Practical application of Monte Carlo methods, examples of the standardization of $^{55}$Fe

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Activity (of a radionuclide)

Mean number of spontaneous transitions per unit of time
Unit: becquerel

1 Bq = 1 s\(^{-1}\)

There is no method to directly observe (and measure) the occurrence of the disintegration of an atom… but the radiation emitted after the transition can be detected and quantified.
Direct measurement method

• Analyze the radionuclide decay scheme in order to identify the radiation following each decay path (nature, energy, emission probability…)
• Detect this radiation using an ad-hoc detector
• Measure the detector counting rate, \( N \)
• Calculate the detection efficiency, \( R \)

Activity \( A = \frac{N}{R} \)

Uncertainty of \( A = f (N, R) \)
$^{55}$Fe decay scheme
Neglected emissions:
Gamma transition I ~ 10^{-9}
Inner bremsstrahlung I ~ 3 \times 10^{-5}
Radiation detection

Liquid scintillation counter (LSC) :
  • transformation of the ionizing radiation energy in light pulses
  • Light pulse detection with 3 photomultiplier tubes (PMT) in triple and double coincidences

The detection efficiency is a function of the triple to double coincidence ratio (TDCR method)
3 PMT LS counter
TDCR counter (LNHB)

Optical chamber
Detection efficiency, the free parameter model

If an energy $E$ is absorbed in the scintillator, a mean number of photons, $m$, are created and the probability of emission of exactly $x$ photons is:

$$P(x/m) = \frac{m^x e^{-m}}{x!}$$

Detection efficiency is one minus non detection efficiency:

$$R = 1 - P(0/m) = 1 - \frac{m^0 e^{-m}}{0!} = 1 - e^{-m}$$

Detection efficiency is a function of only one parameter, $m$, which is the mean number of photons produced per unit of energy absorbed in the scintillator.
Reality is a little more complicated: the light emission is not proportional to the energy, the PMT’s are not similar, radiation is not monoenergetic and what can be observed is not a photon but a photoelectron produced in a PMT…

* Detection efficiency for 2 PMT’s in coincidence: 

\[ R_D = \int_0^{E_{\text{max}}} S(E) (1 - e^{-\frac{\nu \eta}{3}})^2 \, dE \]

* Detection efficiency for 3 PMT’s in coincidence: 

\[ R_T = \int_0^{E_{\text{max}}} S(E) (1 - e^{-\frac{\nu \eta}{3}})^3 \, dE \]

\[ \eta = \int_0^E \frac{A \, dE}{1 + kB \frac{dE}{dx}} \]

Knowledge of the free parameter \( \nu A \) allows the calculation of the detection efficiency

but how to find out \( \nu A \)?
... using the Triple to Double Coincidence Ratio

\[
\frac{R_T}{R_D} = \frac{\int_{\text{spectrum}} S(E)(1 - e^{-\frac{v\eta}{3}})^3 \, dE}{\int_{\text{spectrum}} S(E)(1 - e^{-\frac{v\eta}{3}})^2 \, dE}
\]

\[\eta = \int_0^E \frac{A dE}{1 + kB \frac{dE}{dx}}\]

For a large number of observations:

\[\frac{R_T}{R_D} \rightarrow \frac{T_{\text{experimental}}}{D_{\text{experimental}}}\]

Numerical solution \[\rightarrow\] \(vA\) \[\rightarrow\] \(R_D\) \[\rightarrow\] Activity
In the real world, the 3 PMT’s are not similar

\[
\begin{align*}
\frac{R_T}{R_{AB}} &= \frac{\int_{\text{spectrum}} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})(1-e^{-\eta_C}) \, dE}{\int_{\text{spectrum}} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B}) \, dE} \\
\frac{R_T}{R_{BC}} &= \frac{\int_{\text{spectrum}} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})(1-e^{-\eta_C}) \, dE}{\int_{\text{spectrum}} S(E)(1-e^{-\eta_B})(1-e^{-\eta_C}) \, dE} \\
\frac{R_T}{R_{AC}} &= \frac{\int_{\text{spectrum}} S(E)(1-e^{-\eta_A})(1-e^{-\eta_B})(1-e^{-\eta_C}) \, dE}{\int_{\text{spectrum}} S(E)(1-e^{-\eta_A})(1-e^{-\eta_C}) \, dE}
\end{align*}
\]

Solution: minimize

\[
\left( \frac{T_{\exp}}{AB_{\exp}} - \frac{T_{\calc}}{AB_{\calc}} \right)^2 + \left( \frac{T_{\exp}}{BC_{\exp}} - \frac{T_{\calc}}{BC_{\calc}} \right)^2 + \left( \frac{T_{\exp}}{AC_{\exp}} - \frac{T_{\calc}}{AC_{\calc}} \right)^2
\]

e.g. by the downhill simplex method
### Spectrum calculation (KLM model)

