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Treatment of uncertainties using Monte Carlo (UncTools)

Atomic Radiations in ENSDF (NS_RadList)

T. Kibèdi, B. Tee and B. Coombes (ANU)

Two-state mixing model

E0 strength parameter, ρ^2(E0):

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

^{40}Ca 3353 keV E0

ρ^2(E0)=0.0259(16)

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

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

- ☐ From min/max values of ρ^2(E0) and $\Delta(\beta^2)$
  $\alpha^2_{1,2}$ = 0.31(19) or 0.69(19)
- ☐ Python Uncertainty (analytical, from numerical derivatives)
  $\alpha^2_{1,2}$ = 0.3 (4) or 0.7(4)
- ☐ NIST Uncertainty Machine (Monte Carlo)
  Could not run; negative "b^2-4ac" detected
- ☐ UncTools (Monte Carlo)
  $\alpha^2_{1,2}$ = 0.18(+12-7) or 0.82(+7-12)

Experimental quantitates 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 DX/X values
  - c) Correlations neglected

For multi-variant functions (BrIcc, Ruler, Gabs, Gtol) uncertainty propagation is difficult

Solution: Bayesian (Monte Carlo) uncertainty propagation

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

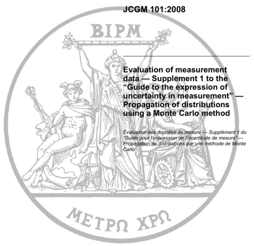
GUM framework

Joint Committee for Guides in Metrology

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 Functions (PDF)
  - Symmetrical UNC: normal
  - Asymmetric UNC: Skewed Normal
  - Limit: rectangular (uniform)

to the values of the input quantities.



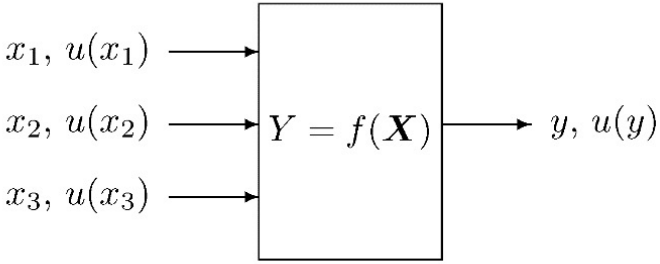
JCGM 101:2008

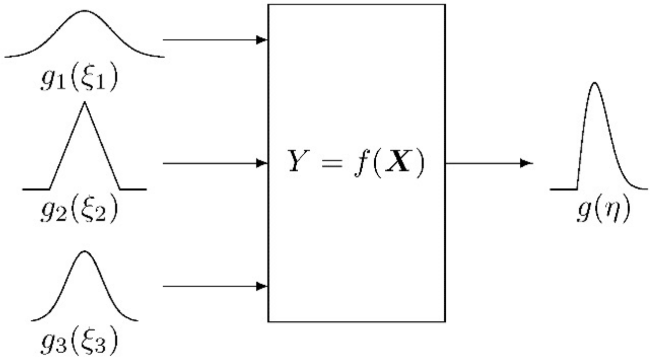
BIPM

Evaluation of measurement data — Supplement 1 to the “Guide to the expression of uncertainty in measurement” — Propagation of distributions using a Monte Carlo method

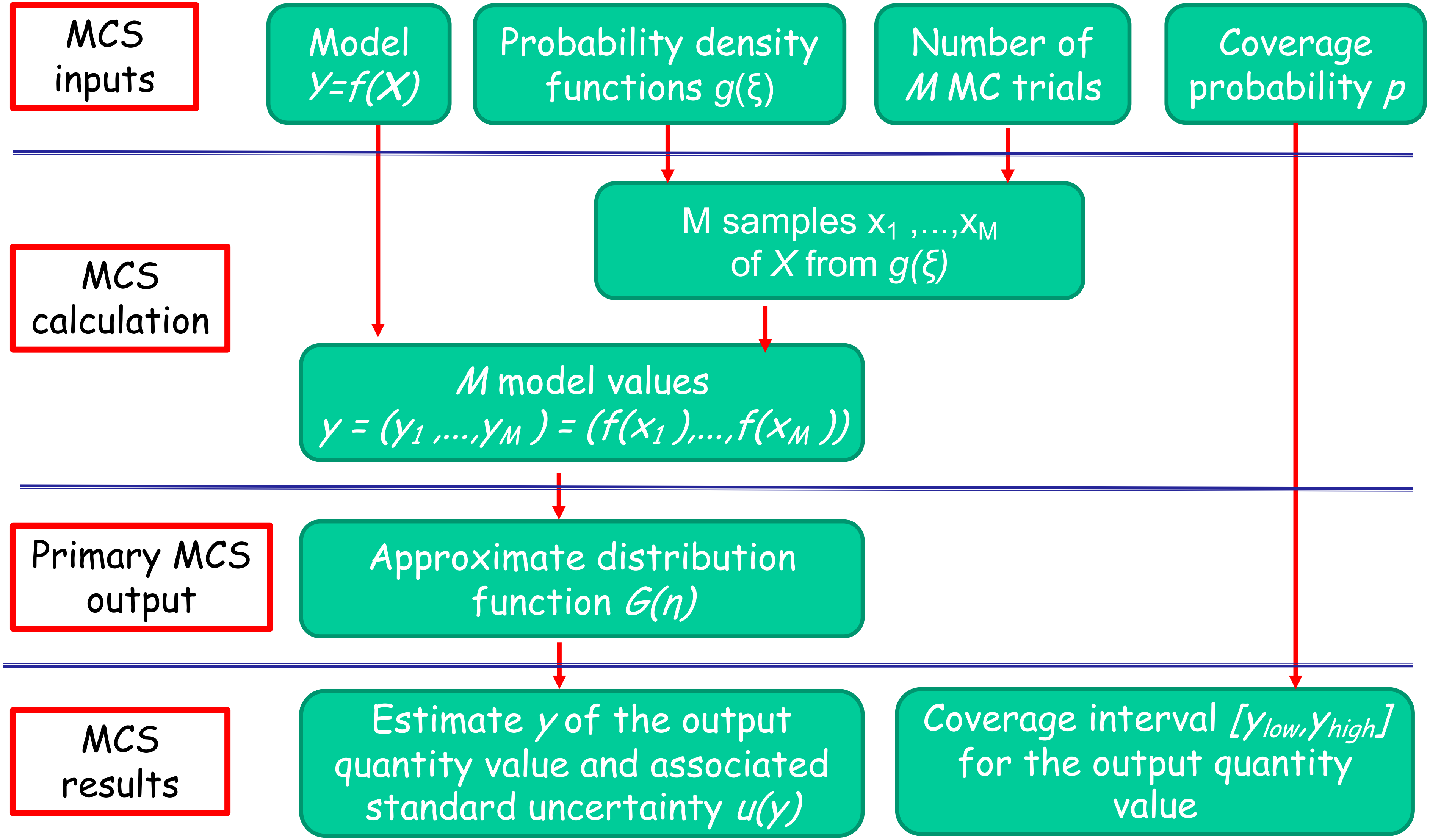
Évaluation des données de mesure — Supplément 1 du “Guide pour l’expression de l’incertitude de mesure” — Propagation de distributions par une méthode de Monte Carlo

