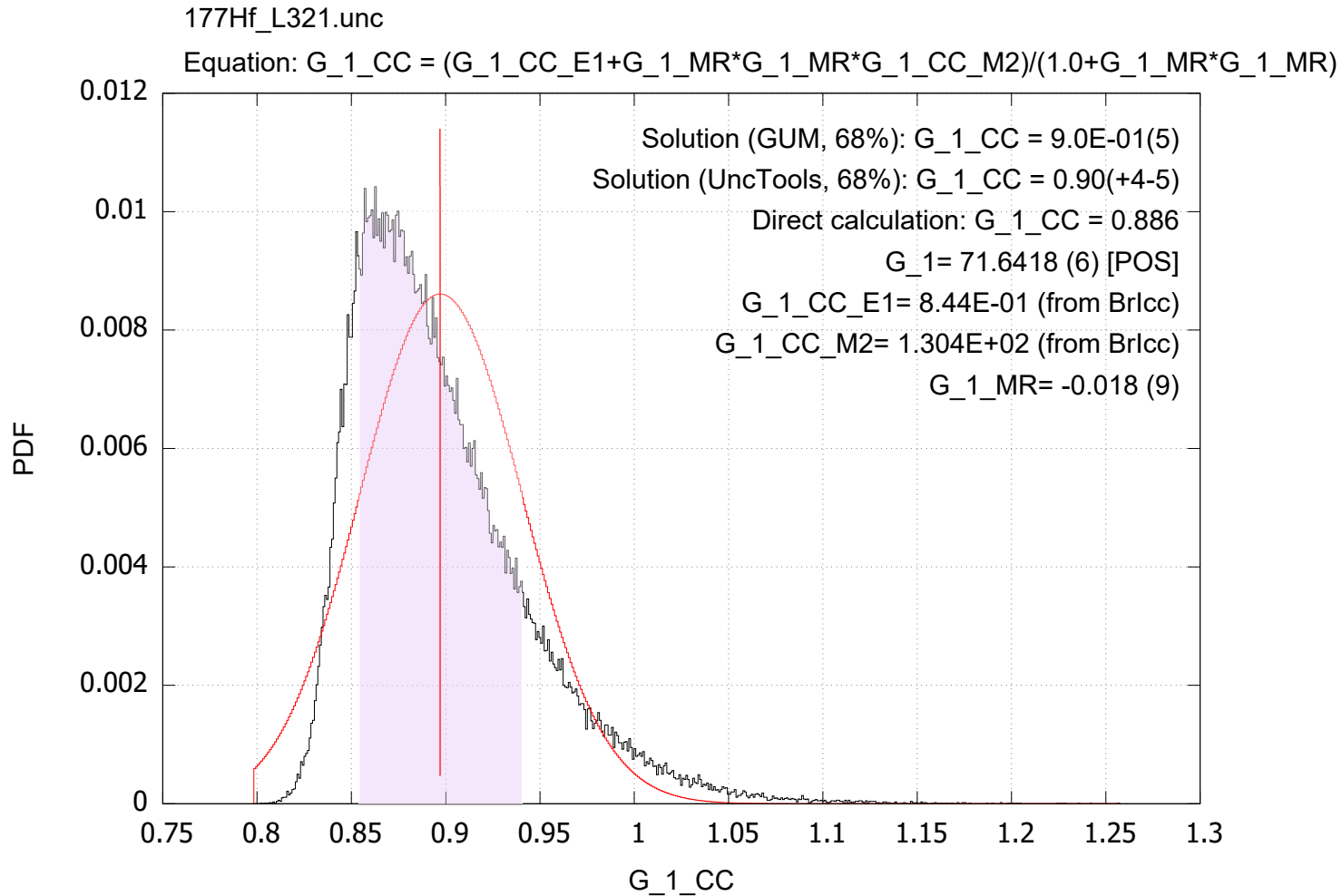




UncTools (NS_Lib) - treatment of uncertainties using Monte Carlo

T. Kibèdi and Ben Coombes (ANU)



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

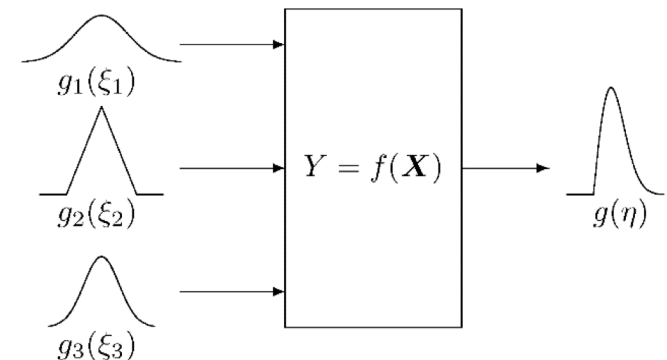
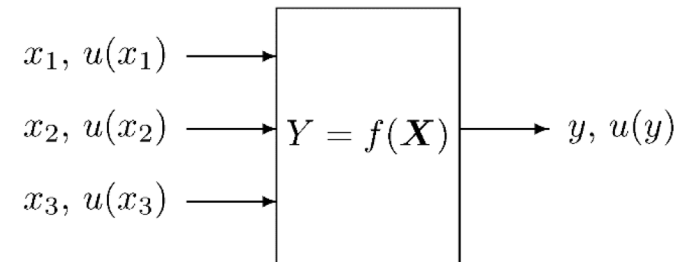
- ❑ Single unsigned number: BR, CC, HF, LOGFT, NB, NP, NR, NT, QP
 - ❑ Single signed number: MR, Q-, QA, SN, SP
