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Proposal to propagate uncertainties in ENSDF using Monte Carlo

T. Kibèdi (ANU)

UncTools was developed with B. Coombes and contributions from B. Tee (ANU)

Proposal: use Monte Carlo in ENSDF

- Single unsigned or signed number
- Standard symmetric or asymmetric uncertainty
- Limits

Uncertainty propagation in ENSDF codes:

- Taylor expansion, only valid for
  a) Linear or nearly-linear relations/equations
  b) small ΔX/X values; ΔX/X < ~10%
  c) Correlations neglected

For multi-variant functions uncertainty propagation is difficult

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For multi-variant functions uncertainty propagation is difficult

Solution: Monte Carlo (MC) uncertainty propagation

- Recognises and express any asymmetry
- Uses the full distribution, not just the standard deviation
- Produces valid coverage intervals

1) Evaluation of measurement data — Supplement 1 to the "Guide to the expression of uncertainty in measurement" — Propagation of distributions, JCGM 101:2008 (Joint Committee for Guides in Metrology)
2) M. Cox, A. O`Hagan, Accreditation and Quality Assurance 27 (2022) 19-37
3) A. Possolo, C. Merkatas, O. Bodnar, Metrologia 56 (2019) 045009

Two statistical paradigms

- **Frequentist methods** are based on the frequency definition of probability, where the probability of an event is defined to be the frequency with which that event occurs in the long run, over many repetitions. The Type A procedures given in the GUM are based on frequentist statistical theory, and accordingly the resulting standard uncertainties quantify how variable the estimate of a measurand will be over many repetitions of the measurement process.
- **Bayesian methods** employ a subjective definition of probability, whereby the probability of an event is a subjective judgement representing a person's rational degree of belief that it will occur. Type B evaluation in the GUM is a subjective judgement and the resulting standard uncertainty quantifies the metrologist's uncertainty about the measurand.

Ref: O'Hagan, Anthony, and Maurice Cox. "Simple Informative Prior Distributions for Metrology." (2021).

GUM: **Guide to the expression of uncertainty in measurement**, Working Group 1 of the Joint Committee for Guides in Metrology

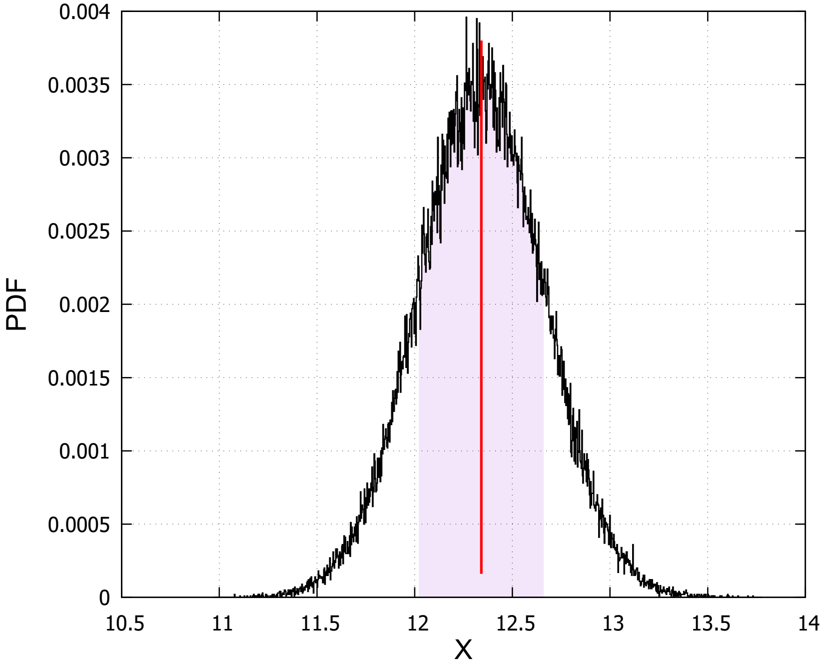
Existing software tools for Monte Carlo uncertainty propagation

- NIST Uncertainty machine: https://uncertainty.nist.gov
- Error Propagation Calculator (python)
- GUM_MC (application)

Many more at:
https://en.wikipedia.org/wiki/List_of_uncertainty_propagation_software

Symmetric uncertainty

Representation in ENSDF: X(u)



X = 12.34(32)

PDF: Normal distribution

$$PDF(x) = \frac{1}{\sigma\sqrt{2\pi}} \times \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

μ = mean = 12.34 mode

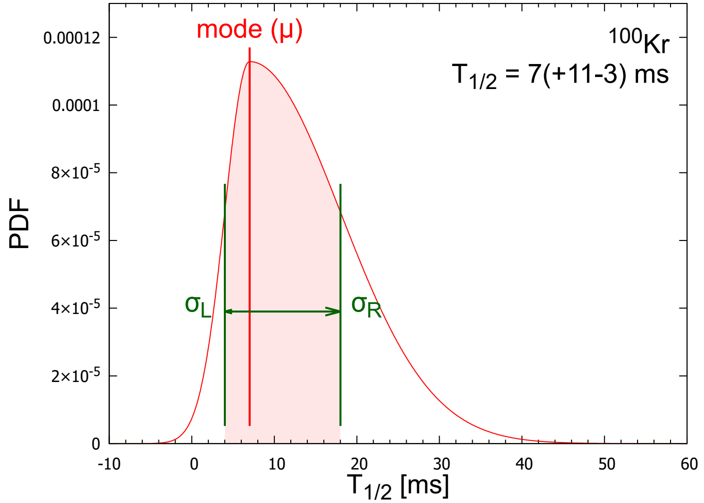
σ = 0.32 standard deviation

Asymmetric uncertainty

Representation in ENSDF: $X(+u_R\ -u_L)$

Symmetrizing: Audi et al, NUBASE2016, C. Phys. C Vol. 41, No. 3 (2017) 030001

$X\ (+u_R\ -u_L) \rightarrow$ value: $X+(u_R-u_L)/2$, symmetric uncertainty: $(u_R+u_L)/2$



- ❑ 1σ (68%) coverage intervals on the left and right are not equal!
- ❑ For best performance: $0.645 < u_R/u_L < 1.55$
- ❑ An alternative: Generalized Extreme Value distribution works well in the tail section. But no easy parametrisation from $X\ (+u_R\ -u_L)$

X = 7(+11,-3)

PDF: Split normal distribution

$$PDF(x) = A \times \exp\left(-\frac{(x-\mu)^2}{2u_L^2}\right) \quad X < \mu$$

$$PDF(x) = A \times \exp\left(-\frac{(x-\mu)^2}{2u_R^2}\right) \quad X \geq \mu$$

$$A = \frac{\sqrt{2}}{\sqrt{\pi}(\sigma_L+\sigma_R)}$$

$\mu = 7$ mode

$u_L = 3$ left uncertainty (σ_L)

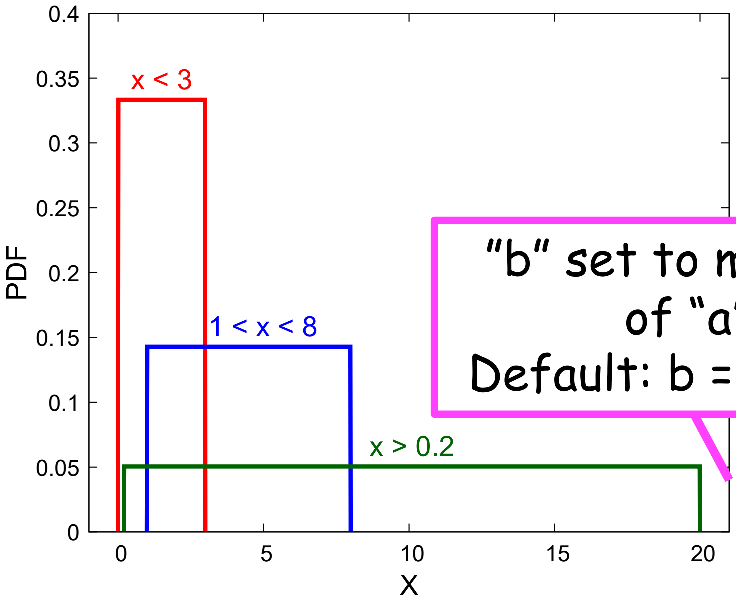
$u_R = 11$ right uncertainty (σ_R)

$$mean = \mu + \sqrt{2/\pi}(u_R - u_L)$$

Representation in ENSDF: X & LE/LT/GE/GT

Q: What the limit means?

- $T_{1/2}$ < 13 ns   Can`t be negative: ICC, E, RI, etc. Non-physical!



"b" set to multiple of "a"
Default: b = 100 * a

X < 1.27; or general a < X , b

PDF: rectangular distribution

$$PDF(x) = \frac{1}{b-a} \quad for\ a < x < b$$

0 otherwise

a or b could not be infinity, or zero (singularity)

Current practice in ENSDF

- LT/LE: 50% of the limit value & 50% symmetric UNC
- GT/GE: 50% of multiple (100-1000) of limit value & 50% symmetric UNC
- The effect of PDF completely ignored!

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Limits – Sign does matter

Quantities are always:

- Positive: Q-, SP, QA, QP, E, RI, TI, CC, NR, NT, BR, IB, LOGFT
- Positive or Negative: MR

	Limit	Range	Range for MC
UPPER	<0.5	[0 : +0.5]	[0 : +0.5]
	<+0.5	[-infinity : +0.5]	[-499.5:+0.5]
	<-0.5	[-infinity : -0.5]	[-500.5:-0.5]
LOWER	>0.5	[+0.5:+infinity]	[+0.5:+500.5]
	>+0.5	[+0.5:+infinity]	[+0.5:+500.5]
	>-0.5	[-0.5:+infinity]	[-0.5:+499.5]

Using a multiplier of 1000

APproximate, CAlculated and SYstematcs

Representation in ENSDF: X & AP/CA/SY

- AP – value approximate, UNC=50%
- CA – value calculated, UNC=50%
- SY – value from systematics, UNC=50%

X = 12 AP

PDF: Normal distribution

$$PDF(x) = \frac{1}{\sigma\sqrt{2\pi}} \times \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

μ = mean = 12 mode

σ = 6 standard deviation

Doing Monte Carlo uncertainty propagation in the nutshell

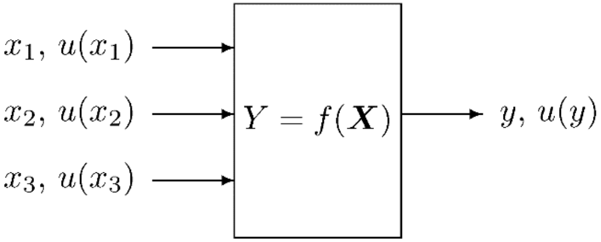
- Develop a model, f(X) relating the output quantity to the input quantities.
- Based on the available knowledge, assign a Probability Density Function (PDF) for each input quantity.
- Evaluate the mathematical model N* times and build the PDF of the output quantity
- Deduce statistical properties of the output quantity from its PDF. NO assumptions on the output UNC from the input.

  Recommended value: central value

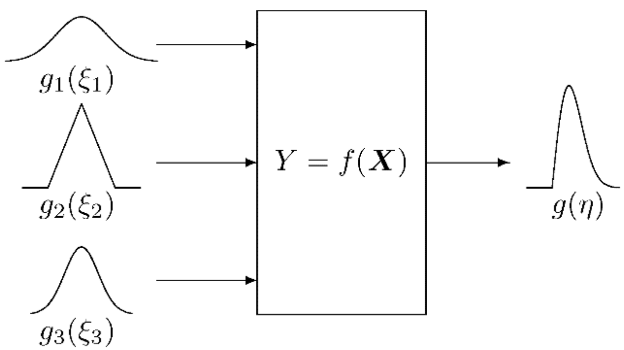
  Left (u_L) and right (u_R) uncertainties from 1s coverage interval