<table>
<thead>
<tr>
<th>Energy Process</th>
<th>Energy Contribution</th>
<th>Probability Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{K}_x )</td>
<td>( \text{Compton+photoelectric} + \frac{X_L}{A_L} )</td>
<td>( P_{K} \omega_{K} R_{K}^{x} \frac{PK_{x}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{K}_\beta )</td>
<td>( \text{Compton+photoelectric} )</td>
<td>( P_{K} \omega_{K} R_{K}^{\beta} \frac{PK_{\beta}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{Auger K}_\alpha )</td>
<td>( \frac{X_L}{A_L} )</td>
<td>( P_{K} \omega_{K}(1-R_{K}^{\alpha}) \frac{PK_{\alpha}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{Auger K}_\beta )</td>
<td>0</td>
<td>( P_{K} \omega_{K}(1-R_{K}^{\alpha}) \frac{PK_{\beta}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{Auger K}_{XY} )</td>
<td>( \frac{A_{KLL} + \frac{X_L}{A_L} + \frac{X_L}{A_L}}{PK_{\text{tot}}} )</td>
<td>( P_{K}(1-\omega_{K}) \frac{PK_{KLL}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{Auger K}_{LX} )</td>
<td>( \frac{A_{KLL} + \frac{X_L}{A_L}}{PK_{\text{tot}}} )</td>
<td>( P_{K}(1-\omega_{K}) \frac{PK_{KLL}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{Auger K}_{XY} )</td>
<td>( \frac{A_{KXY}}{PK_{\text{tot}}} )</td>
<td>( P_{K}(1-\omega_{K}) \frac{PK_{KXY}}{PK_{\text{tot}}} )</td>
</tr>
<tr>
<td>( \text{L Auger} )</td>
<td>( \frac{X_L}{A_L} )</td>
<td>( P_{L} )</td>
</tr>
<tr>
<td>( \text{M, N} )</td>
<td>0</td>
<td>( 1-(P_{K}+P_{L}) )</td>
</tr>
</tbody>
</table>
### $^{55}$Fe decay data

*Table des radionucléides, LNHB 2002*

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mean value</th>
<th>Standard deviation</th>
<th>Parameter</th>
<th>Mean value</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_K$</td>
<td>0.8853</td>
<td>0.0016</td>
<td>Relative intensity $X_{K\alpha}$</td>
<td>0.8804</td>
<td>0.014</td>
</tr>
<tr>
<td>$P_L$</td>
<td>0.0983</td>
<td>0.0013</td>
<td>Relative intensity Auger KLL</td>
<td>0.775</td>
<td>0.025</td>
</tr>
<tr>
<td>$P_{M,N}$</td>
<td>1-(P$_K$+P$_L$)</td>
<td>0.0008</td>
<td>Relative intensity Auger KLX</td>
<td>0.211</td>
<td>0.006</td>
</tr>
<tr>
<td>$\omega_K$</td>
<td>0.321</td>
<td>0.007</td>
<td>Relative intensity Auger KXY</td>
<td>0.0141</td>
<td>0.0004</td>
</tr>
<tr>
<td>$\omega_L$</td>
<td>0.0053</td>
<td>0.0004</td>
<td>$X_{K\alpha}$ energy</td>
<td>5.895 keV</td>
<td></td>
</tr>
<tr>
<td>$\omega_{M,N}$</td>
<td>0</td>
<td>0</td>
<td>$X_{K\beta}$ energy</td>
<td>6.153 keV</td>
<td></td>
</tr>
<tr>
<td>Auger L energy</td>
<td>0.57 keV</td>
<td></td>
<td>Auger KLL energy</td>
<td>5.08 keV</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Auger KLX energy</td>
<td>5.78 keV</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Auger KXY energy</td>
<td>6.42 keV</td>
<td></td>
</tr>
</tbody>
</table>
Calculation of the energy absorbed by the scintillator

Hypothesis:

• Auger electrons: totally absorbed
• $X_L$: totally absorbed
• $X_K$: absorbed energy calculated by MC model

Dominant parameters:

• $P_K$, $P_L$, $P_{M,N}$ (available energy after electron capture)
• $\omega_K$ ($X_K$ emission probability)
Stochastic model of X ray absorption
Penelope (Salvat et al.)

- Aluminum
- Polymer
- Air
- Glass
- Liquid scintillator
Scintillator composition
(ICRM LSCWG web page)

**Elementary composition of the samples**

It is useful to have the elementary composition of the scintillator in order to calculate the electron linear energy transfer and photon-interaction cross-sections.

It is necessary to calculate the scintillator-water sample composition individually, using for example, the following compositions kindly provided by J. Thomson, Perkin-Elmer (formerly Packard Bioscience).