 - ❑ Standard symmetric uncertainty; two character field (ENSDF Manual V.11):
 - ❑ an up to two digits integer, up to 99, preferable less than 25
 - ❑ LT, GT, LE, GE, AP, CA, S
DBR, DCC, DE,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



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

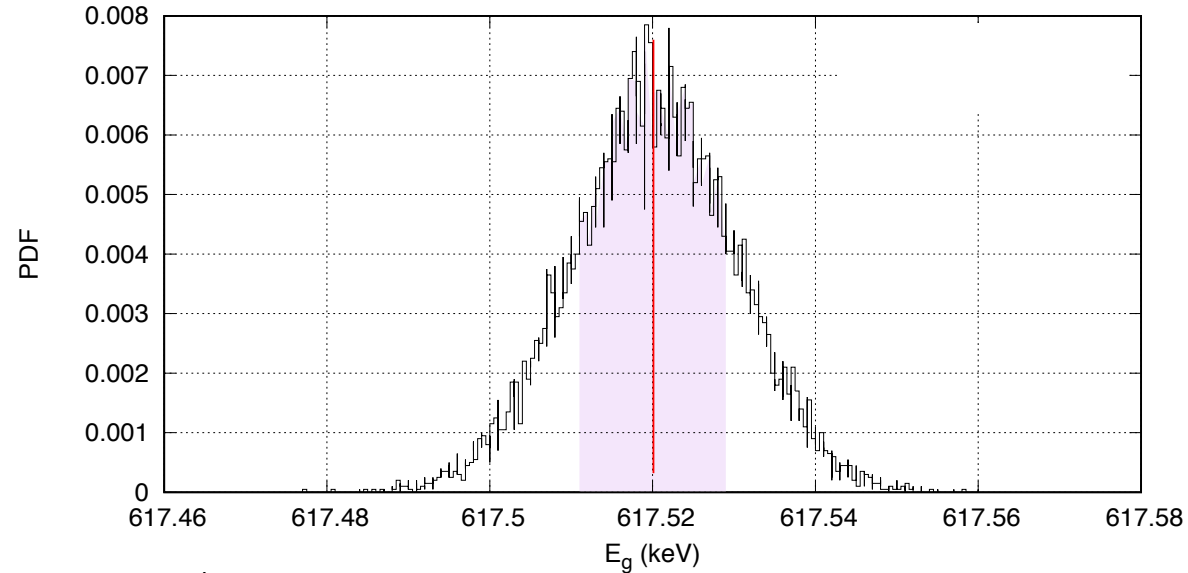
Concept

- 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.