METPΩ XPΩ





Monte Carlo simulations to obtain the output quantity



MCS inputs

Model $Y=f(X)$

Probability density functions $g(\xi)$

Number of M MC trials

Coverage probability p

MCS calculation

M samples $x_1,\ldots,x_M$ of X from $g(\xi)$

M model values $y=(y_1,\ldots,y_M)=(f(x_1),\ldots,f(x_M))$

Primary MCS output

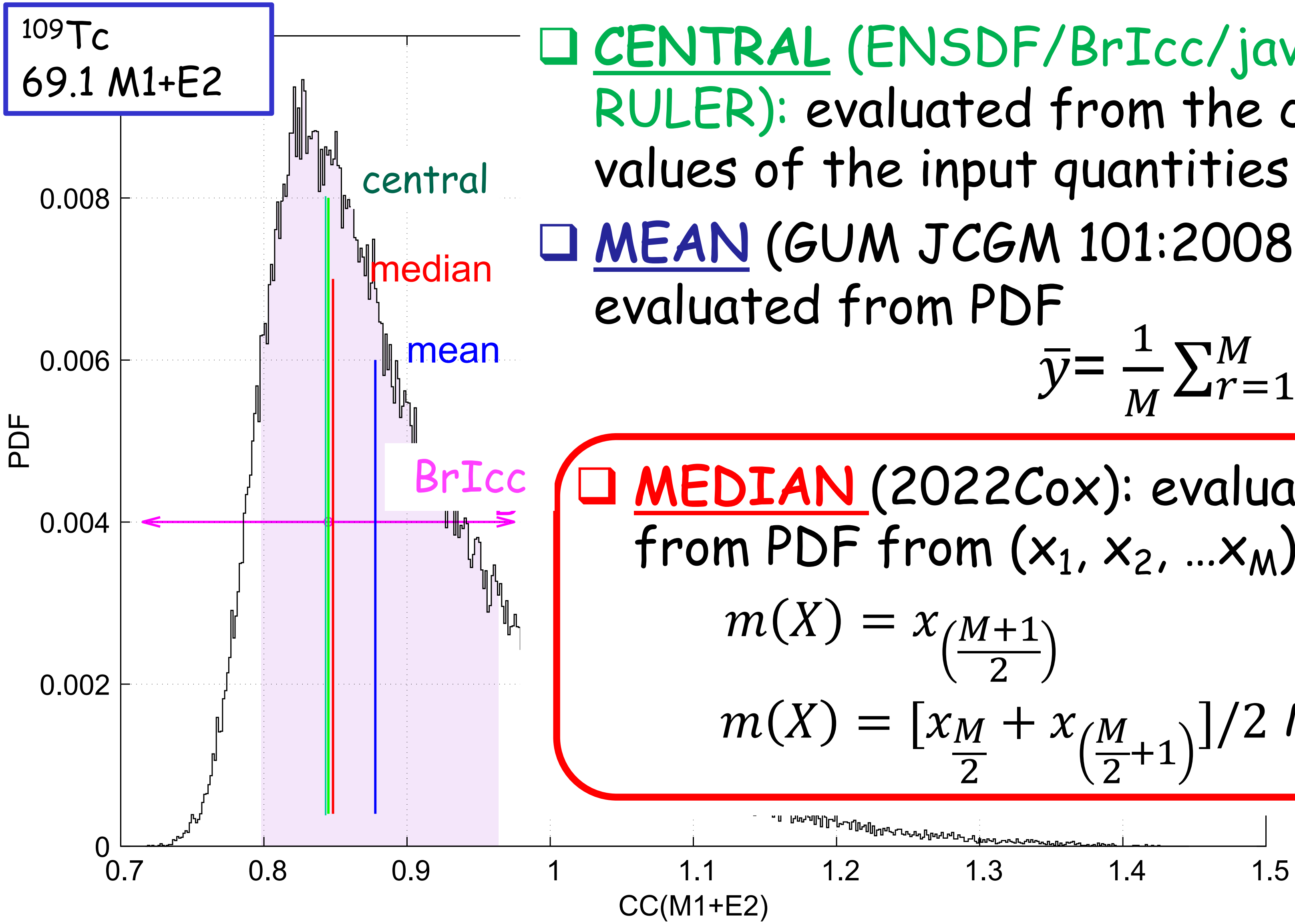
Approximate distribution function $G(\eta)$

MCS results

Estimate y of the output quantity value and associated standard uncertainty $u(y)$

Coverage interval $[y_{low},y_{high}]$ for the output quantity value

Value of the output quantity



- **CENTRAL** (ENSDF/BrIcc/java-RULER): evaluated from the central values of the input quantities
- **MEAN** (GUM JCGM 101:2008): evaluated from PDF

