5)	100 (1)	7.70E−02	$\lvert\delta\rvert = 0.92(8)$			
					M1				4.7 (5)E−15	1.81 (18)E+12	5	283 (6)
					E2				4.0 (4)E−15	4.2 (5)E+9	4	254 (7)
			4^+	0^+	E2	897.848 (7)	44.9 (6)	1.70E−02	3.90 (23)E−15	1.09 (7)E+10	4	323 (5)

$$\Gamma_\gamma^j = \frac{\hbar}{\tau_\gamma^j} = \frac{\hbar}{\tau^{exp}} \times \frac{I_\gamma^j}{\sum_{k=1}^{N} I_\gamma^k \times (1 + \alpha_T^k)}.$$

Furthermore, the strength $|M|^2$ of an individual transition in single-particle (Weisskopf) units (W.u.) is related to its widths, lifetimes and B values, and to the inverse of its hindrance factor (F_W) by:

$$|M|^2\,(W.u.) = \Gamma_\gamma/\Gamma_W = \tau_W/\tau_\gamma = B_\gamma\downarrow/B_{sp}\downarrow = 1/F_W. \qquad (14)$$

For transitions that are (in principle) forbidden, the degree of K forbiddenness, ν, is defined as:

$$\nu = \Delta K - \lambda, \qquad (15)$$

where $\Delta K = |K_i - K_f|$ is the difference between the K quantum numbers of the initial and final states, and λ is the multipole order of the transition. The *reduced* hindrance per degree of K forbiddenness is given by:

$$f_\nu = F_W^{\frac{1}{\nu}}. \qquad (16)$$

TRuler - transition strength

Table 1 (*continued*)

E_i [keV]	$T_{1/2}^{exp}$	K_i^π [ħ]	J_f^π [ħ]	K_f^π [ħ]	σλ	E_γ [keV]	I_γ	α_T	Γ_γ [eV]	F_w	ν	f_ν
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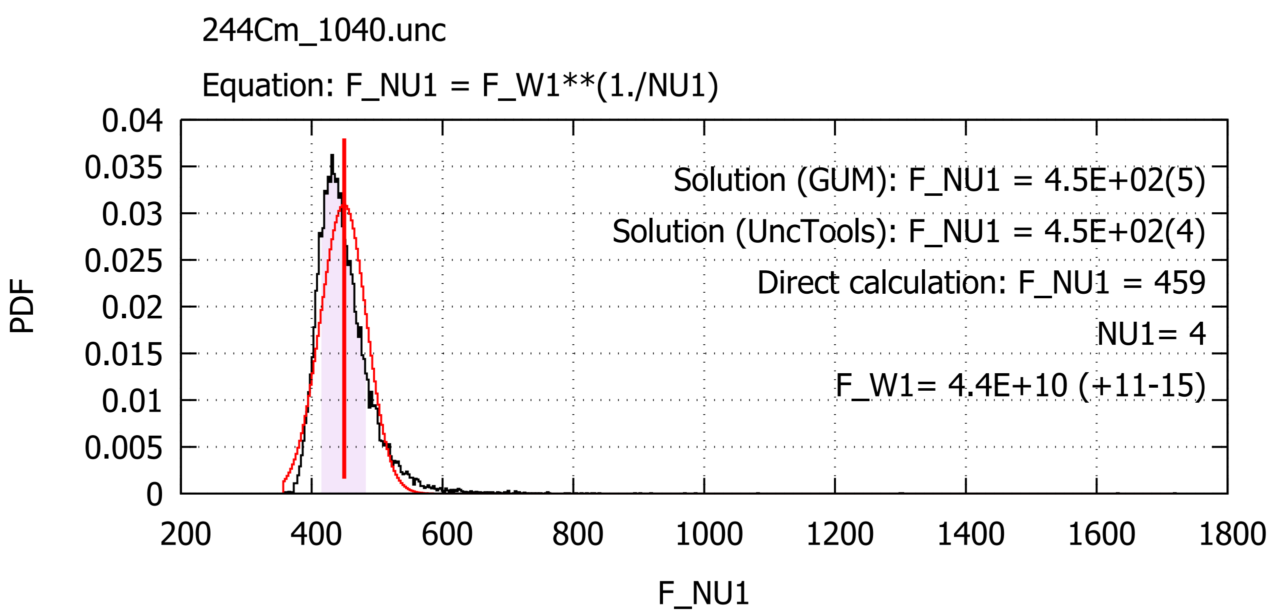
			6^+	0^+	M1 + E2	743.971 (5)	100 (1)	7.70E−02	|δ| = 0.92(8)			
					M1				4.7 (5)E−15	1.81 (18)E+12	5	283 (6)
					E2				4.0 (4)E−15	4.2 (5)E+9	4	254 (7)
			4^+	0^+	E2	897.848 (7)	44.9 (6)	1.70E−02	3.90 (23)E−15	1.09 (7)E+10	4	323 (5)



2015Ko14 (Python)
f_ν=440(30)

GUM
f_ν=4.5 (5)E+2

UncTools
f_ν=4.5 (4)E+2

Directly calculated
f_ν=4.59E+2?????

Proposal of propagation uncertainties including limits using MC

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Advantage

- Consistent treatment of all cases, much simpler program logic (no more jungle of IF statements)
- Sound statistical approach even for larger relative uncertainties and limits

Disadvantage

- CPU intensive
- Mean value may not agree with directly calculated value

Questions/Problems

- Sampled / output values could be nonphysical: $T1_{/2}$=0.15(7) ns
- Some uncertainties in ENSDF expected to be symmetrical (DBR, DCC, DE, DHF, DIA, DIB, DIE, DIP, DNB, DNR, DNP, DNT, DQP, DQ-, DS, DSP, DTI)