Number of recommended MC trials: 10 k to 1 M

Mathematical model



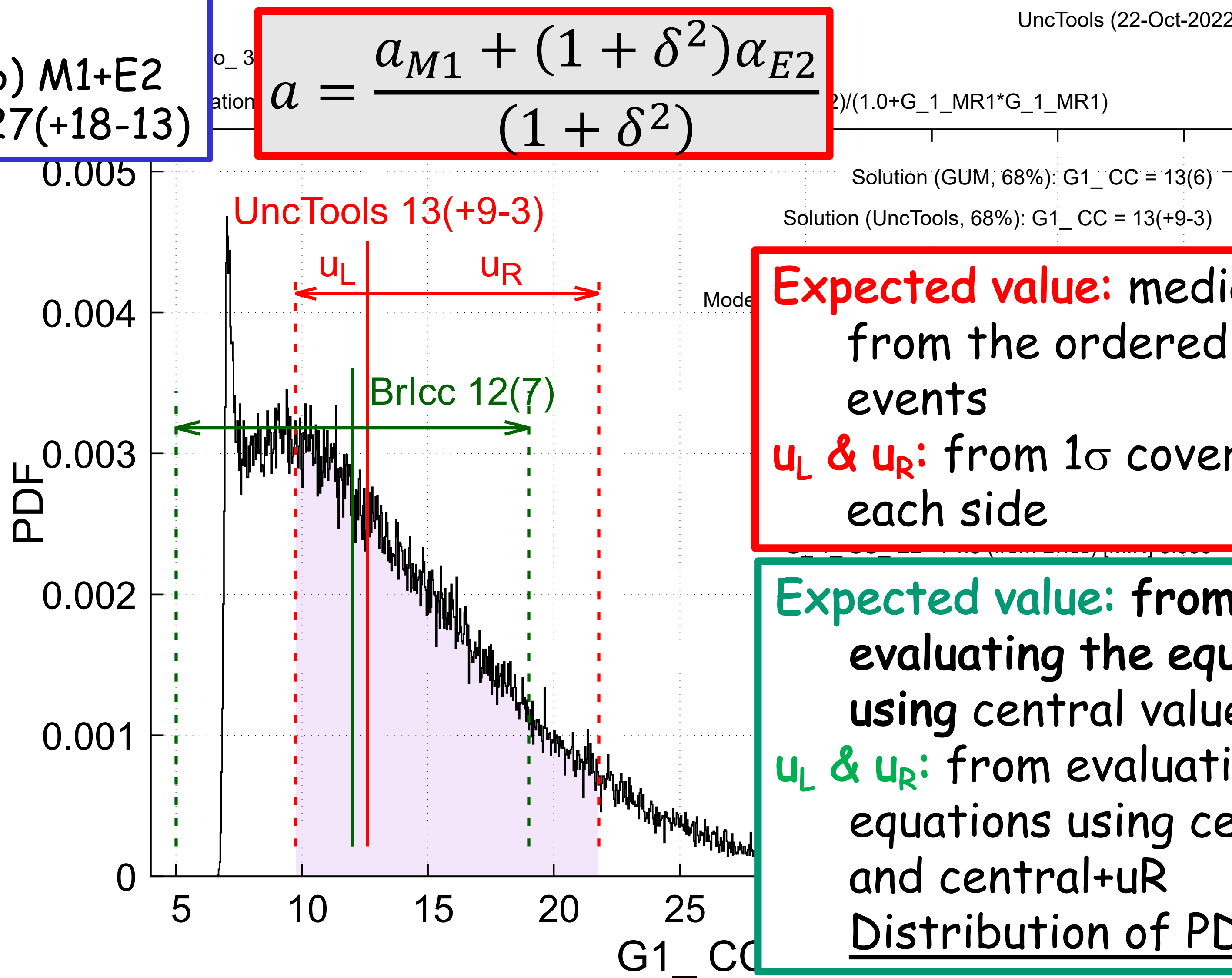
Monte Carlo using PDF



Value of the output quantity

^{87}Mo
31.55(6) M1+E2
MR=0.27(+18-13)

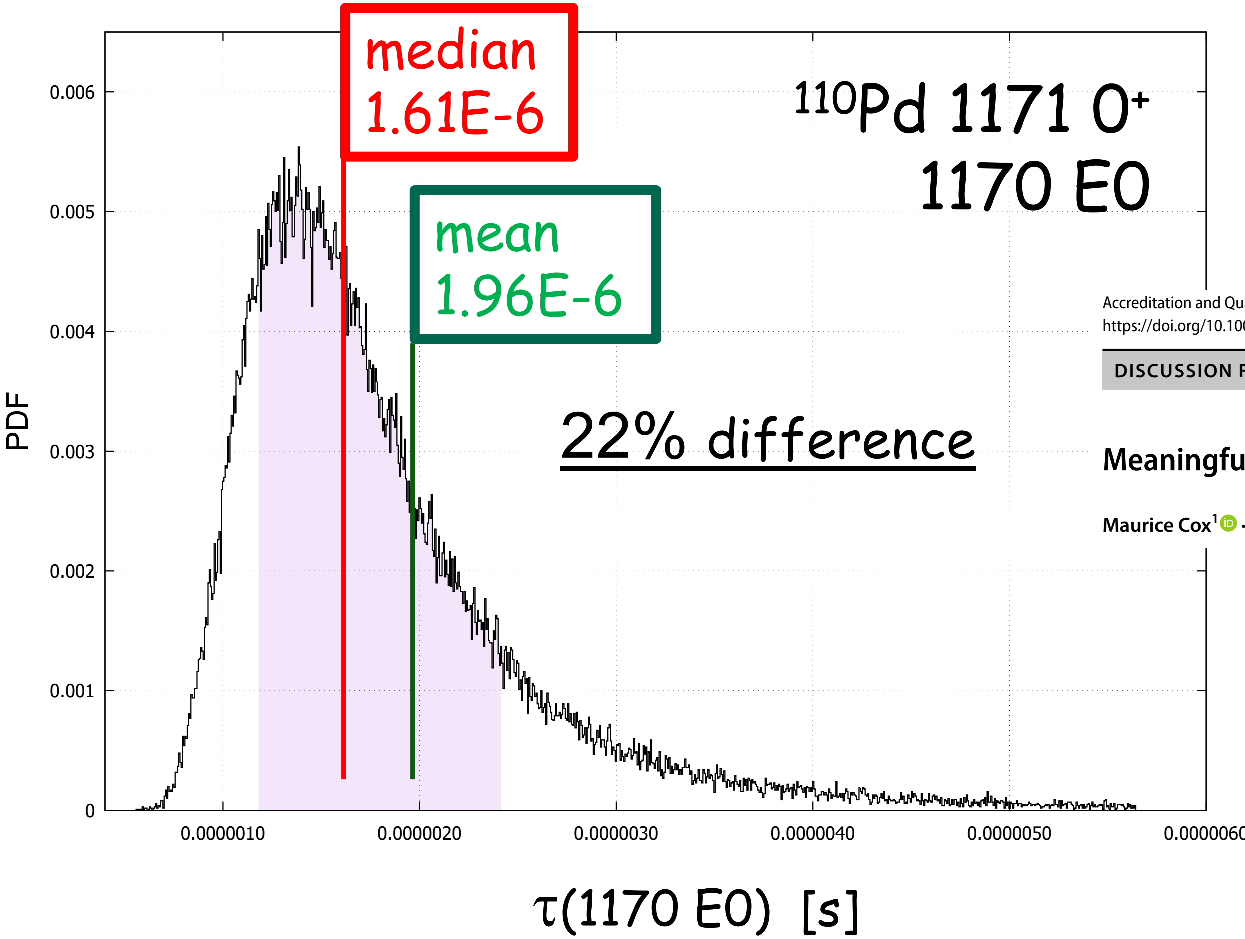
$$a = \frac{a_{M1} + (1+\delta^2)\alpha_{E2}}{(1+\delta^2)}$$



Expected value: median value from the ordered list of MC events
u_L & u_R: from 1σ coverage on each side

Expected value: from evaluating the equation using central values.
u_L & u_R: from evaluating equations using central-uL and central+uR
Distribution of PDF ignored

Value of the output quantity
Mean vs. Median



Accreditation and Quality Assurance (2022) 27:19–37
https://doi.org/10.1007/s00769-021-01485-5

DISCUSSION FORUM

Meaningful expression of uncertainty in measurement

Maurice Cox[1] · Anthony O'Hagan[2]

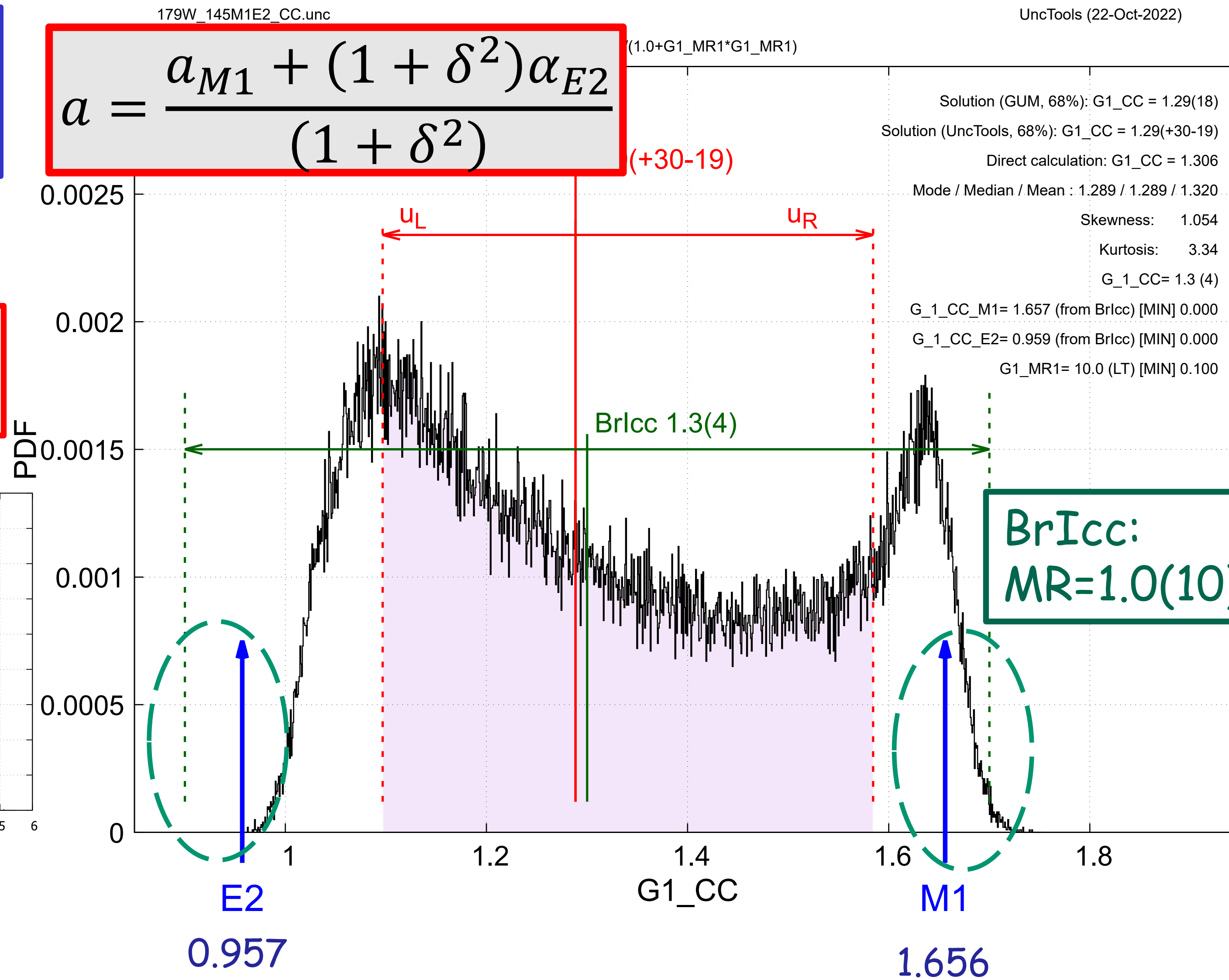
Unknown MR

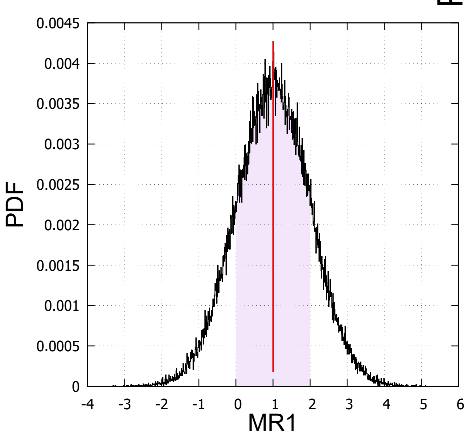
^{179}W
144.66 M1+E2
MR= not known

$$a = \frac{a_{M1} + (1+\delta^2)\alpha_{E2}}{(1+\delta^2)}$$

MC:
MR = 1.0(10)

BrIcc:
MR=1.0(10)



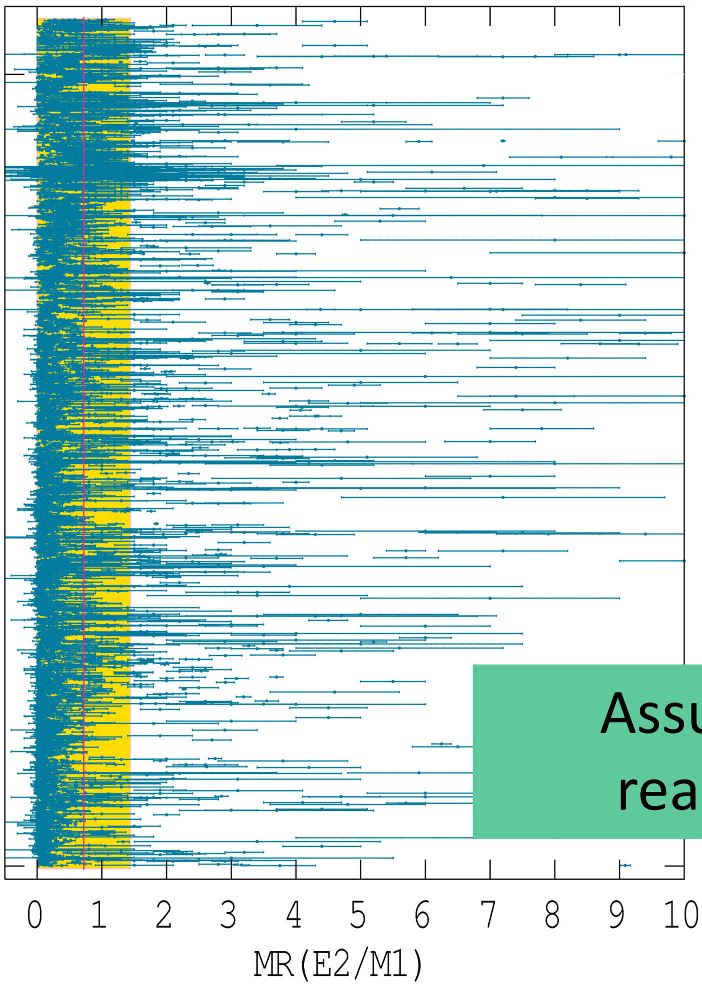


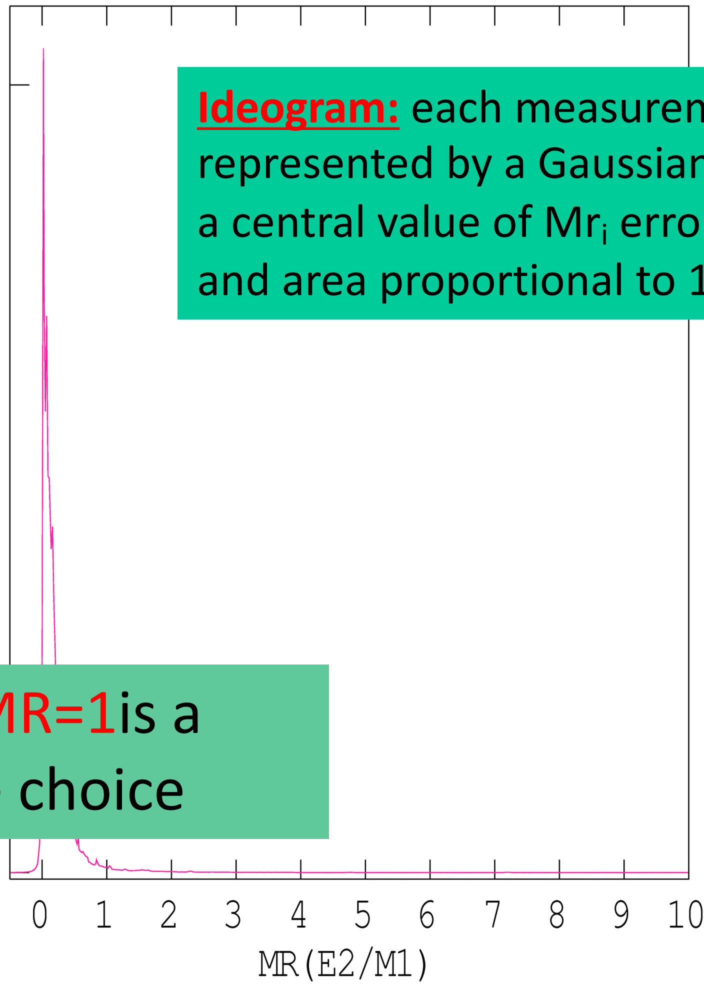
Experimental systematics of MR values NSDD 2011