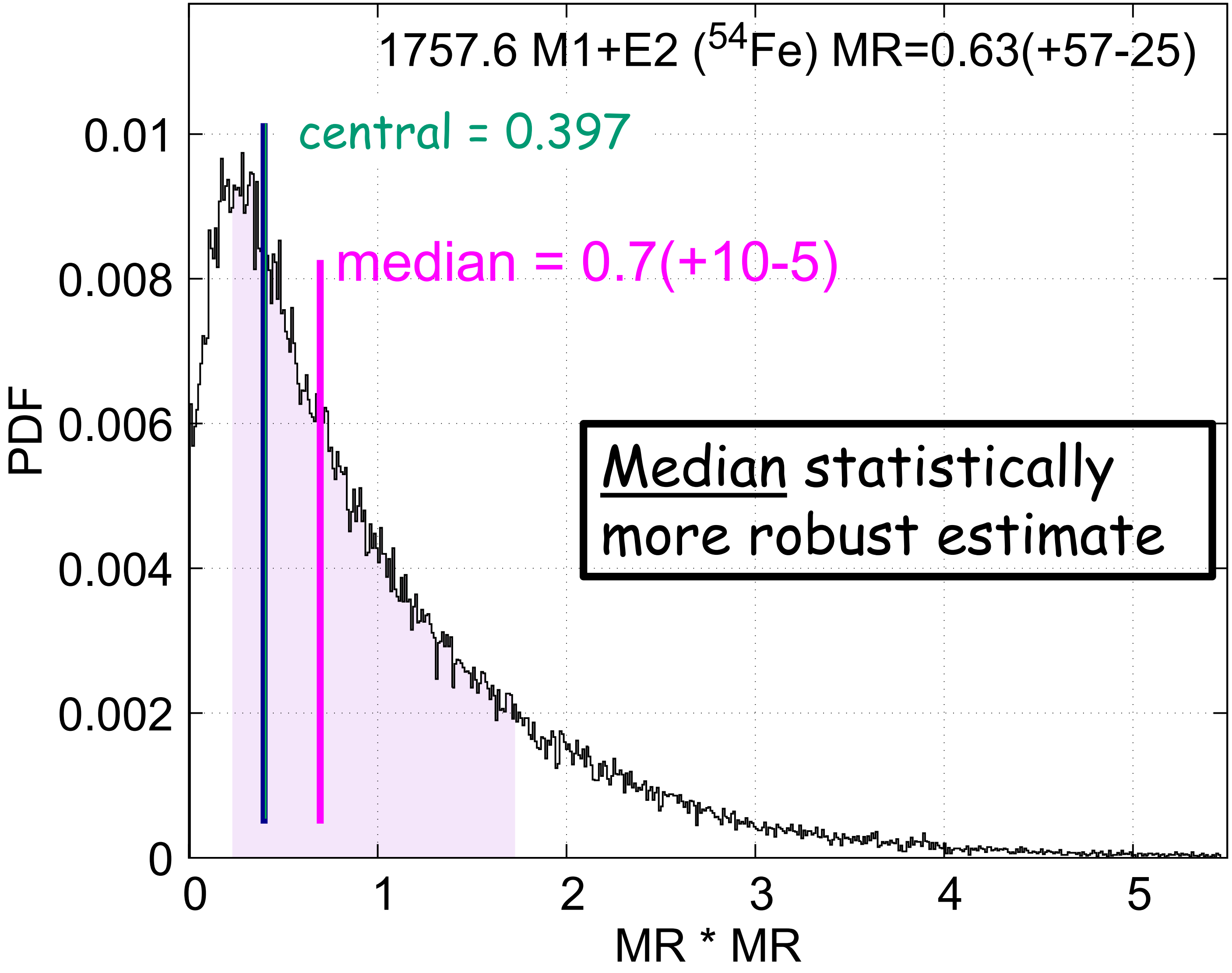
$$\bar{y} = \frac{1}{M}\sum_{r=1}^{M} y_r$$

- **MEDIAN** (2022Cox): evaluated from PDF from $(x_1, x_2, \ldots x_M)$ as

$$m(X) = x_{\left(\frac{M+1}{2}\right)} \quad \text{M odd}$$

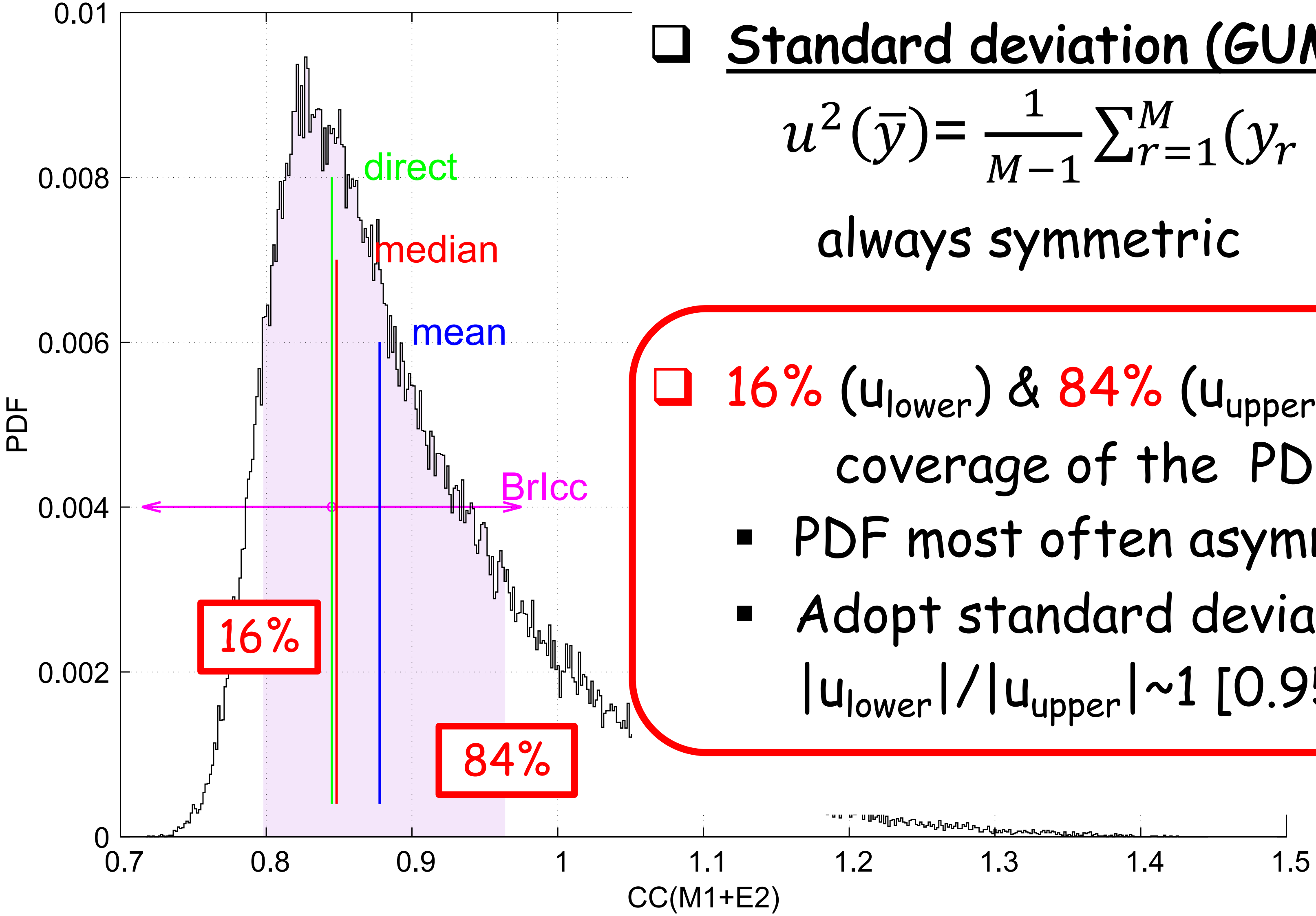
$$m(X) = \left[x_{\frac{M}{2}} + x_{\left(\frac{M}{2}+1\right)}\right]/2 \quad \text{M even}$$