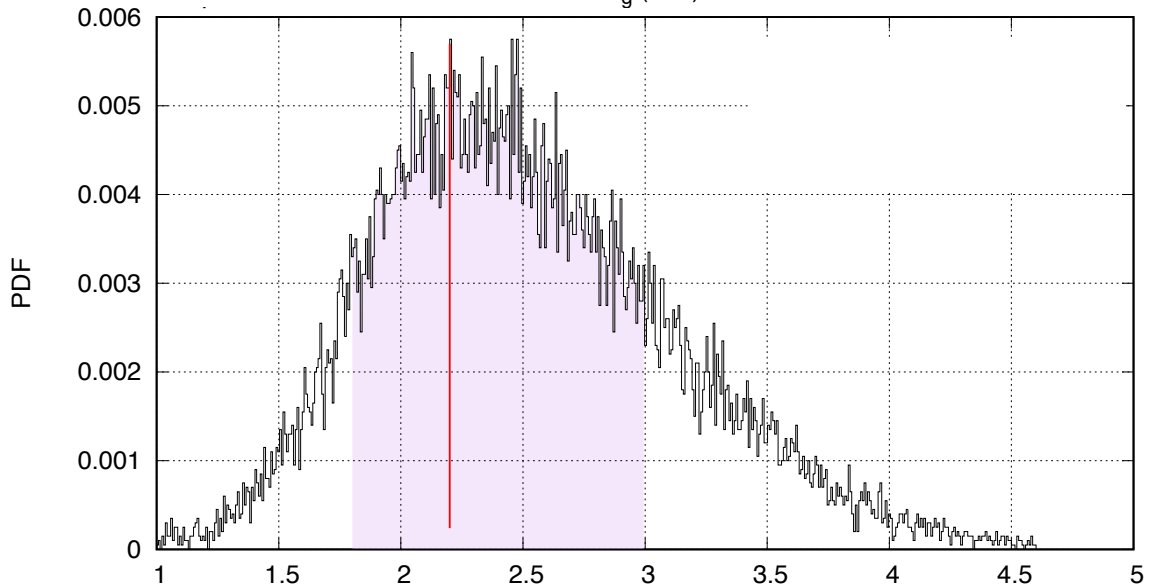


Probability Density Function (PDF)

Symmetric Normal Distribution:
 $E_\gamma = 617.520(10) \text{ keV}$



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



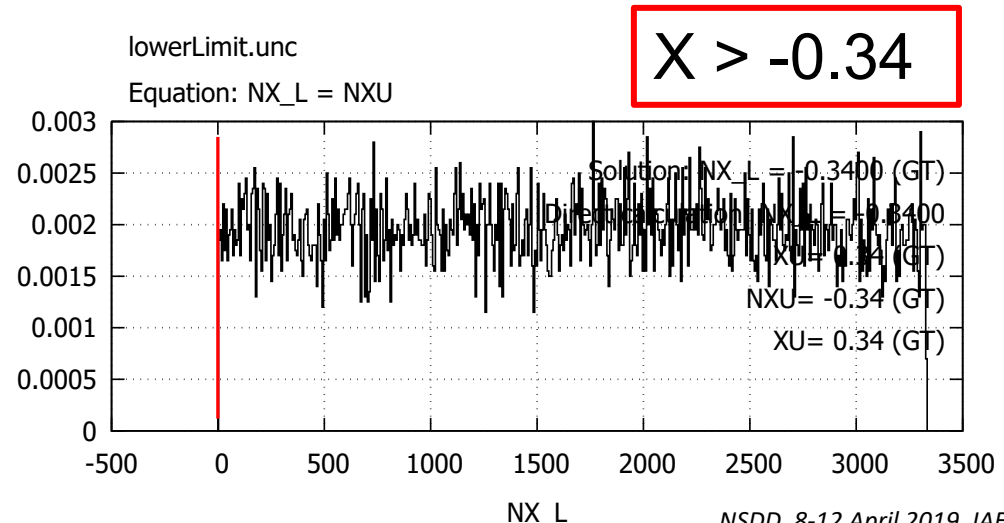
Probability Density Function (PDF)