- Only consider ADOPTED LEVELS, GAMMAS data sets
- MR must be numeric, absolute value of MR was used
- Exclude MR if:
  - (a) No DMR given
  - (b) DMR is a limit
  - (c) DMR is an asymmetric uncertainty

	Total	MR ±DMR
E2/M1	9760	6414
M3/E2	313	240
E4/M3	6	4
M5/E4	None	None
M2/E1	1104	862
E3/M2	80	60
M4/E3	9	4
E5/M4	5	3

MR(E2/M1): N=6414; LWM=0.72(72)





Ideogram: each measurement is represented by a Gaussian with a central value of Mr_i error DMR_i and area proportional to $1/MR_i$

Assuming MR=1is a reasonable choice

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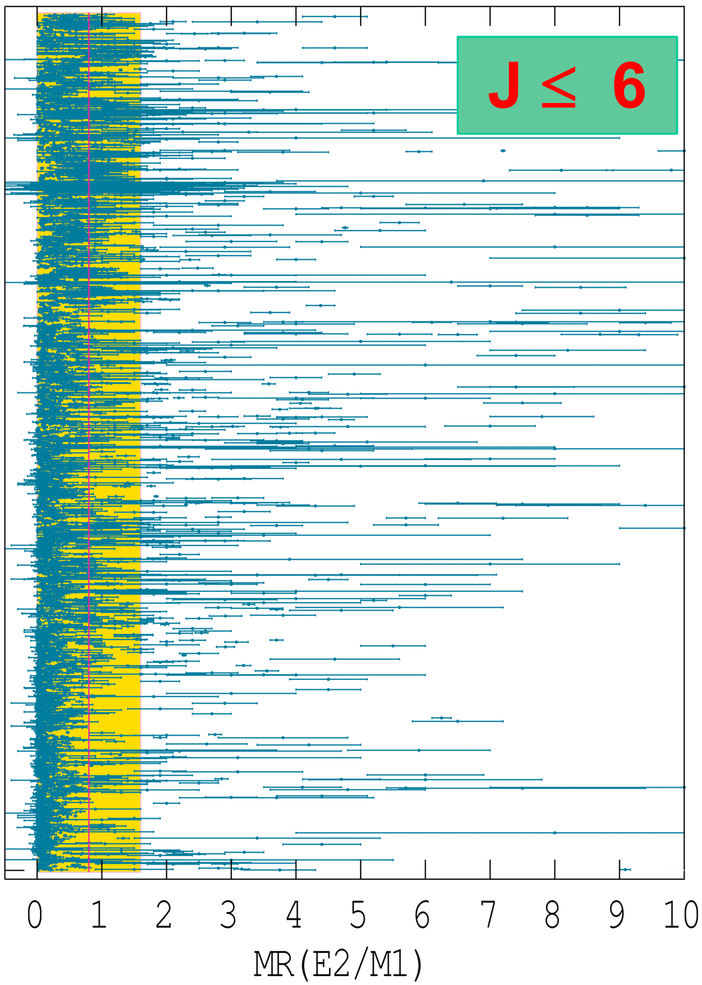
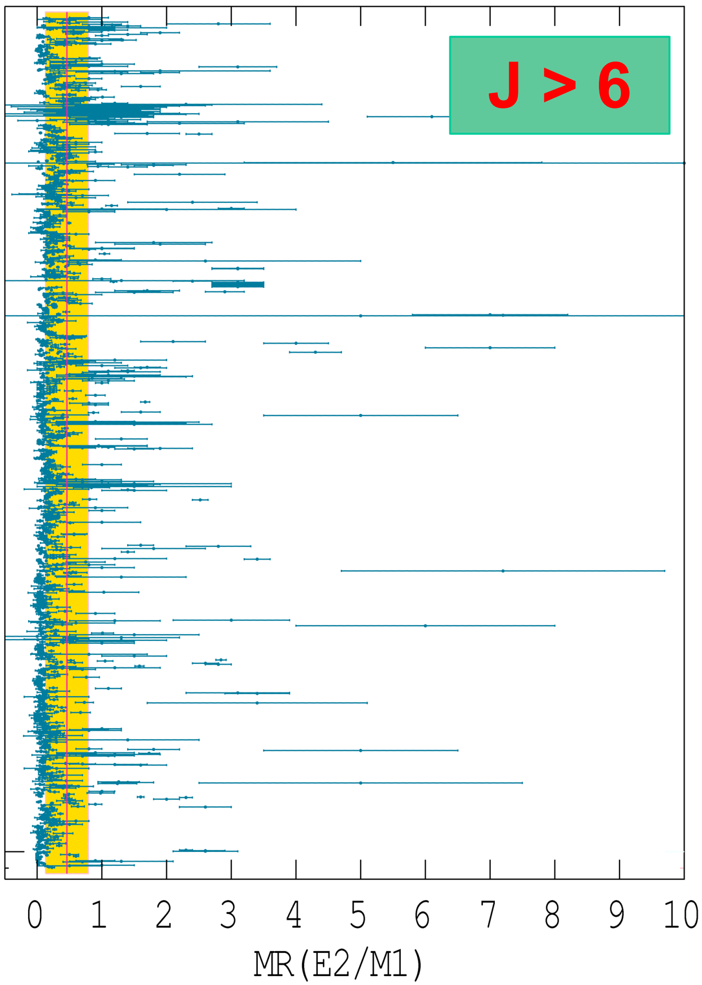
E2/M1
NSDD 2011

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

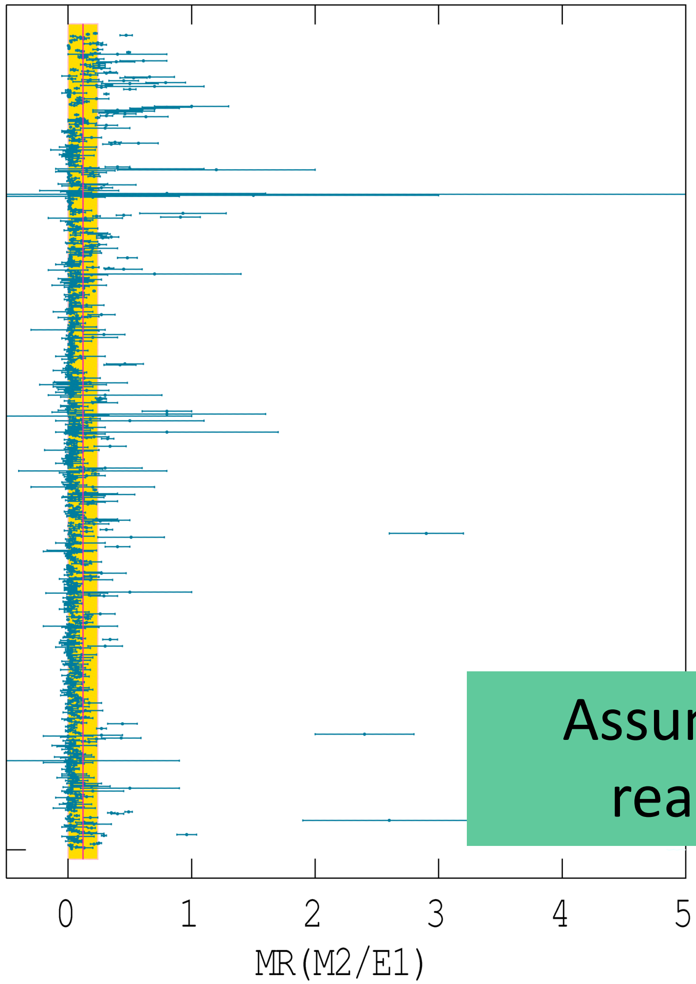


~A, ~N, ~Z Nuclear Structure effects?

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

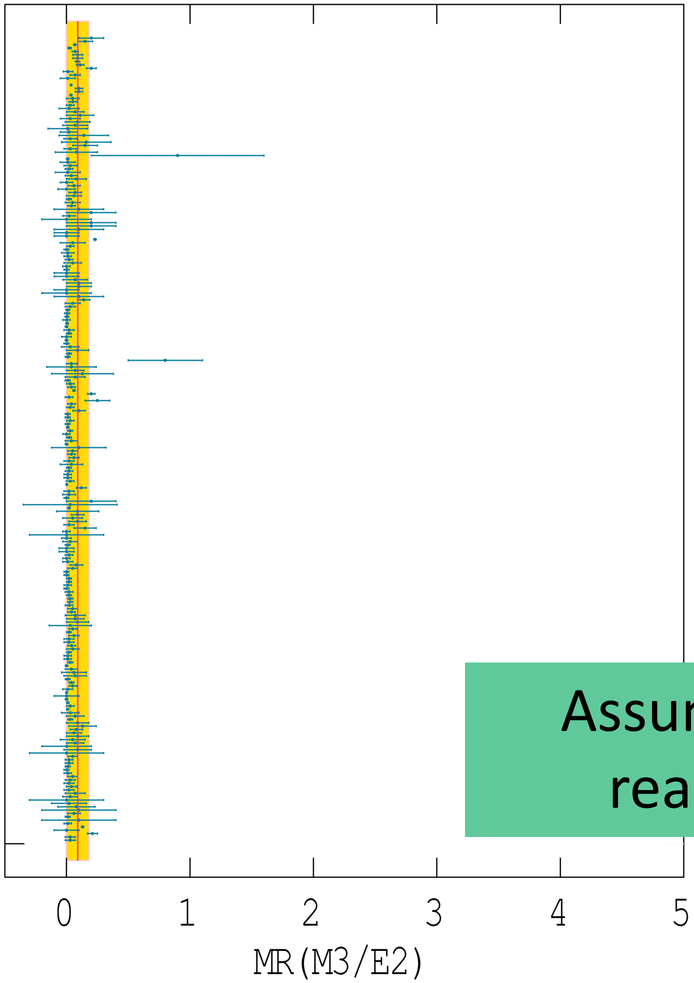


MR(M2/E1): N=862; LWM=0.12(12)



Assuming MR=0.1 is a reasonable choice

MR(M3/E2): N=240; LWM=0.09(9)