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 $|u_{lower}|/|u_{upper}|$~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

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

BrIcc - calculating mixed ICC MR is unknown

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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%]

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

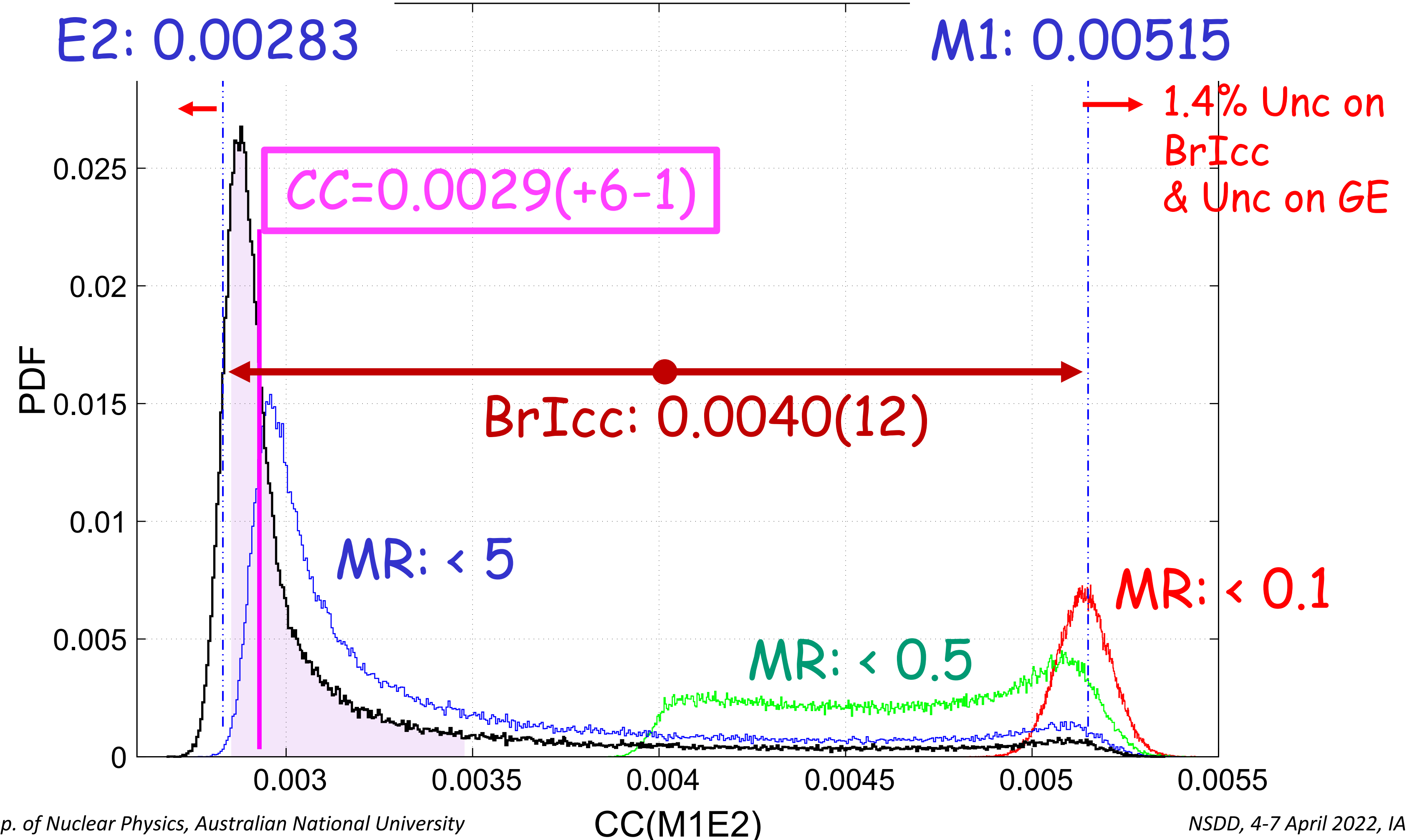
CC = 0.0029(+6-1)

- ☐ 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-record

```
[G_1_E]
[G_1_CC_E2]
[G_1_RI]
```

Samples parameters from G-record, calling BrIcc

```
[EQN]       G1_TI = G_1_RI * (1. + G_1_CC_E2)
```

Calculates TI

```
[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
```

TI to g.s.

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

Calculates NR, BR=1

```
[EQN]       G1_pTI = G_1_RI * NR
```

Calculates %IG

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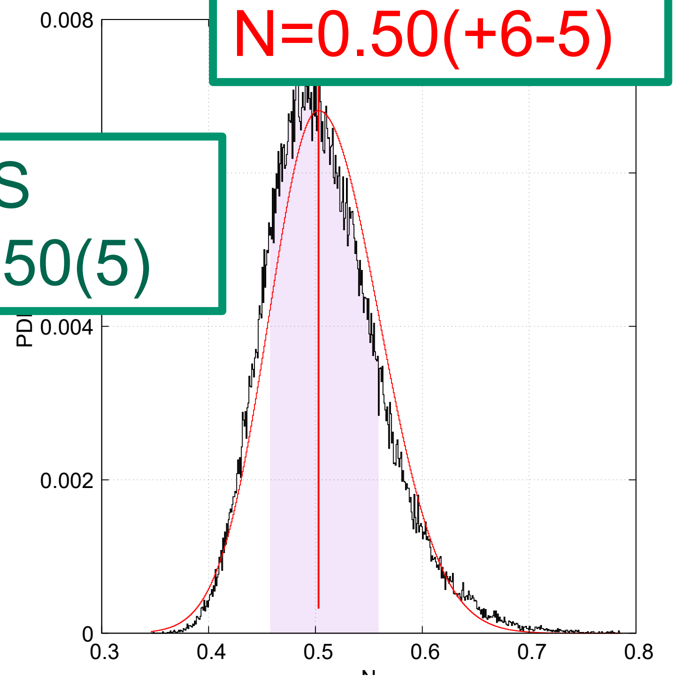
UncTools results

```
[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
```