Limits

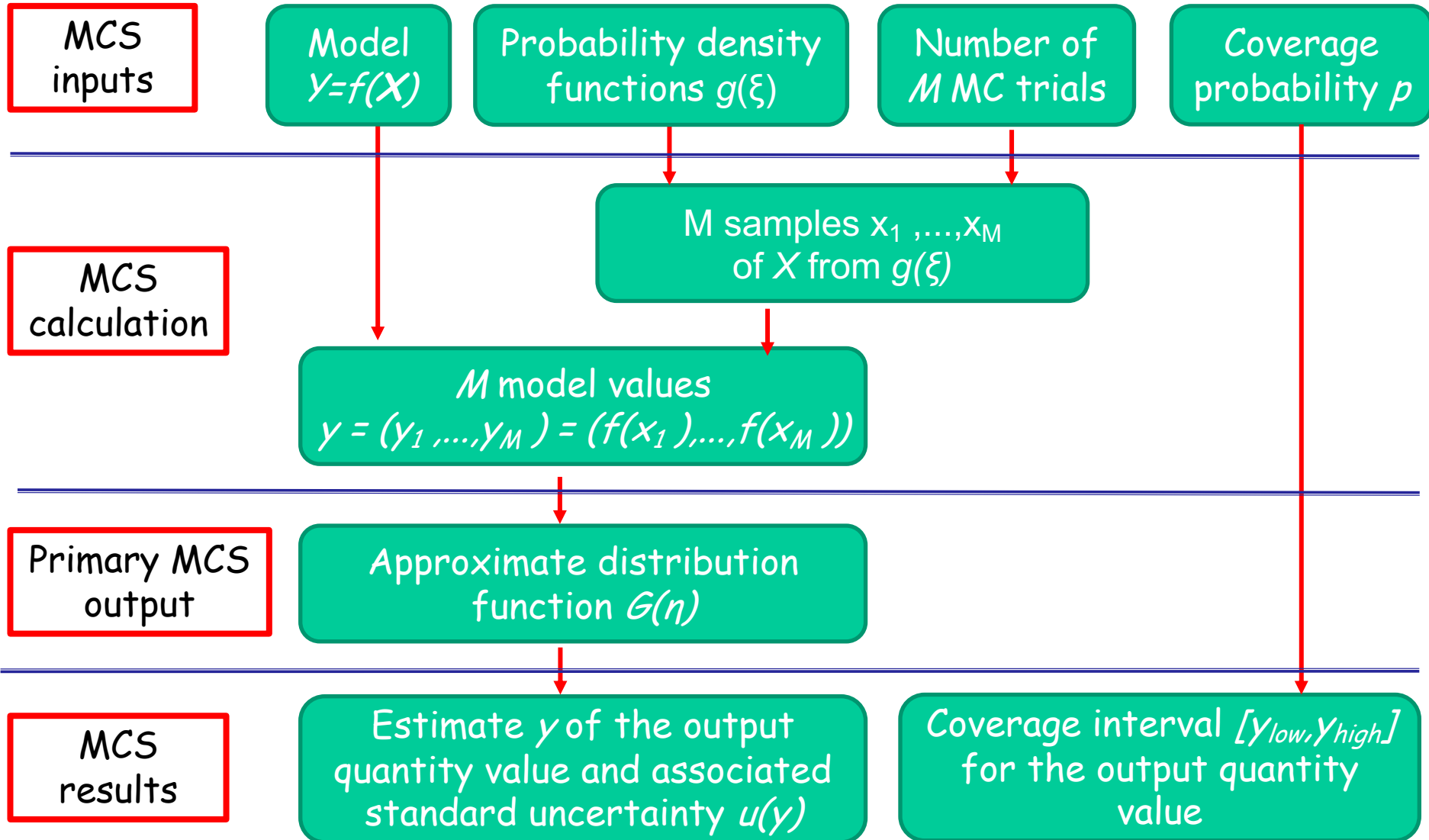
	Limit	Range	Range Used in MC
UPPER	<0.5	[0 : +0.5]	[0 : +0.5]
	<+0.5	[-infinity : +0.5]	[-4999.5:+0.5]
	<-0.5	[-infinity : -0.5]	[-5000.5:-0.5]
LOWER	>0.5	[+0.5:+infinity]	[+0.5:+5000.5]
	>+0.5	[+0.5:+infinity]	[+0.5:+5000.5]
	>-0.5	[-0.5:+infinity]	[-0.5:+4999.5]