Assuming MR=0.1 is a reasonable choice

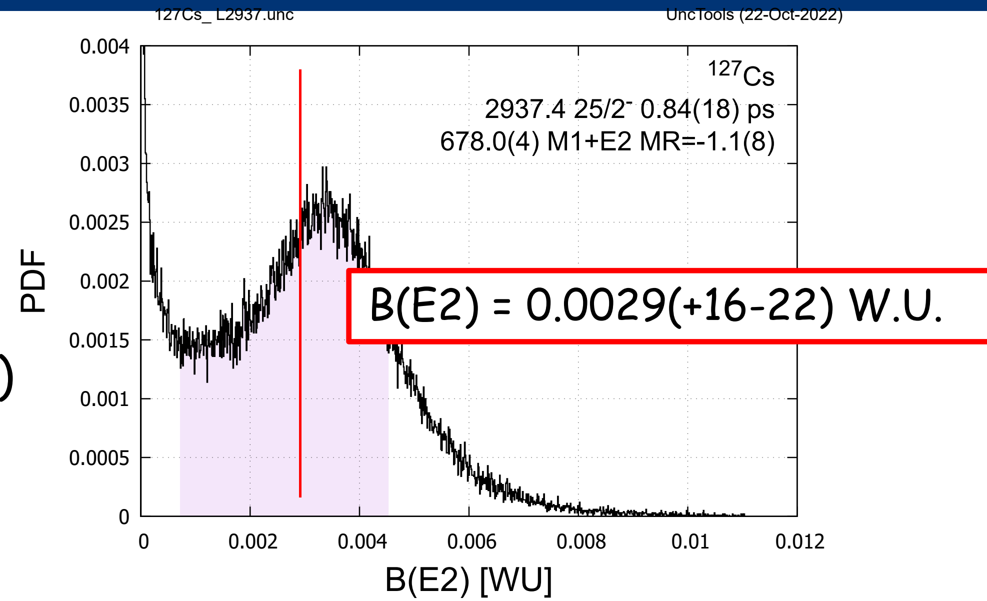
Reduced transition rates

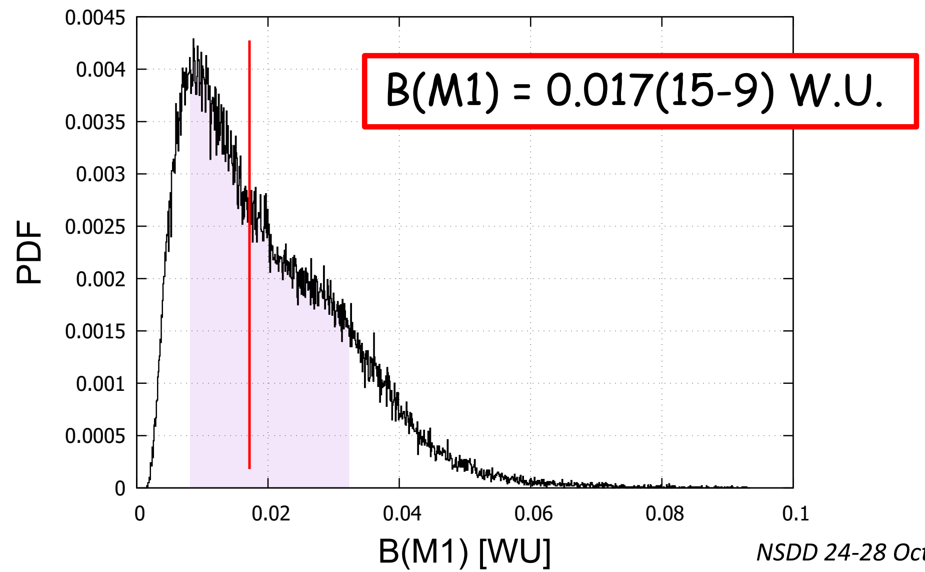
^{127}Cs

level: 2937.4 keV 25/2^{-} 0.84(18) ps

G1: 678.0(4) RI=3.6(4) M1+E2 MR=1.1(8)

G2: 819.3(4) RI=4.5(2) E2





Proposal of propagation uncertainties including limits using MC

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
  Solution: through away non-physical MC trials
- Some uncertainties in ENSDF expected to be symmetrical
  Solution: symmetrize output quantities using the GUM procedure

Symmetrizing output quantities

X(+a −b)

- ❑ Audi et al., NUBASE 2016: 2 methods:
  - Only use X, a and b, ignores the distribution (PDF) of X
- ❑ GUM – statistically more sound approach

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

mean value

replace with median

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

characteristic uncertainty

(standard deviation)

Comparison with java-Ruler

(version 4-Apr-2022)

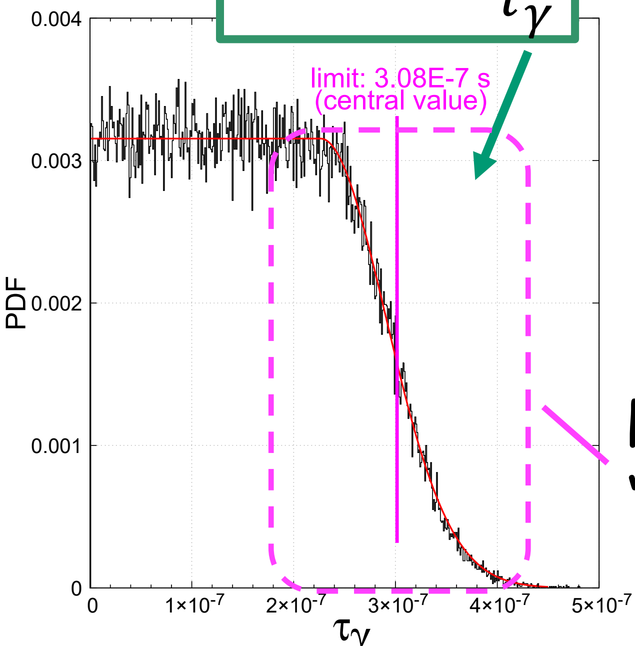
```
184RE  L 825.47    15 (9-)          5 NS    LT                  D
184RE  G 379.6     2  3.8    3 (E1)
184RE  G 637.5     2  158    19(E1)
```

	Java-Ruler	UncTools
BE1W	>2.08E-8	4E-8(+8-1)
BE1W	**>1.76E-7**	**3.E-7(+7-1)**

$$B(E1) = \frac{\tau_W}{\tau_\gamma}$$

$$\tau_W = \frac{9.756E-15}{E_\gamma^3 \times A^{2/3}} = 5.513(9)\text{E-15 s}$$

~0.016% UNC from E_γ



Propagation of the DRI`s "smoothers" the limit

Comparison with java-Ruler
(version 4-Apr-2022)

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184RE L 825.47 15 (9-) 5 NS LT D
184RE G 379.6 2 3.8 3 (E1)

	Java-Ruler	UncTools
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	Java-Ruler	UncTools
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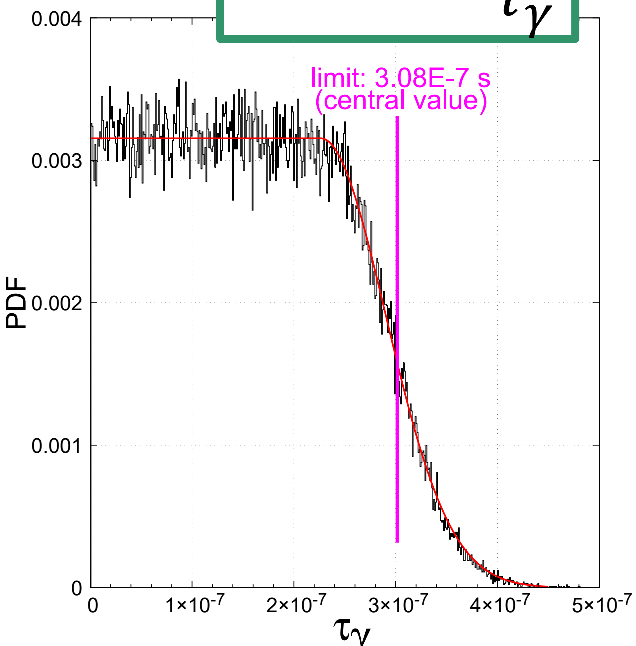
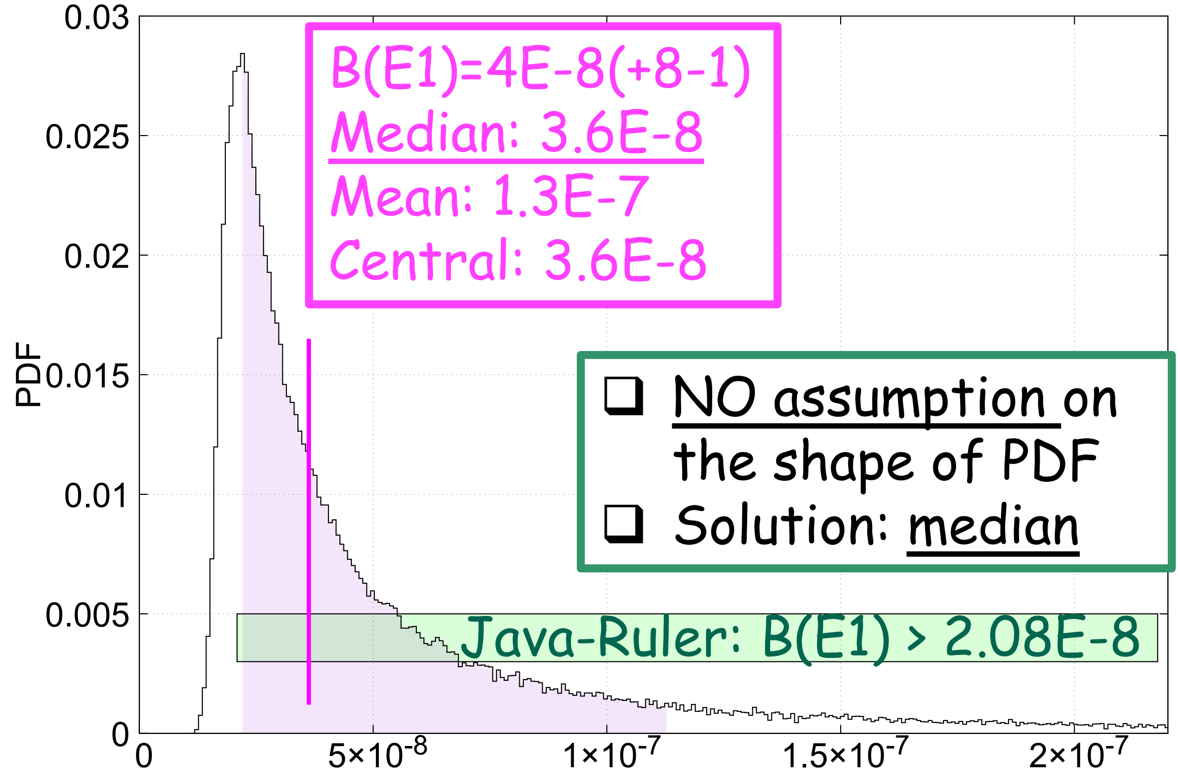
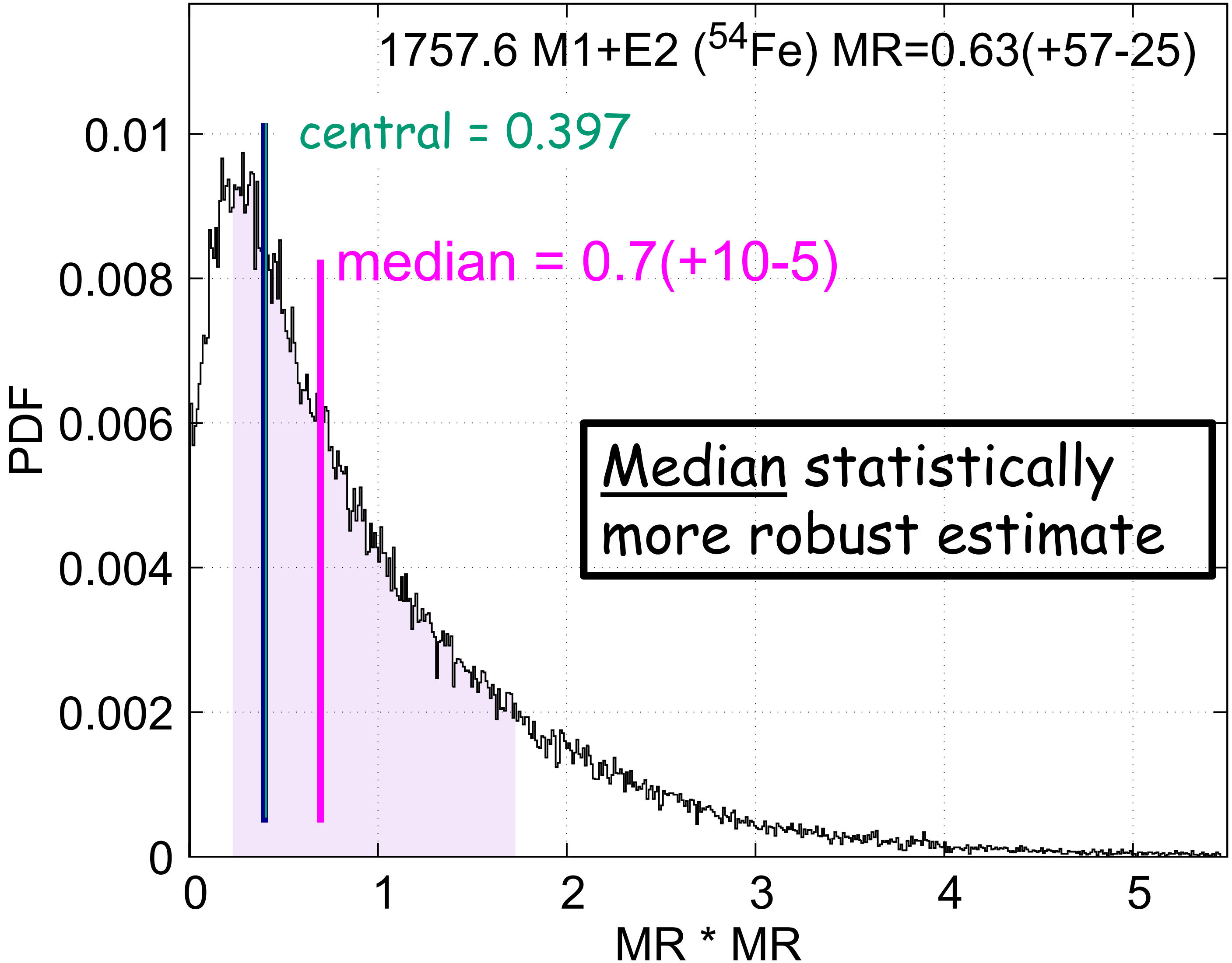
$$B(E1) = \frac{\tau_W}{\tau_\gamma}$$