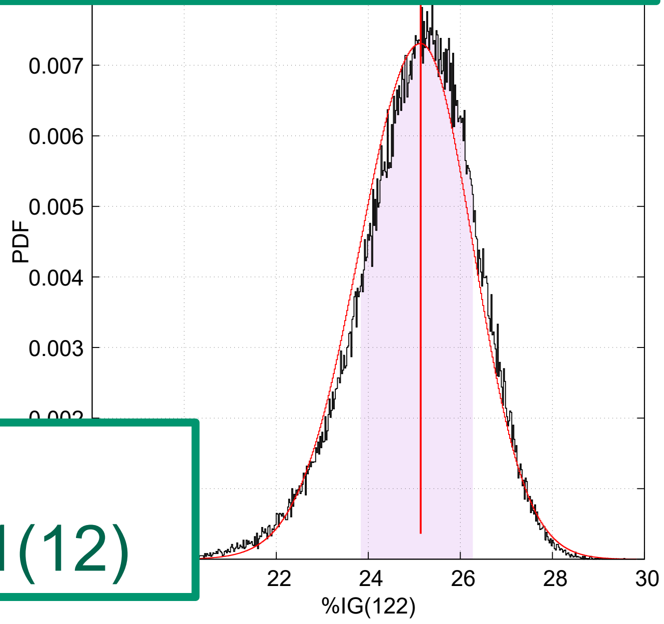
N=0.50(+6-5)

GABS
NR= 50(5)

1

0

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



GABS
%IG(122)=25.1(12)

Tibor Kibèdi, Dep. of Nuclear Physics, Australian National University

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)

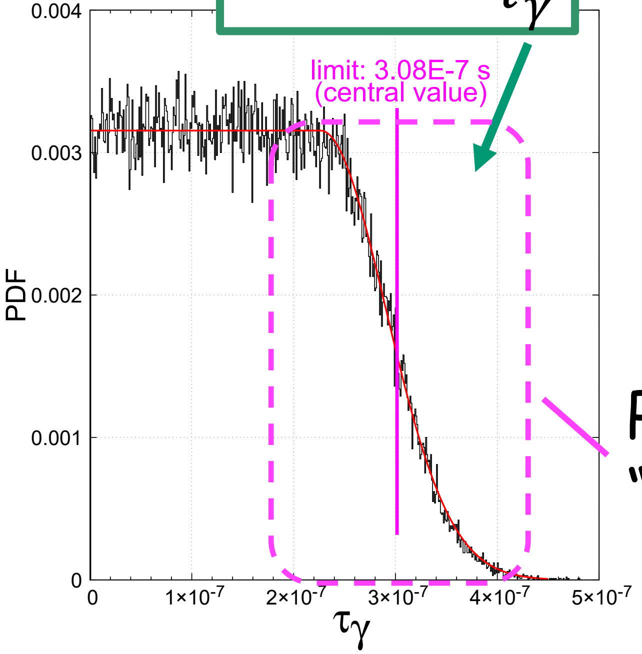
184RE G 637.5   2 158   19(E1)

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

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

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

~0.016% UNC from E_γ



Propagation of the DRI`s "smoothers" the limit

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Comparison with java-Ruler

(version 4-Apr-2022)

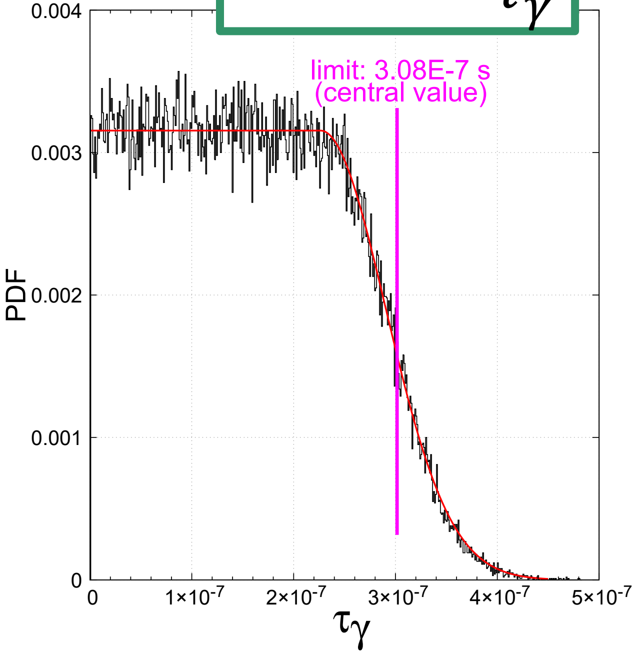
184RE L 825.47 15 (9-) 5 NS LT D

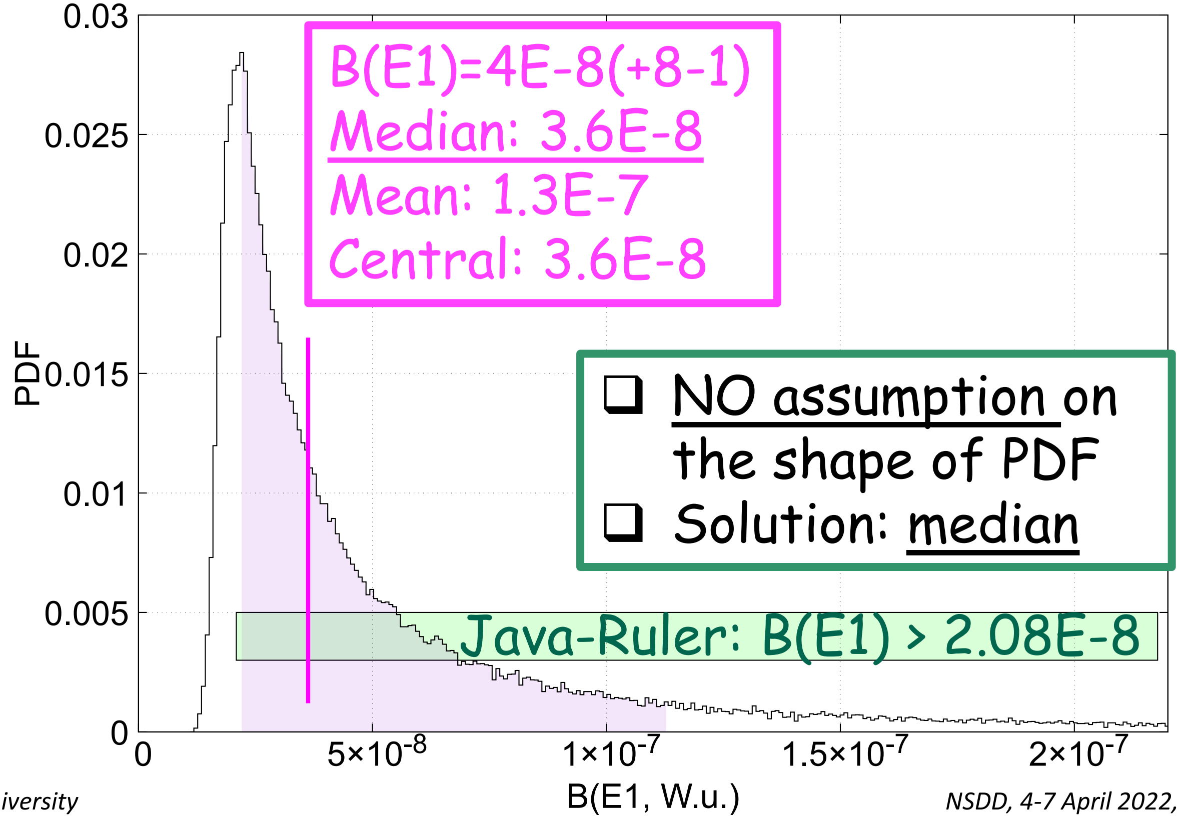
184RE G 379.6 2 3.8 3 (E1)