PDF uniform over the entire range

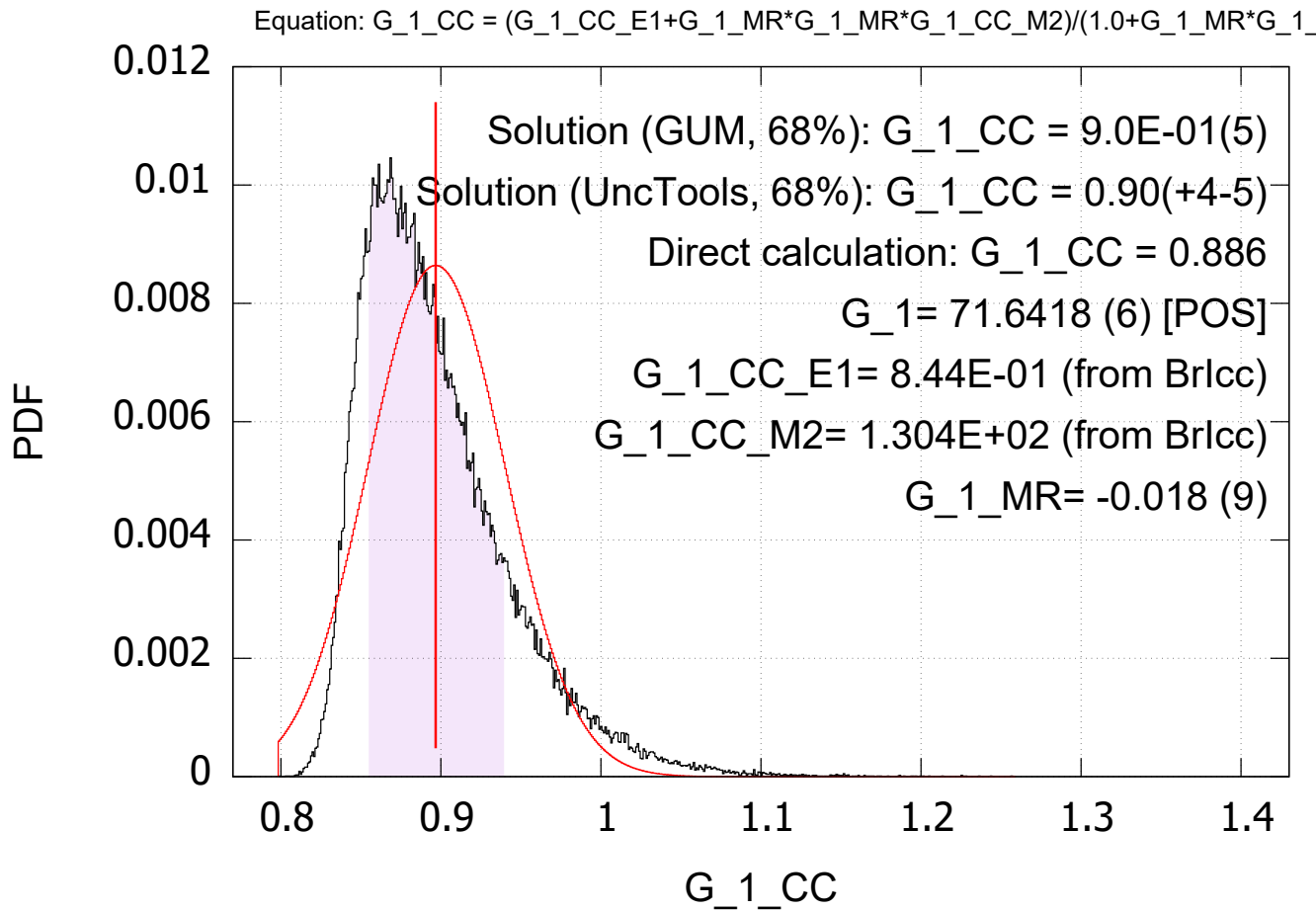
- ❑ Infinite range: PDF = Zero
- ❑ Replace infinity with a sufficiently large range:
Infinity ~ **10000** Limit value^{PDF}