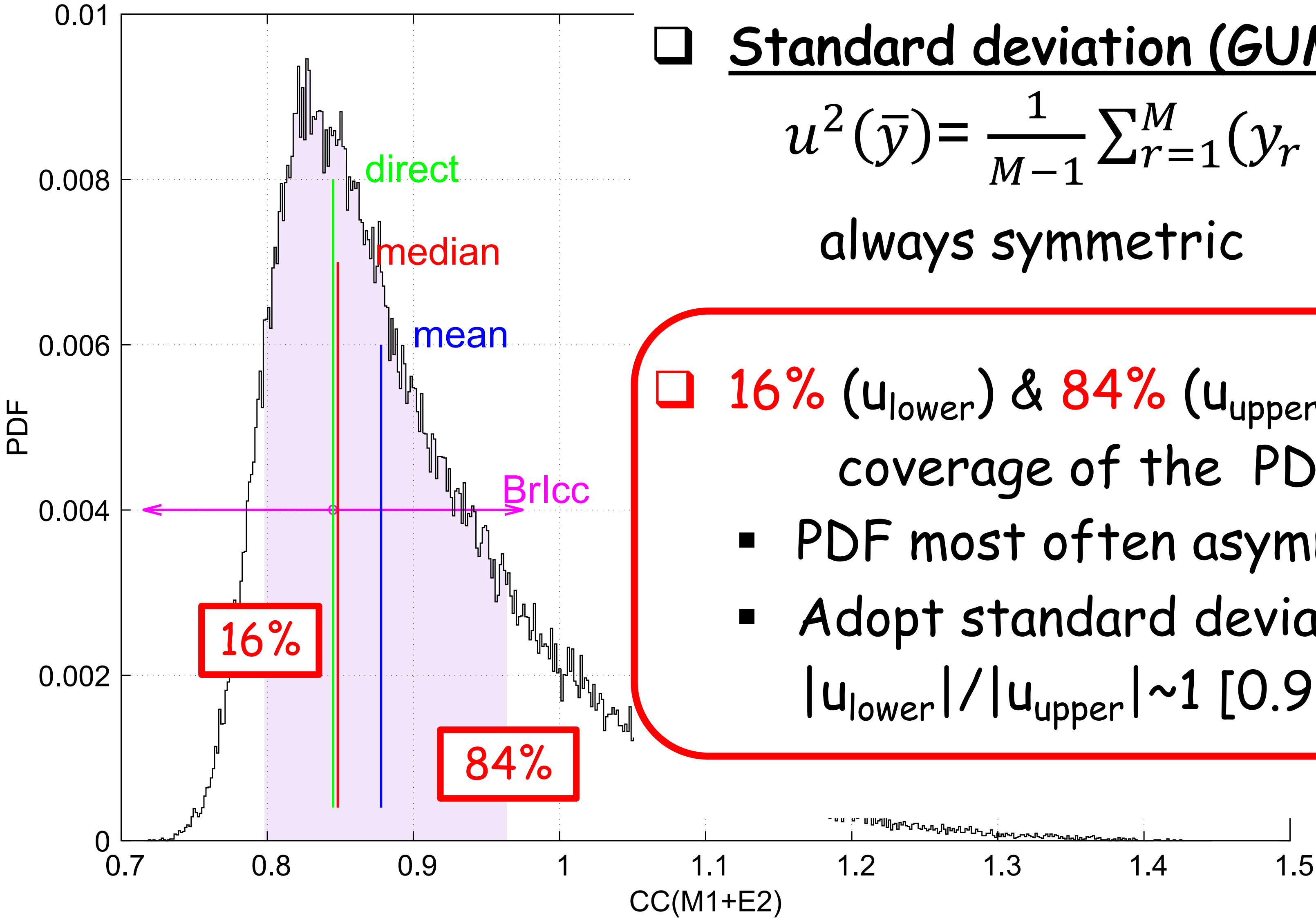
- NO assumption on the shape of PDF
- Solution: median

Value of the output quantity



Median statistically more robust estimate

Uncertainty of the output quantity



- **Standard deviation (GUM)**

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

always symmetric

- 16% (u_{lower}) & 84% (u_{upper}) coverage of the PDF
  - PDF most often asymmetric
  - Adopt standard deviation if $|u_{lower}|/|u_{upper}| \sim 1$ [0.95 : 1.05]

BrIcc - calculating mixed ICC MR is unknown

^{168}Yb 1144.9(6) M1+E2

- ENSDF assigned as E2+E0, but M1 could not be excluded

<u>BrIcc:</u>

CC=[CC(M1)+CC(E2)]/2

DCC=|CC(M1)-CC(E2)|/2

<u>CC = 0.0040(12)</u>

CC(M1)=0.00515

CC(E2)=0.00283

BrIcc - calculating mixed ICC MR is unknown

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- ENSDF assigned as E2+E0, but M1 could not be excluded

BrIcc: CC=[CC(M1)+CC(E2)]/2

DCC=|CC(M1)-CC(E2)|/2

CC = 0.0040(12)

CC(M1)=0.00515

CC(E2)=0.00283

UncTools: MR uniform in [0 : 10]

M1 [100% : 1%];

E2 [0% : 99%]

$$CC = \frac{(CC(M1) + MR^2 \times CC(E2))}{1 + MR^2}$$

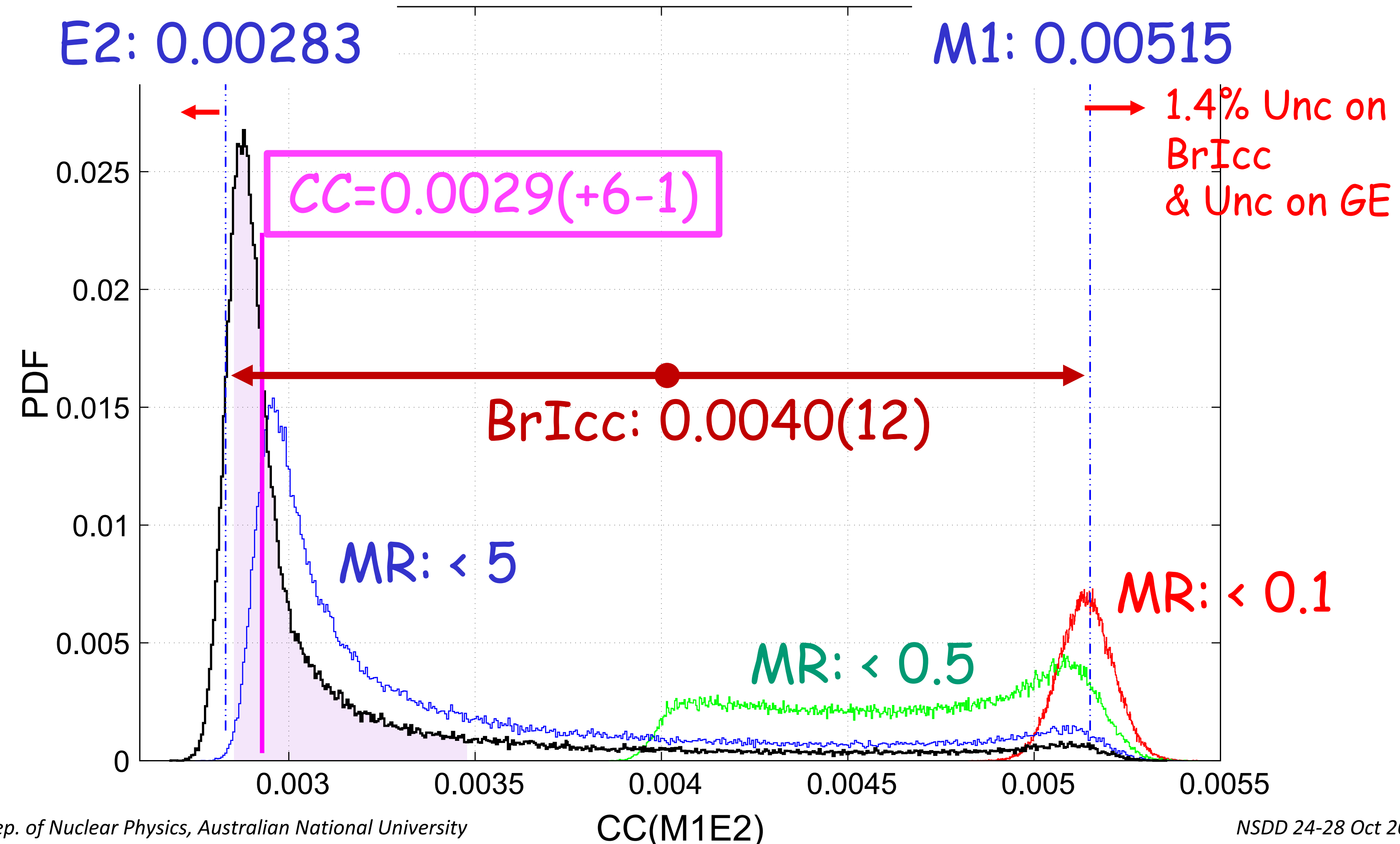
CC = 0.0029(+6-1)

- Closer to E2 than M1
- Uncertainty significantly smaller & asymmetric

UncTools - calculating mixed ICC MR is unknown

^{168}Yb 1144.9(6) M1+E2

$$CC = \frac{(CC(M1) + MR^2 \times CC(E2))}{1 + MR^2}$$



Is the GABS calculation correct?

Shamsu Basunia

^{186}Ta β^- decay scheme normalisation (GABS): NR=0.50(5)

E	RI	%IG
122.3	50(7) 14%	25.1(12) 4.8%
737.5	58(4) 6.9%	29.1(32) 11%
1284.0	0.5(25)	0.3 (13)
1322.0	0.60(30)	0.30 (15)

← **Is this correct?**

NUDAT/LiveChart:

%IG=25(4) 16%

CalibSinglesDS.f90: lines 254-266:

$$\%IG_i = \frac{(100 - IGS)\times RI_i}{\sum_j^{1,N} RI_j \times (1 + CC_j)}$$

Calculating %DIG(122), DRI(122) is used in the nominator and denominator

%DIG could be overestimated!

Filip`s talk on absolute gamma intensities

UncTools Script

```
[MAXTALLY]     100000
[G_1] 186W   G 122.3     1      50   7   E2                     1.79
[G_1_E]
[G_1_CC_E2]
[G_1_RI]
[EQN]        G1_TI = G_1_RI * (1. + G_1_CC_E2)

[G_2] 186W   G 737.5     3       58 4E2                         0.00850
[G_2_E]
[G_2_CC_E2]
[EQN]        G2_TI = G_2_RI * (1. + G_2_CC_E2)

[G_3] 186W   G 1284.0    15     0.5 25E2                        0.00278
[G_3_E]
[G_3_CC_E2]
[EQN]        G3_TI = G_3_RI * (1. + G_3_CC_E2)

[G_4] 186W   G     1322.015   0.60 30
[EQN]        G4_TI = G_4_RI

[EQN]        TI = G1_TI + G2_TI + G3_TI + G4_TI

[EQN]        NR = 100. / TI    (no g.s. feeding)

[EQN]        G1_pTI = G_1_RI * NR
```

G-record

Samples parameters from G-record, calling BrIcc

Calculates TI

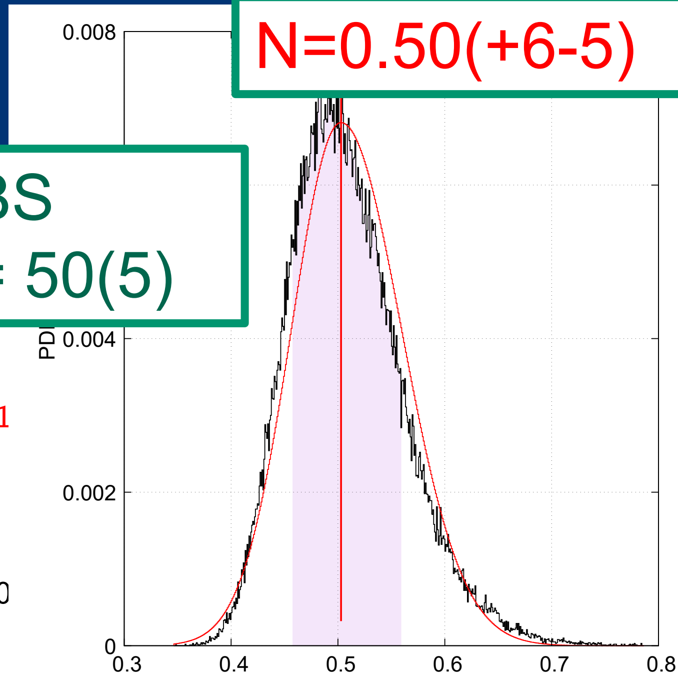
TI to g.s.