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

☐ 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

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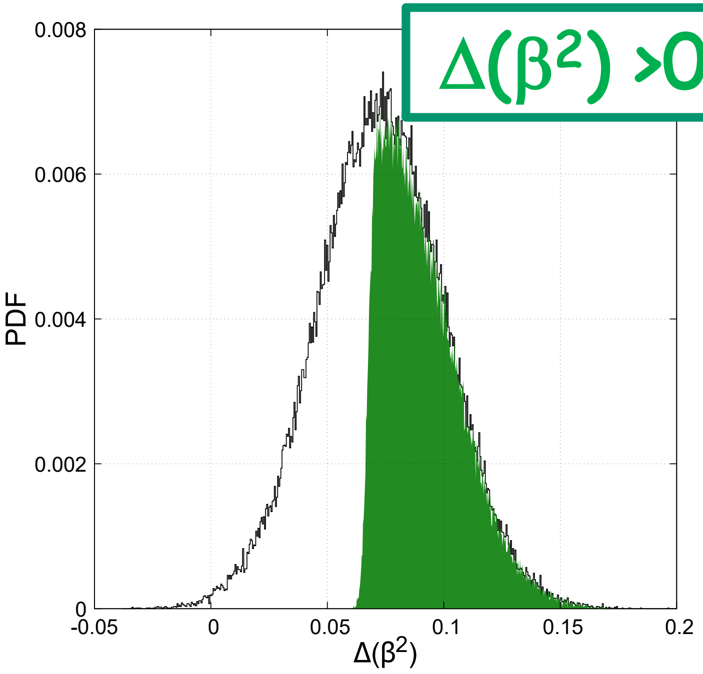
Handling non-physical solutions

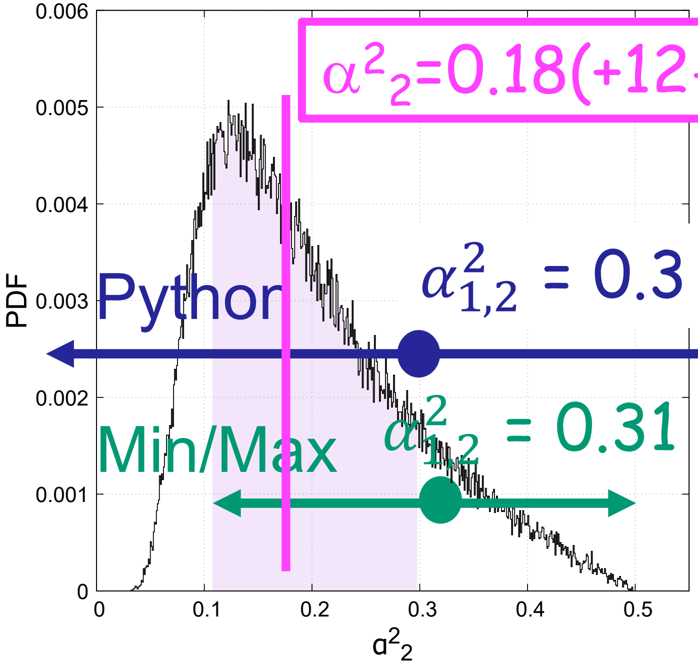
$$\rho^2(E0) = \left(\frac{3}{4\pi}Z\right)^2 \alpha^2(1-\alpha^2)[\Delta(\beta^2)]^2$$

^{40}Ca 3353 keV E0
$\rho^2(E0)=0.0259(16)$
$\Delta(\beta^2)=0.073(27)$

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



$\Delta(\beta^2) > 0.06$



$\alpha^2_2=0.18(+12-7)$

Python $\alpha^2_{1,2}$ = 0.3 (4)

Min/Max $\alpha^2_{1,2}$ = 0.31 (19)

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:

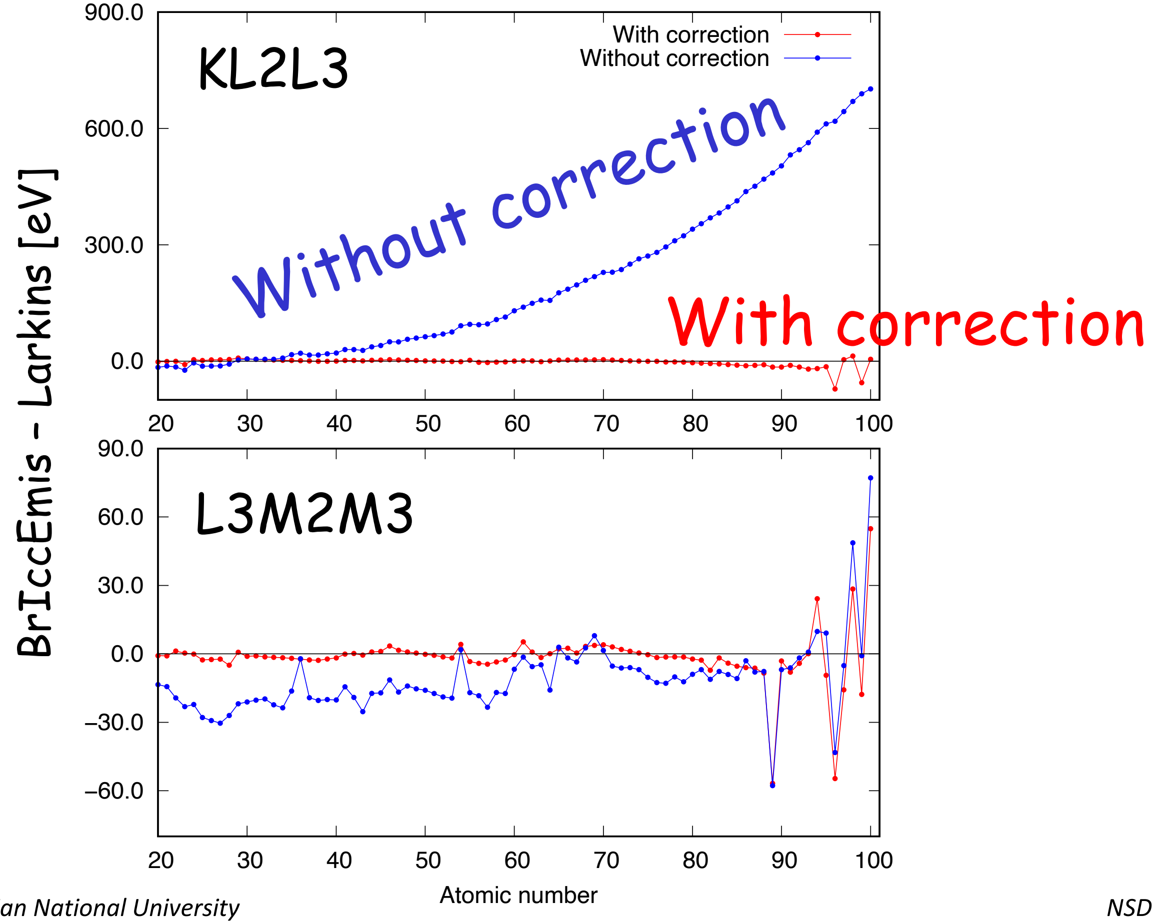
```
unctools <input script> -x
```

- 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

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

```
# 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