Monte Carlo simulations to obtain the output quantity



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

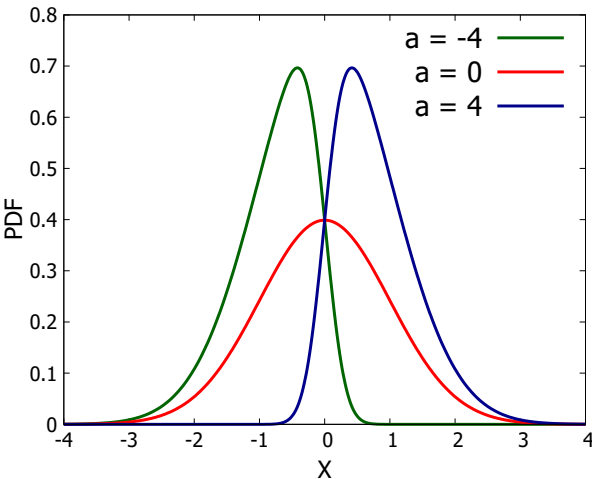


BrIcc
CC=0.89(6)

GUM
CC=0.90(5)

UncTools
CC=0.90(+4-5)

Skewness & Kurtosis



Symmetrical:

$$|\gamma_1| < 0.01; k \approx 3$$

Asymmetric:

$$0.01 < |\gamma_1| < 0.995272$$

Limits:

$$|\gamma_1| = 0; k < 3 ?$$

Skewness - degree of distortion from any symmetrical, like normal distribution

$$\gamma_1 = \frac{\sum_{i=1}^N (x - \bar{x})^3}{\sigma^3}$$

- Mean - arithmetic mean
- Median - middle number of the ordered list
- Mode - where PDF has maximum