Calculates NR, BR=1

Calculates %IG

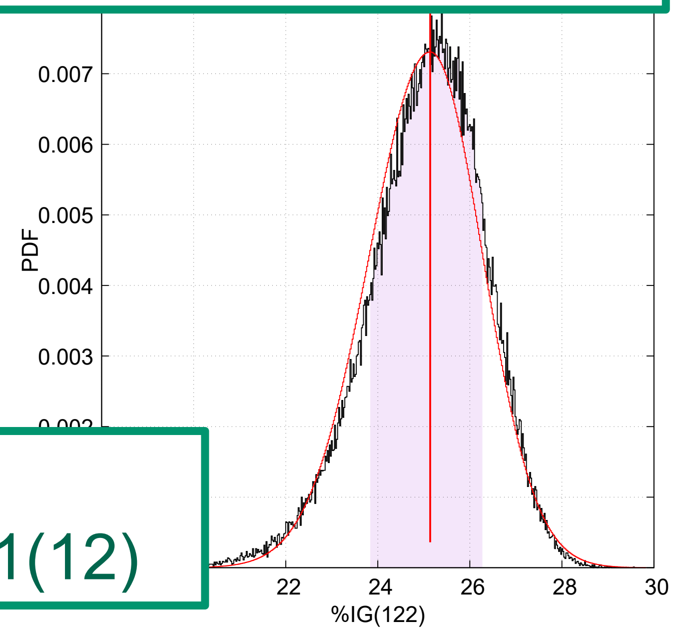
UncTools results

```
[MAXTALLY]     100000
[G_1] 186W   G 122.3      1      50   7   E2
[G_1_E]
[G_1_CC_E2]
[G_1_RI]
[EQN]        G1_TI = G_1_RI * (1. + G_1_CC_E2)
[G_2] 186W   G 737.5      3        58 4E2
[G_2_E]
[G_2_CC_E2]
[EQN]        G2_TI = G_2_RI * (1. + G_2_CC_E2)
[G_3] 186W   G 1284.0     15     0.5 25E2
[G_3_E]
[G_3_CC_E2]
[EQN]        G3_TI = G_3_RI * (1. + G_3_CC_E2)
[G_4] 186W   G      1322.015   0.60 30
[EQN]        G4_TI = G_4_RI
[EQN]        TI = G1_TI + G2_TI + G3_TI + G4_TI
[EQN]        N = 100. / TI
[EQN]        G1_pTI = G_1_RI * N
```



N=0.50(+6-5)

GABS
NR= 50(5)



%IG(122)=25.1(+11-13)

GABS
%IG(122)=25.1(12)

Comparison with java-Ruler
(version 4-Apr-2022)

177HF L 321.3162   4 9/2+   0.665 NS 16
177HF G 71.6418   6   1.58 5E1+M2   -0.018 9   0.89   6

	Java-Ruler	UncTools
CC	0.89(6)	0.89(+5-3)
BE1W	1.24E-5(5)	1.24E-5(5)
BM2W	3.6(+45-27)	4(+5-3)

177HF G 208.3662 4   100.0 14E1+M2   +0.076 19   0.068 9

CC	**0.068(9)**	**0.068(+8-6)**
BE1W	3.17E-5(8)	3.17E-5(8)
BM2W	19.3(+104-85)	19(+11-8)

177HF G 321.3159 6   2.10 4 E1+M2   +0.175 10   0.0354 21

CC	**0.0354(21)**	**0.0354(+20-19)**
BE1W	1.77E-7(6)	1.77E-7(6)
BM2W	0.242(+29-28)	0.241(+29-27)

Comparison with java-Ruler
(version 4-Apr-2022)

184RE L 825.47 15 (9-) 5 NS LT D

184RE G 379.6 2 3.8 3 (E1)

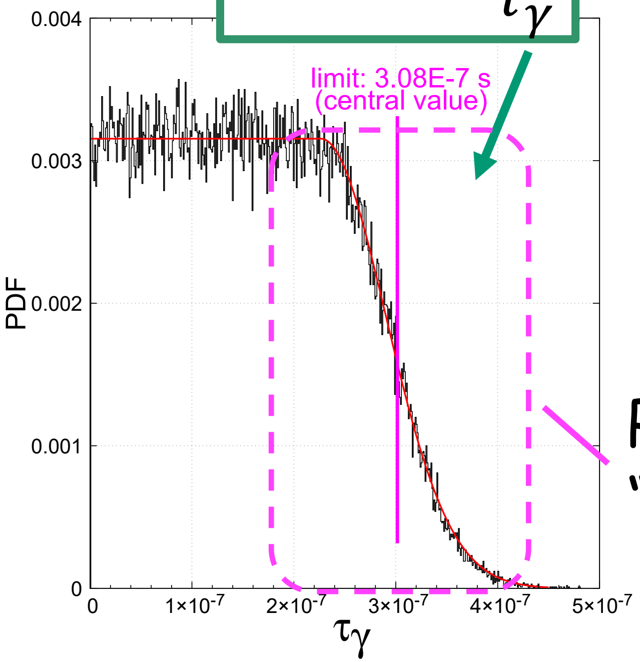
184RE G 637.5 2 158 19(E1)

	Java-Ruler	UncTools
BE1W	>2.08E-8	4E-8(+8-1)
BE1W	**>1.76E-7**	**3.E-7(+7-1)**

$$B(E1) = \frac{\tau_W}{\tau_\gamma}$$

$$\tau_W = \frac{9.756E-15}{E_\gamma^3 \times A^{2/3}} = 5.513(9)\text{E-15 s}$$

~0.016% UNC from E_γ



Propagation of the DRI`s "smoothers" the limit

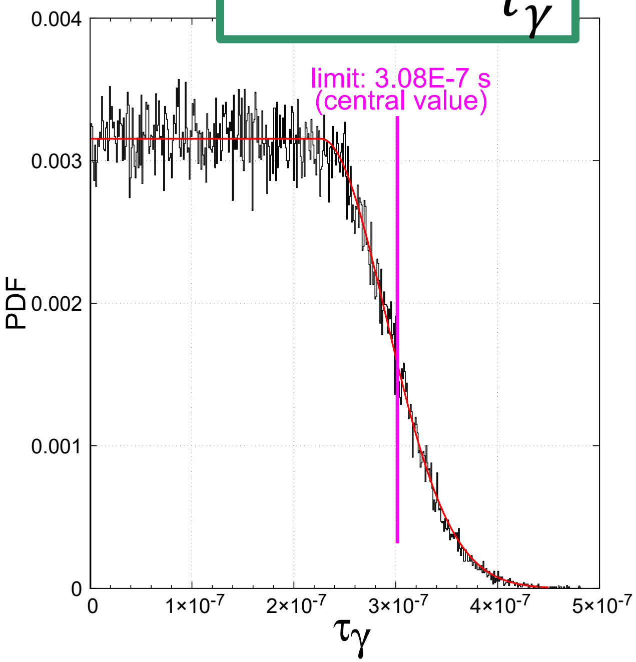
Comparison with java-Ruler
(version 4-Apr-2022)

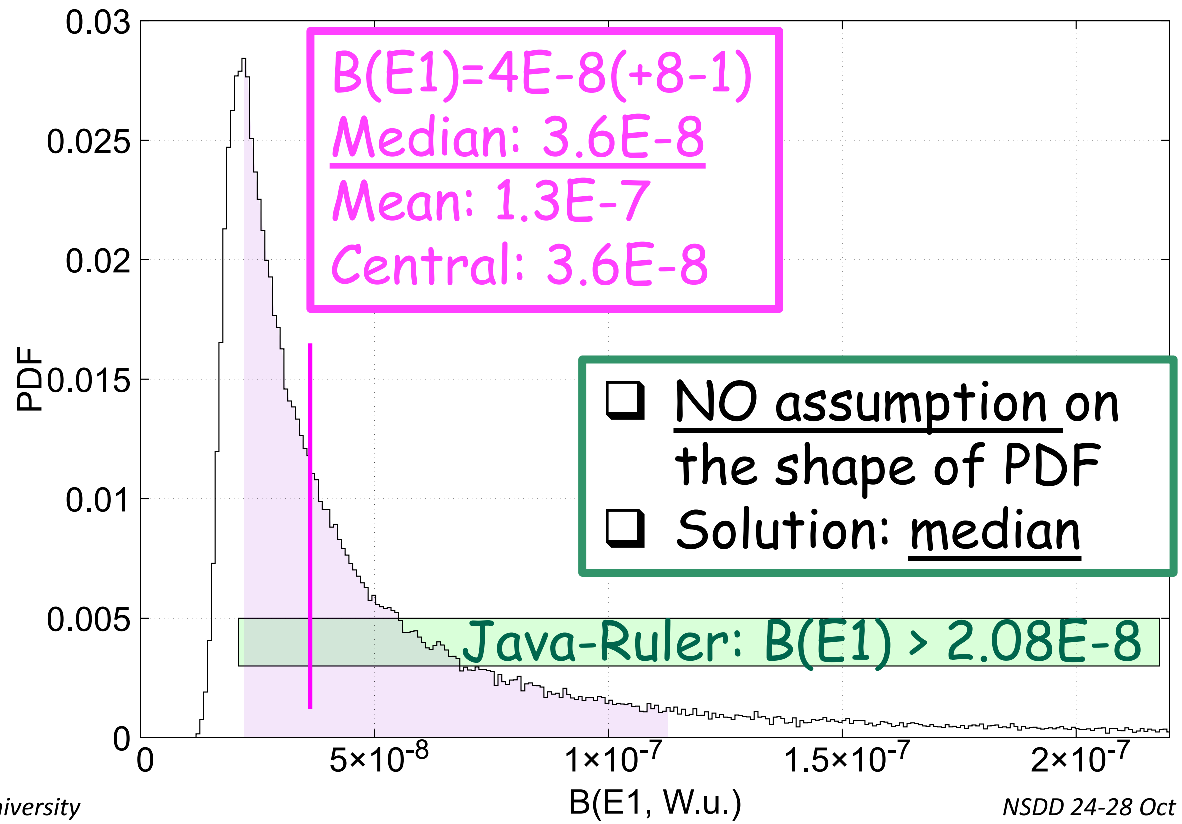
184RE L 825.47 15 (9-) 5 NS LT D
184RE G 379.6 2 3.8 3 (E1)

184RE G 637.5 2 158 19(E1)

	Java-Ruler	UncTools
BE1W	>2.08E-8	4E-8(+8-1)
BE1W	>1.76E-7	3.E-7(+7-1)

$$B(E1) = \frac{\tau_W}{\tau_\gamma}$$





B(E1)=4E-8(+8-1)
Median: 3.6E-8
Mean: 1.3E-7
Central: 3.6E-8

- ❑ NO assumption on the shape of PDF
- ❑ Solution: median

Java-Ruler: B(E1) > 2.08E-8

Handling non-physical solutions

$$\rho^2(E0) = \left(\frac{3}{4\pi}Z\right)^2 \alpha^2(1-\alpha^2)[\Delta(\beta^2)]^2$$

^{40}Ca 3353 keV E0

$\rho^2(E0)=0.0259(16)$

$\Delta(\beta^2)=0.073(27)$

Solution: $\alpha_{1,2}^2 = \frac{b \pm \sqrt{b^2-4ac}}{2a}$ $a=+1; b=-1;$ $c = \frac{\rho^2(E0)(4\pi)^2}{(3Z\Delta(\beta^2))^2}$

- Input parameters sampled up to +/- 5σ are all valid.

  Plugging them into the equation gave non-physical solution:

  $\Delta(\beta^2) < 0.06 \rightarrow [b^2 - 4ac] < 0$

  - NIST uncertainty machine: DO NOT proceed
  - UncTools: Dump this trial and take a new sample of the input parameters

Handling non-physical solutions

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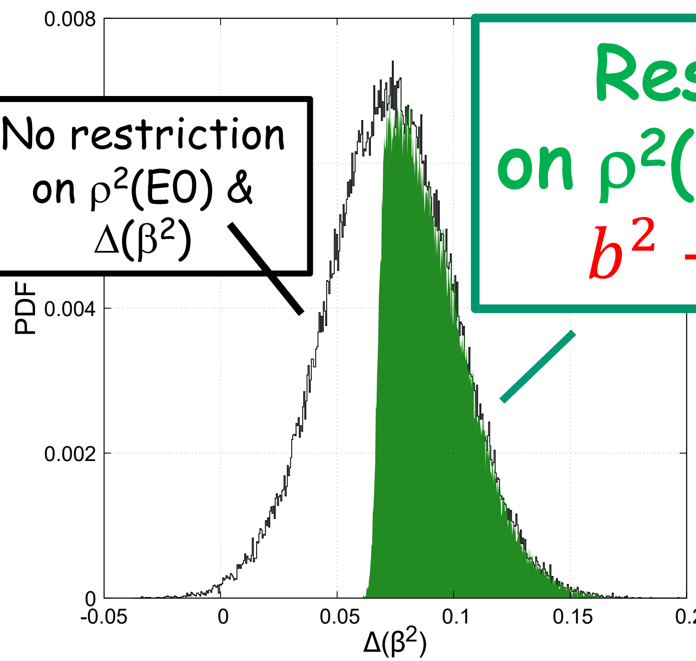
$$\rho^2(E0) = \left(\frac{3}{4\pi}Z\right)^2 \alpha^2(1-\alpha^2)[\Delta(\beta^2)]^2$$

^{40}Ca 3353 keV E0

$\rho^2(E0)=0.0259(16)$

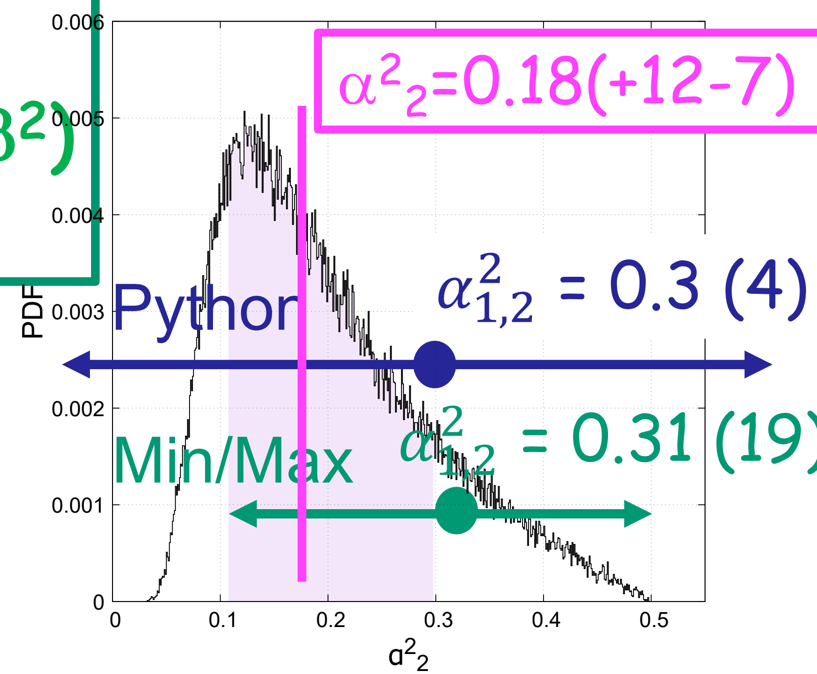
$\Delta(\beta^2)=0.073(27)$

Solution: $$\alpha^2_{1,2} = \frac{b \pm \sqrt{b^2-4ac}}{2a}$$ $$a=+1;\, b=-1;\; c=\frac{\rho^2(E0)(4\pi)^2}{(3Z\Delta(\beta^2))^2} > 0$$