```
# X-rays =====================================================
# Transition           Energy [keV]               Probability
#               Mean     95% Confidence range  [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)
```

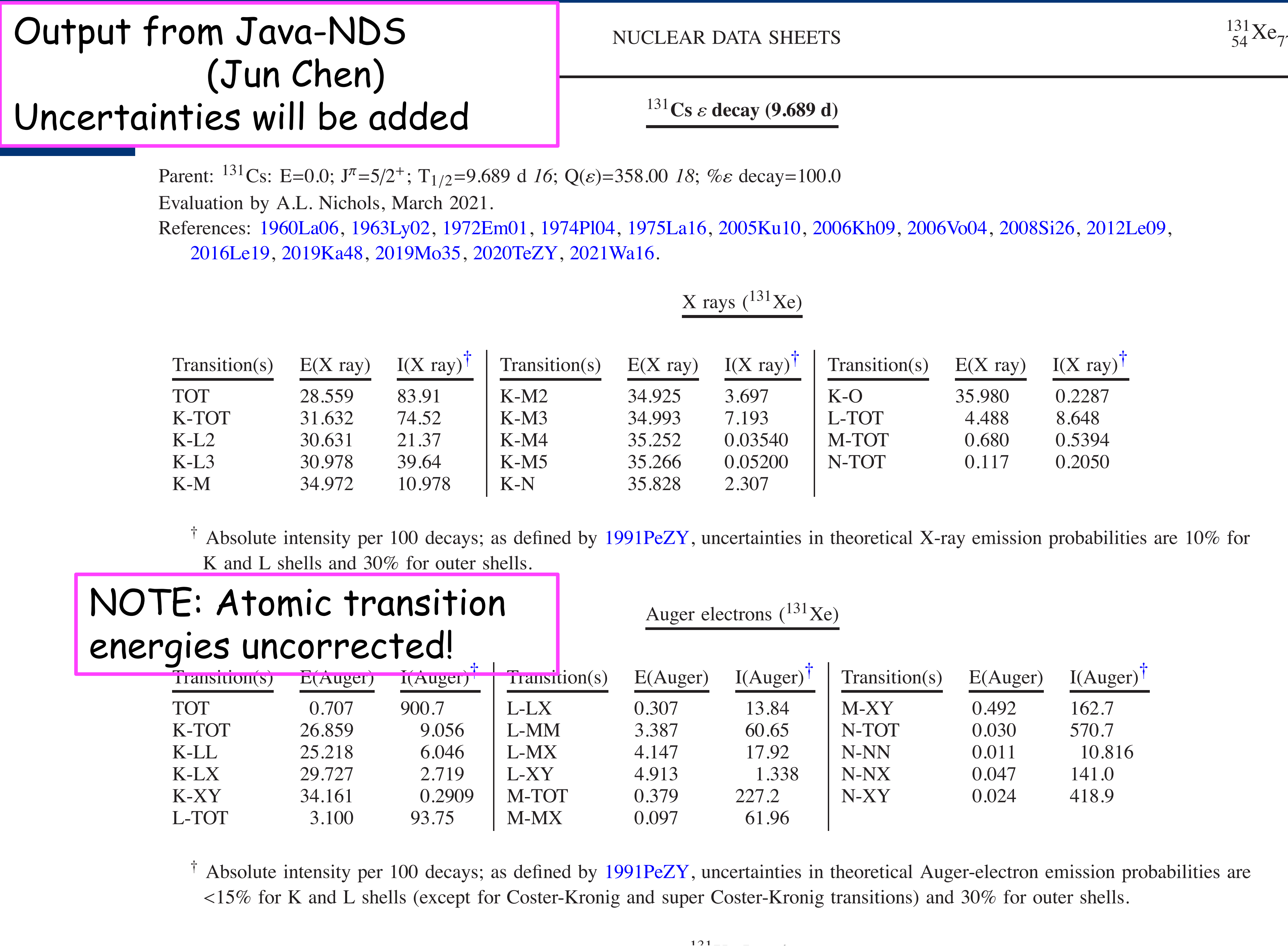
Evaluated from 1 eV binned spectra

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.

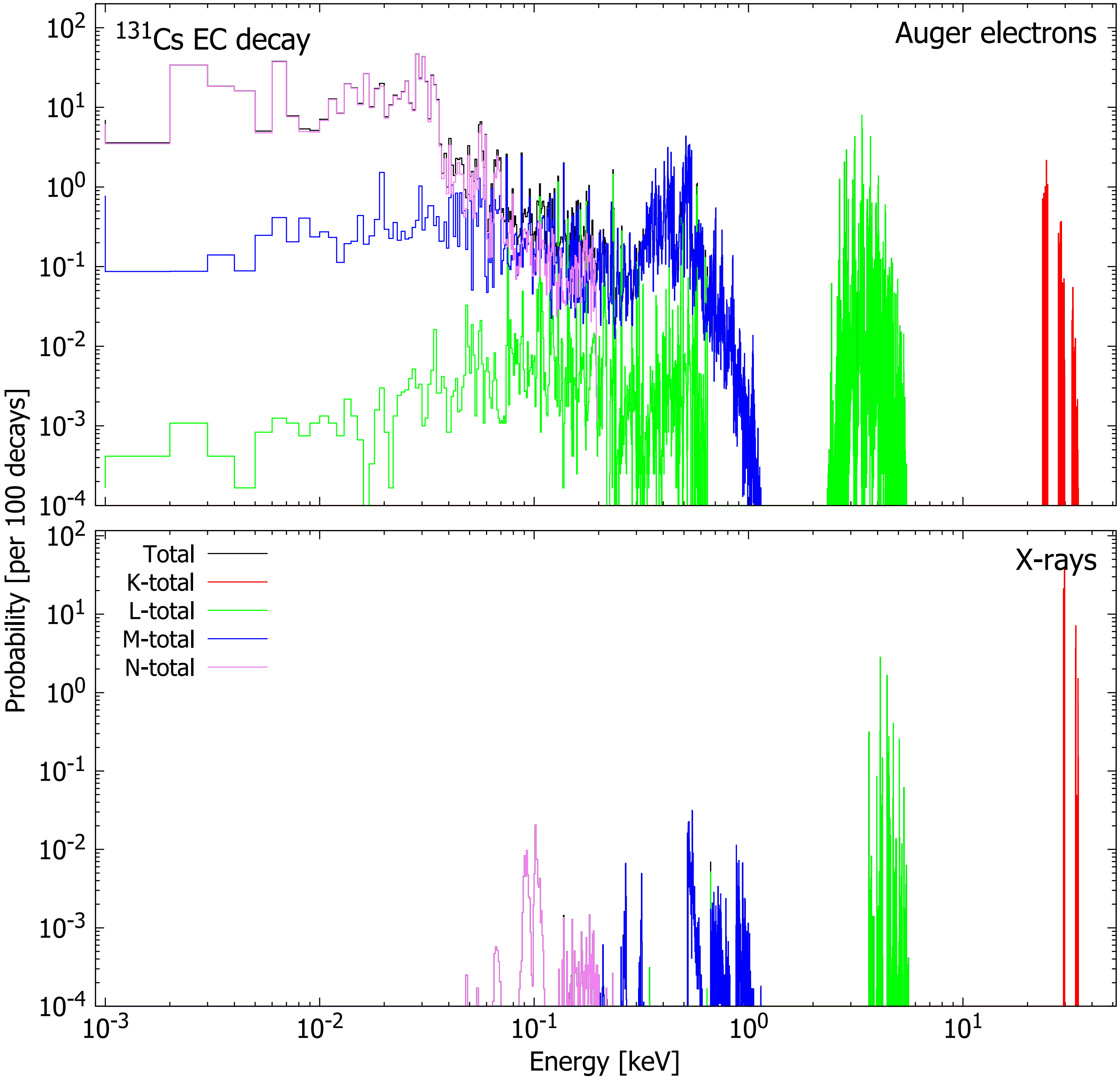
NOTE: Atomic transition energies uncorrected!

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)



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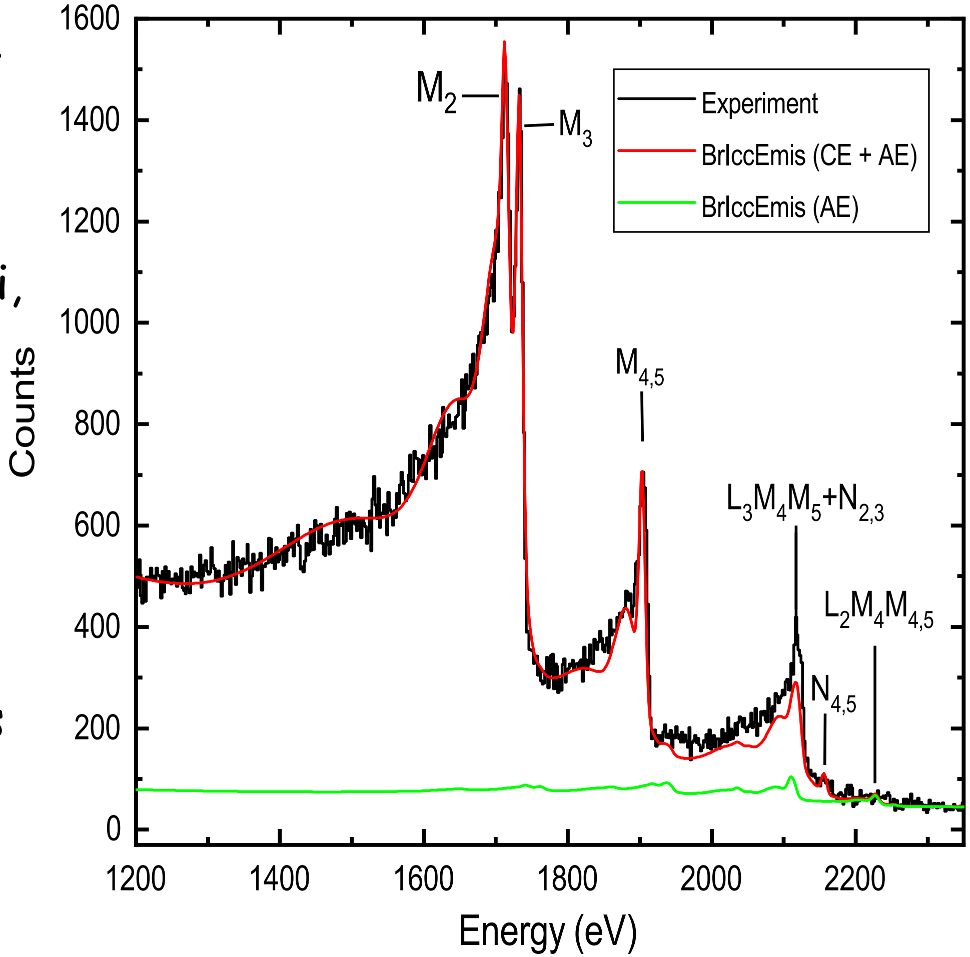
Recent low energy electron measurements – ^{99}Mo/^{99m}Tc

^{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



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NS_RadList & UncTools

- ❑ UncTools: Full MC uncertainty propagation implemented

  output quantity
  - Symmetric: median(standard deviation)
  - Asymmetric: median($+\sigma_{\mathrm{Upp},84\%}$ $-\sigma_{\mathrm{Low},16\%}$)
  - 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