Normal distribution: **mode = median = mean**

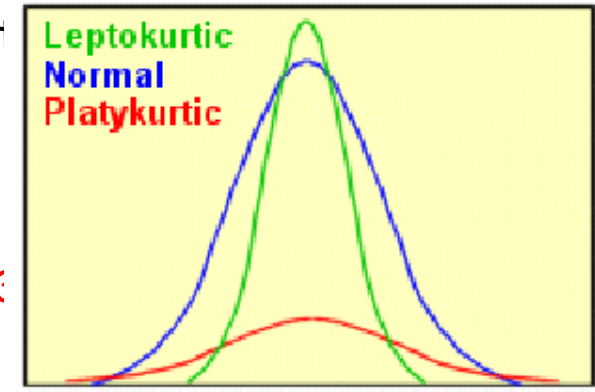
Skew positive: **mode < median < mean**

Skew negative: **mode > median > mean**

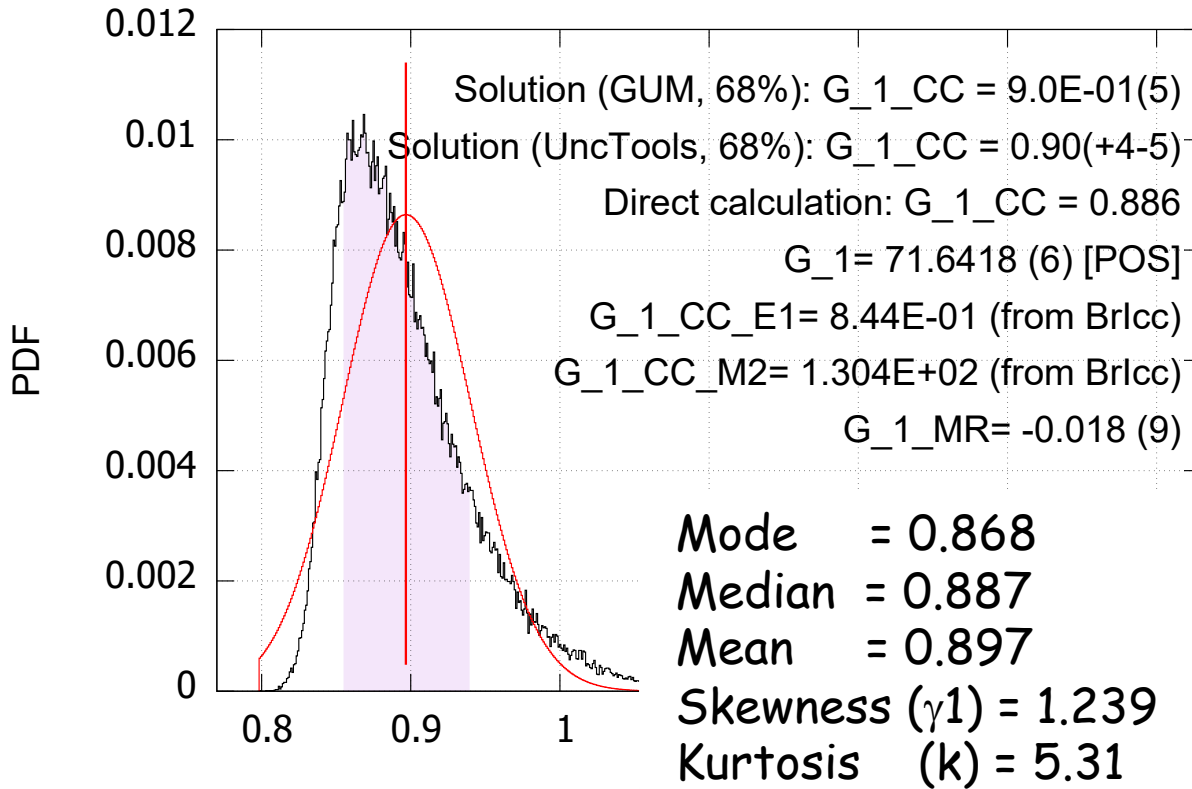
Kurtosis (from Greek: κυρτός, *kyrtos* or *kurtos*, meaning "curved, arching") is a measure of the "tailedness" of the probability

$$k = \frac{1}{N} \sum_{i=1}^N (x - \bar{x})^4}{\sigma^4}$$

- Normal distribution: **k = 3**
- Platykurtic: **k < 3**
- Leptokurtic: **k > 3**



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)**

Symmetrical:

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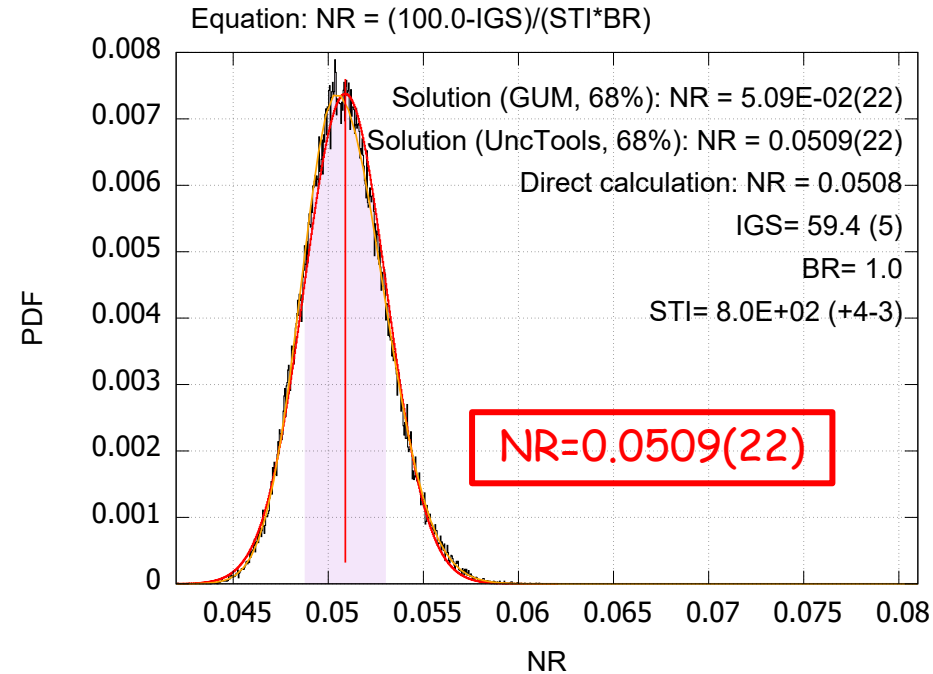
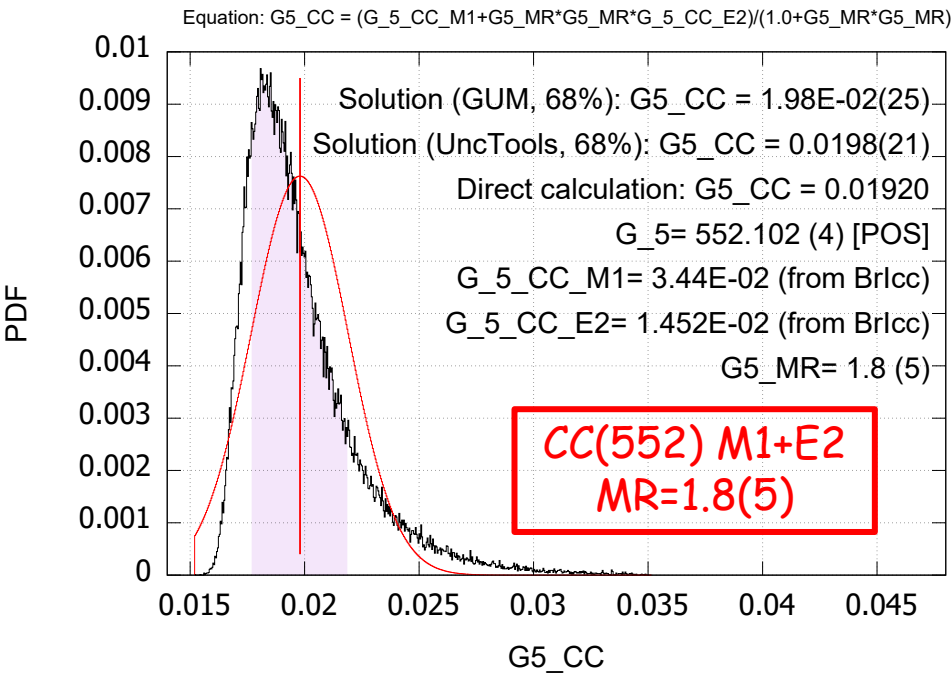
Limits:

$|\gamma_1| = 0; k < 3 ?$

**$\alpha_T(71.6418)$
negative skew: Mode < Median < Mean
 $|\gamma_1| > 1$ not an asymmetric normal distribution**

^{177}Lu B-
12 G's for
normalisation

	GABS	Python	UncTools
Input file	<code>gabs-test.ens</code>	<code>pycalc-test.py</code>	<code>gabs-test.unc</code>
NR	0.0508(21)	0.0508(21)	0.0509(22)
%IG(150.399)	18.0 (5)	18.0 (5)	18.0 (5)



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: $T_{1/2}=0.15(7)$ 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)