Restriction on $\rho^2(E0)$ & $\Delta(\beta^2)$

$b^2 - 4ac > 0$



UncTools - Summary

- A script driven tool to propagate uncertainties using Monte Carlo
- Input parameters (normal, skewed normal and limits, max 8000) sampled and propagated through equations (max 1000)
- Parse full ENSDF records & checks for errors
- Probability Density Function (PDF) of the output used to determine the value and uncertainty; based in input quantities no assumption is made
- Output = median (recommended); in most cases median & central value are close
- Uncertainty from 16% : 84% coverage intervals (asymmetric PDF) or standard deviation (symmetric or nearly symmetric PDF)
- Can be called from any application, return values in XML:

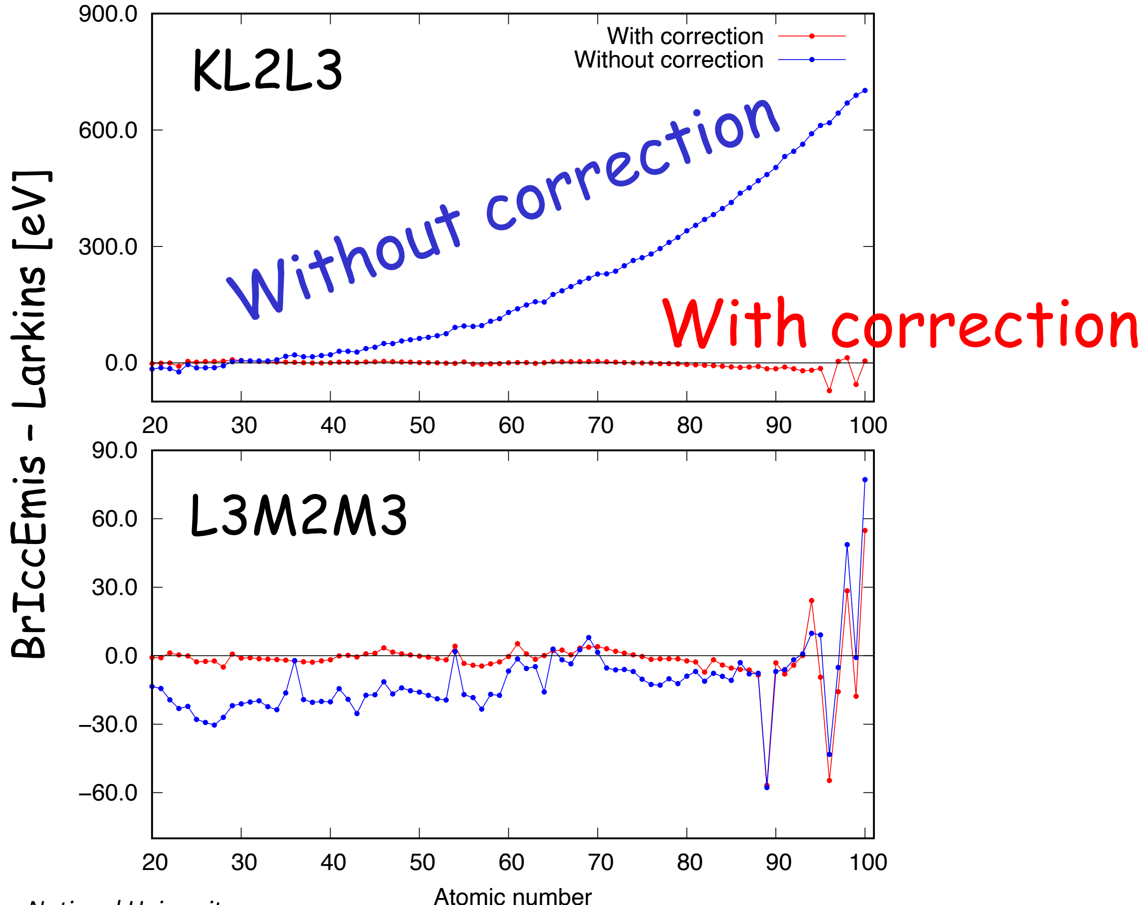
  unctools <input script> -x

- Publication quality plots:

  unctools <input script> -g

NS_RadList - beta version with B. Tee

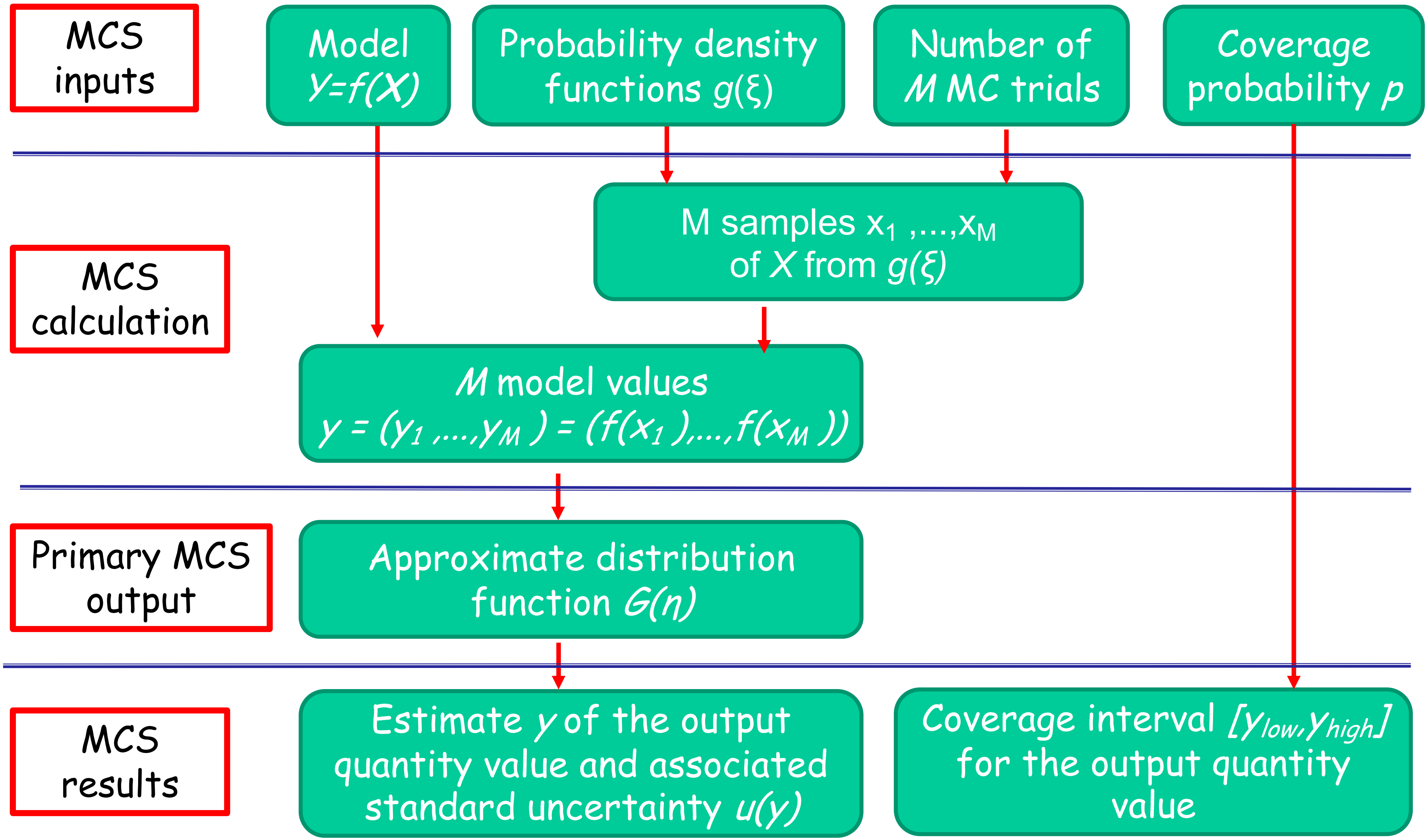
- Atomic transition rates from EADL (1991PeZY)
- Atomic transition energies calculated using RAINE (2002Ba85), with semi-empirical corrections (2020TEZY)



NS_RadList - beta version with B. Tee

- Initial atomic vacancy from
  - EC & IC (nuclear decay mode);
  - Electron/positron bombardment
  - User specified distribution (from file)
- BrIccEmisDB (219 MB)
  - precalculated atomic spectra for Z=6 to 100 by putting an initial vacancy on K to O shells; 1 million simulations
  - Binned with 1 eV
  - X-rays and Auger electrons
  - Unbinned "raw" data 3.5 GB - for expert use

Monte Carlo simulations to obtain the output quantity



NS_RadList – nuclear decay mode with B. Tee

Ns_radlist –n <ENSDF.file> -u -g

- Reads and parses ENSDF file; comprehensive error detection
- Evaluates EC rates using EC probabilities from 1995SzZY (planned to use BetaShape)
- Evaluates IC rates using BrIcc v3, Z up to 126 (2008Ki07, 20212Ki04), new Ω(E0) tables (2020Do01)
- "-u" propagates uncertainties in nuclear structure parameters (energy, intensity, mixing ratio, etc) using UncTools (10,000 MC trials)
- "-g" generates spectrum plots of the PDF
- Generates new ENSDF records

NS_RadList - calculation report with B. Tee

Ns_radlist -n 125I_EC.ens -u -g

```
#    Program version: NS_RadList v1.0 (23-Mar-2022)
#    BrIccEmis: BrIccEmis (02-Mar-2021)
#    NSR Key: 2012Le09
#    Command line: -n 125I_EC.ens -g -u
#    ENSDF file: 125I_EC.ens
#    Parent: 125I
#    Daughter: 125TE
#    DecayMode: EC
#    Half Life: 59.400 D
#    $Atomic relaxation from BrIccEmis (26-May-2021) 2016Le19
#      IM$Absolute intensity per 100 decays; as defined by 1991PeZY,
#      uncertainties in theoretical X-ray emission probabilities are 10% fo
#      K and L shells and 30% for outer shells.
#      IM$Absolute intensity per 100 decays; as defined by 1991PeZY,
#      uncertainties in theoretical Auger-electron emission probabilities
#      are <15% for K and L shells (except for Coster-Kronig and super
#      Coster-Kronig transitions) and 30% for outer shells.
```

NOTE: uncertainties in atomic transition probabilities are NOT propagated

NS_RadList - calculation report with B. Tee

```
# NUCLEAR TRANSITIONS ========================================
# ELECTRON CAPTURE ===========================================
# Trans   E-decay       E_f            EC Prob.       Shell EC Prob.
#           [keV]        [keV]          [/100 dec]      (1998Sc28)
EC -  1   150.27(6)    35.4925(5)   100
K  -  1                                                 0.8007(+17-18)
L1 -  1                                                 0.1519(+13-12)
L2 -  1                                                 0.004133(34)
M1 -  1                                                 0.0339(+7-6)
M2 -  1                                                 0.000994(+20-19)
N1 -  1                                                 0.0077(4)
N2 -  1                                                 0.000214(12)
O1 -  1                                                 0.000473(27)
# EM transitions (Intensity cutoff:  1.00E-03% ==============
# Transition               Energy [keV]              Probability
#                                                  [per 100 decays]
G_1                        35.4925(5)                 6.68(13)
G_1_CK                      3.6725(5)                78.1(19)
G_1_CL                     30.5945(+24-20)           10.67(+26-25)
G_1_CM                     34.4996(+10-9)             2.14(5)
G_1_CN                     35.3244(6)                 0.421(10)
G_1_CO                     35.4752(5)                 0.0440(10)
```

NS_RadList - calculation report with B. Tee

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```
# AUGER electrons =============================================
# Transition          Energy [keV]                         Probability
#                 Mean     95% Confidence range          [per 100 decays]
Auger_Tot         0.598       [0.001 : 3.610]          1895(19)
Auger_Ktot       23.913      [21.795 : 29.947]           19.13(23)
Auger_KLL        22.516      [21.795 : 22.976]           12.91(+16-15)
Auger_KLX        26.450      [25.812 : 27.334]            5.63(7)
Auger_KXY        30.307      [29.751 : 31.452]            0.589(7)
Auger_Ltot        2.774       [0.124 : 3.983]           184.2(18)
CK_LLX            0.285       [0.063 : 0.533]            26.82(21)
Auger_LMM         3.044       [2.471 : 3.720]           121.1(+13-12)
Auger_LMX         3.673       [3.307 : 4.258]            33.95(35)
Auger_LXY         4.305       [4.027 : 4.799]             2.366(24)
Auger_Mtot        0.323       [0.021 : 0.626]            450(5)
CK_MMX            0.096       [0.009 : 0.246]           130.0(13)
Auger_MXY         0.416       [0.254 : 0.640]           319.8(33)
Auger_Ntot        0.016       [0.001 : 0.077]          1242(12)
SCK_NNN           0.016       [0.002 : 0.057]           181.6(18)
CK_NNX            0.033       [0.001 : 0.107]           110.4(11)
Auger_NXY         0.013       [0.001 : 0.076]            950(9)
```

Evaluated from 1 eV binned spectra

NS_RadList - calculation report with B. Tee

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X-rays ==

# Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
X-ray tot	25.432	[3.778 : 31.693]	155.6(18)
X-ray Ktot	28.039	[27.203 : 31.693]	139.0(17)
X-ray KL2	27.203	[27.203 : 27.203]	40.1(5)
X-ray KL3	27.473	[27.473 : 27.473]	74.3(9)
X-ray KM	30.980	[30.944 : 30.995]	20.19(24)
X-ray KM2	30.944	[30.944 : 30.944]	6.81(8)
X-ray KM3	30.995	[30.995 : 30.995]	13.24(16)
X-ray KN	31.701	[31.693 : 31.704]	4.20(5)
X-ray KN2	31.693	[31.693 : 31.693]	1.398(17)
X-ray KN3	31.704	[31.704 : 31.704]	2.772(33)
X-ray Ltot	3.933	[3.339 : 4.590]	14.77(15)
X-ray Mtot	0.554	[0.250 : 0.882]	0.782(8)
X-ray Ntot	0.100	[0.078 : 0.167]	1.007(11)

Evaluated from 1 eV binned spectra

New ENSDF records

```
125TE1 AM E(Tot)= 0.598$ I(Tot)= 1895(19)$
125TE2 AM E(Ktot)= 23.913$ I(Ktot)= 19.13(23)$
125TE3 AM E(KLL)= 22.516$ I(KLL)= 12.91(+16-15)$
125TE4 AM E(KLX)= 26.450$ I(KLX)= 5.63(7)$
125TE5 AM E(KXY)= 30.307$ I(KXY)= 0.589(7)$
125TE6 AM E(Ltot)= 2.774$ I(Ltot)= 184.2(18)$
125TE7 AM E(CK_LLX)= 0.285$ I(CK_LLX)= 26.82(21)
125TE8 AM E(LMM)= 3.044$ I(LMM)= 121.1(+13-12)$
125TE9 AM E(LMX)= 3.673$ I(LMX)= 33.95(+35-34)$
125TEa AM E(LXY)= 4.305$ I(LXY)= 2.366(+25-24)$
125TEb AM E(Mtot)= 0.323$ I(Mtot)= 450(+5-4)$
125TEc AM E(CK_MMX)= 0.096$ I(CK_MMX)= 130.0(+13
125TEd AM E(MXY)= 0.416$ I(MXY)= 319.8(+33-32)$
125TEe AM E(Ntot)= 0.016$ I(Ntot)= 1242(12)$
125TEf AM E(SCK_NNN)= 0.016$ I(SCK_NNN)= 181.6(1
125TEg AM E(CK_NNX)= 0.033$ I(CK_NNX)= 110.4(+11
125TEh AM E(NXY)= 0.013$ I(NXY)= 950(+10-9)$
125TE1 XM E(tot)= 25.432$ I(tot)= 155.6(+19-18)$
125TE2 XM E(Ktot)= 28.039$ I(Ktot)= 139.0(+17-16
125TE3 XM E(KL2)= 27.203$ I(KL2)= 40.1(5)$
125TE4 XM E(KL3)= 27.473$ I(KL3)= 74.3(9)$
125TE5 XM E(KM)= 30.980$ I(KM)= 20.19(24)$
125TE6 XM E(KM2)= 30.944$ I(KM2)= 6.81(8)$
125TE7 XM E(KM3)= 30.995$ I(KM3)= 13.24(16)$
125TE8 XM E(KN)= 31.701$ I(KN)= 4.20(5)$
125TE9 XM E(KN2)= 31.693$ I(KN2)= 1.398(17)$
125TEa XM E(KN3)= 31.704$ I(KN3)= 2.772(33)$
```

- Absolut Auger & X-ray intensity
- Inserted before g.s. record
- D record with program version
- C records with notes on uncertainties from EADL

Output from Java-NDS
(Jun Chen)
Uncertainties will be added

^{131}Cs ε decay (9.689 d)

Parent: ^{131}Cs: E=0.0; $J^{\pi}=5/2^{+}$; $T_{1/2}$=9.689 d *16*; Q(ε)=358.00 *18*; %ε decay=100.0

Evaluation by A.L. Nichols, March 2021.

References: 1960La06, 1963Ly02, 1972Em01, 1974Pl04, 1975La16, 2005Ku10, 2006Kh09, 2006Vo04, 2008Si26, 2012Le09, 2016Le19, 2019Ka48, 2019Mo35, 2020TeZY, 2021Wa16.

X rays (^{131}Xe)

Transition(s)	E(X ray)	I(X ray)†	Transition(s)	E(X ray)	I(X ray)†	Transition(s)	E(X ray)	I(X ray)†
TOT	28.559	83.91	K-M2	34.925	3.697	K-O	35.980	0.2287
K-TOT	31.632	74.52	K-M3	34.993	7.193	L-TOT	4.488	8.648
K-L2	30.631	21.37	K-M4	35.252	0.03540	M-TOT	0.680	0.5394
K-L3	30.978	39.64	K-M5	35.266	0.05200	N-TOT	0.117	0.2050
K-M	34.972	10.978	K-N	35.828	2.307			

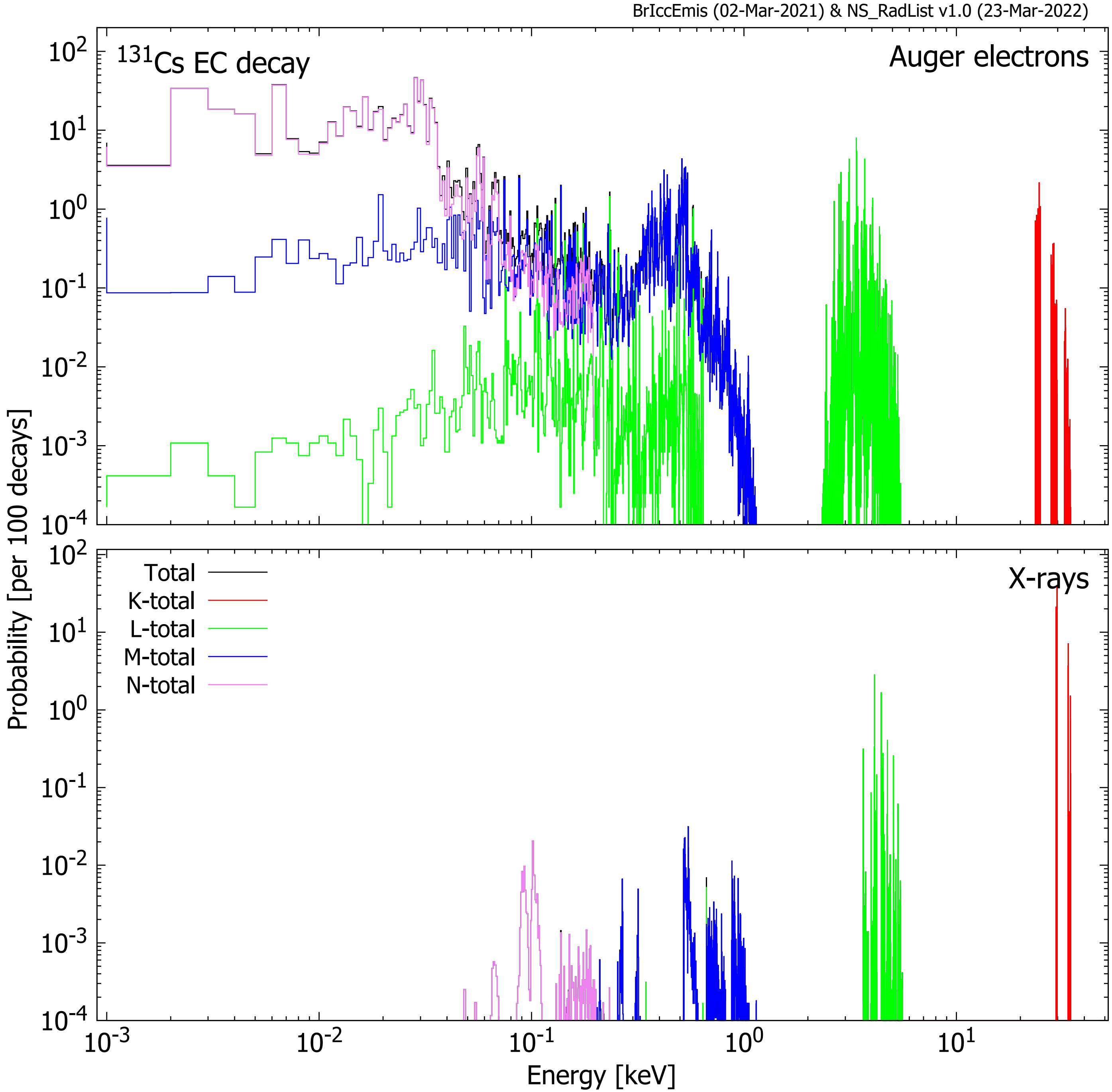
† Absolute intensity per 100 decays; as defined by 1991PeZY, uncertainties in theoretical X-ray emission probabilities are 10% for K and L shells and 30% for outer shells.

NOTE: Atomic transition energies uncorrected!

Auger electrons (^{131}Xe)

Transition(s)	E(Auger)	I(Auger)†	Transition(s)	E(Auger)	I(Auger)†	Transition(s)	E(Auger)	I(Auger)†
TOT	0.707	900.7	L-LX	0.307	13.84	M-XY	0.492	162.7
K-TOT	26.859	9.056	L-MM	3.387	60.65	N-TOT	0.030	570.7
K-LL	25.218	6.046	L-MX	4.147	17.92	N-NN	0.011	10.816
K-LX	29.727	2.719	L-XY	4.913	1.338	N-NX	0.047	141.0
K-XY	34.161	0.2909	M-TOT	0.379	227.2	N-XY	0.024	418.9
L-TOT	3.100	93.75	M-MX	0.097	61.96			

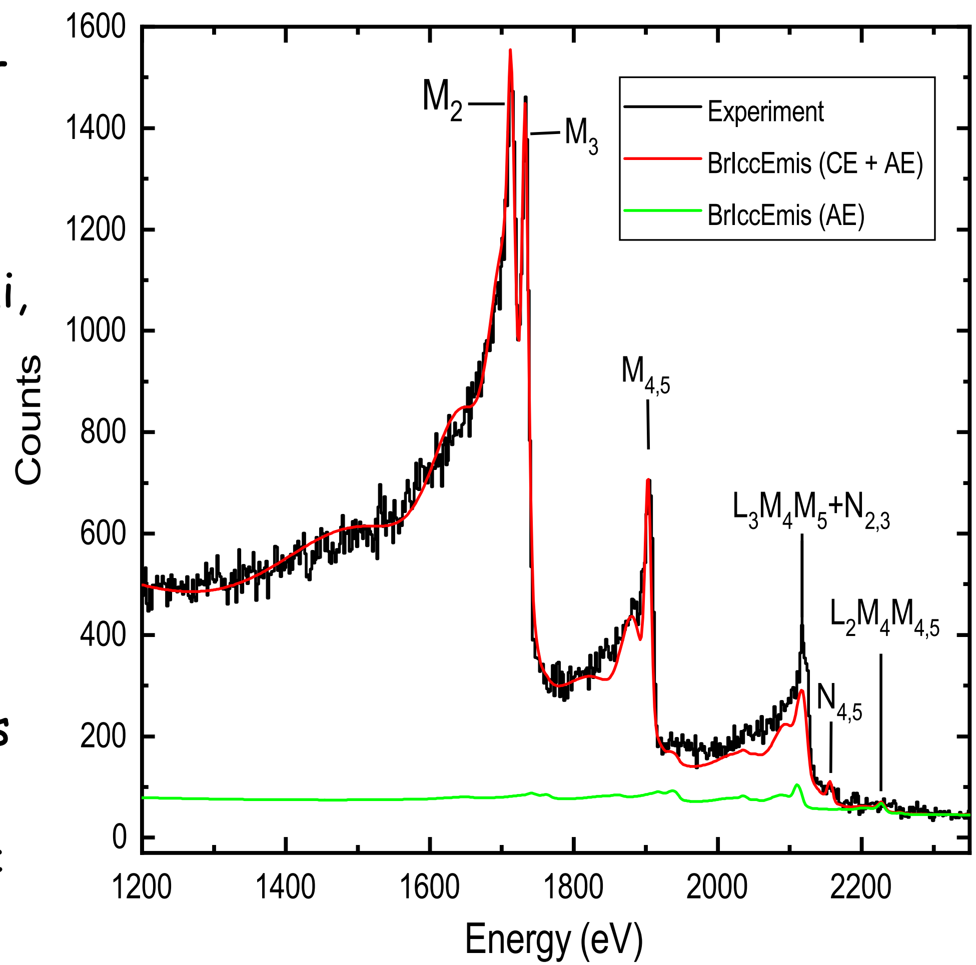
† Absolute intensity per 100 decays; as defined by 1991PeZY, uncertainties in theoretical Auger-electron emission probabilities are <15% for K and L shells (except for Coster-Kronig and super Coster-Kronig transitions) and 30% for outer shells.


BrIccEmis (02-Mar-2021) & NS_RadList v1.0 (23-Mar-2022)
^{131}Cs EC decay
Auger electrons
X-rays
Total
K-total
L-total
M-total
N-total
Probability [per 100 decays]
Energy [keV]
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}

Recent low energy electron measurements - $^{99}Mo/^{99m}Tc$

$^{99}Mo/^{99m}Tc$ source measurements to benchmark BrIccEmis & NS_RadList

- 2.2 MBq source on evaporated Al substrate
- Prepared by M. Roberts, P. Pellegrini, L. Hogan, F. Mansour and I. Greguric (ANSTO, Sydney)
- Experiments & Data analysis: B.P.E. Tee & M. Voss
- Cylindrical Mirror Analyzer (CMA)
- Good agreement, except for the 2.17 keV $N_{2,3}$ CE and L3M4M5 Auger lines
- First ever quantitative comparison of CE and Auger yields from $^{99}Mo/^{99m}Tc$



NS_RadList & UncTools

- UncTools: Full MC uncertainty propagation implemented

  output quantity

  - Symmetric: median(standard deviation)
  - Asymmetric: median($+\sigma_{Upp,84\%}$ $-\sigma_{Low,16\%}$)
  - Limit: direct/central value (shape of PDF examined; under testing)

  NOTE: For symmetric or slightly asymmetric PDF, but median is always more accurate approach

- NS_RadList: Atomic radiation spectrum from ENSFF decay data sets
  - Calibration report, plot, new ENSDF records
  - Use UncTools for uncertainty propagation
  - Energy spectrum for dosimetry calculations

- Both codes will be available for beta testing