**Stoichiometric composition and density of various Perkin-Elmer LS-cocktails (stoichiometric formula)**

(source: J. Thomson, Perkin-Elmer, formerly Packard Bioscience)

<table>
<thead>
<tr>
<th>Element</th>
<th>C</th>
<th>H</th>
<th>N</th>
<th>O</th>
<th>P</th>
<th>S</th>
<th>Na</th>
<th>d at 20 °C g/cm³</th>
<th>Z/A</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ultima Gold</td>
<td>16,81</td>
<td>24,54</td>
<td>0,040</td>
<td>1,52</td>
<td>0,11</td>
<td>0,02</td>
<td>0,02</td>
<td>0,98</td>
<td>0,5459</td>
<td>255,76</td>
</tr>
<tr>
<td>Ultima Gold XR</td>
<td>18,11</td>
<td>29,80</td>
<td>0,035</td>
<td>2,83</td>
<td>0,11</td>
<td>0,03</td>
<td>0,03</td>
<td>0,99</td>
<td>0,5476</td>
<td>297,98</td>
</tr>
<tr>
<td>Ultima Gold AB</td>
<td>18,67</td>
<td>28,49</td>
<td>0,010</td>
<td>2,53</td>
<td>0,01</td>
<td>0,00</td>
<td>0,00</td>
<td>0,98</td>
<td>0,5485</td>
<td>293,47</td>
</tr>
<tr>
<td>Ultima Gold LLT</td>
<td>18,57</td>
<td>28,43</td>
<td>0,010</td>
<td>2,56</td>
<td>0,01</td>
<td>0,00</td>
<td>0,00</td>
<td>0,98</td>
<td>0,5486</td>
<td>292,68</td>
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<tr>
<td>Insta-Gel Plus</td>
<td>18,53</td>
<td>30,93</td>
<td>0,006</td>
<td>3,90</td>
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<td>0,00</td>
<td>0,95</td>
<td>0,5490</td>
<td>315,71</td>
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<tr>
<td>Hionic-Fluor</td>
<td>10,83</td>
<td>18,77</td>
<td>0,060</td>
<td>1,97</td>
<td>0,18</td>
<td>0,04</td>
<td>0,04</td>
<td>0,95</td>
<td>0,5449</td>
<td>188,87</td>
</tr>
</tbody>
</table>
The TDCR method in short

AB, BC, AC

T
kB
$dE\over dx$

Energy spectrum, $S(E)$

Radiation matter interaction calculation (Monte Carlo)

Disintegration scheme $P_K, P_L, P_M, \omega_K, \ldots$
Scintillator composition, geometry

Numerical model

Activity
Uncertainty evaluation
The holly GUM, ca. end of XX century

1. **Measurement model**
   (i.e. transfer function between input data and output results)
   \[
   y = f(x_1, x_2, \ldots, x_n)
   \]

2. **Evaluation of standard deviations of input parameters**
   (experimental values, parameters, *etc.* and covariances)

3. **Combination of standard deviations and covariances**

   \[
   u_c^2(y) = \sum_{i=1}^{n} \left( \frac{\partial f}{\partial x_i} \right)^2 \cdot u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\partial f}{\partial x_i} \cdot \frac{\partial f}{\partial x_j} \cdot u(x_i, x_j)
   \]
Experimental standard deviations, $^{103}\text{Pd}$

- Double coincidences, $D$
- Triple coincidences, $T$
- $\text{TDCR} = \frac{T}{D}$

\[
\begin{align*}
    s_D^2 &= \frac{1}{n-1} \sum_{i=1}^{n} (D_i - \bar{D})^2 \\
    s_T^2 &= \frac{1}{n-1} \sum_{i=1}^{n} (T_i - \bar{T})^2 \\
    s_{DT}^2 &= \frac{1}{n-1} \sum_{i=1}^{n} (D_i - \bar{D})(T_i - \bar{T}) \\
    s_{\text{TDCR}}^2 &= \text{TDCR} \sqrt{\frac{s_T^2}{T^2} + \frac{s_D^2}{D^2} - \frac{2s_{DT}}{DT}}
\end{align*}
\]
Covariance matrix of input data, $^{55}$Fe

<table>
<thead>
<tr>
<th></th>
<th>D</th>
<th>TDCR</th>
<th>$P_K$</th>
<th>$P_L$</th>
<th>$P_M$</th>
<th>$\omega_K$</th>
<th>$\omega_L$</th>
<th>$A_{KLL}/A_K$</th>
<th>$A_{KLX}/A_K$</th>
<th>$A_{KXY}/A_K$</th>
<th>$K_{\alpha}/K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>exp</td>
<td>calc</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TDCR</td>
<td>exp</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$P_K$</td>
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<td></td>
<td>2.5E-06</td>
<td>-6.0E-07</td>
<td>-6.0E-07</td>
<td>0</td>
<td>0</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$P_L$</td>
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<td></td>
<td>1.7E-06</td>
<td>-6.0E-07</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>$P_M$</td>
<td></td>
<td></td>
<td>4.00E-06</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\omega_K$</td>
<td></td>
<td></td>
<td>5.0E-05</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\omega_L$</td>
<td></td>
<td></td>
<td>1.6E-07</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$A_{KLL}/A_K$</td>
<td></td>
<td></td>
<td></td>
<td>6.0E-04</td>
<td>1.0E-04</td>
<td>1.0E-04</td>
<td>0</td>
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<tr>
<td>$A_{KLX}/A_K$</td>
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<td></td>
<td>4.0E-05</td>
<td>1.0E-04</td>
<td>0</td>
<td>0</td>
<td></td>
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</tr>
<tr>
<td>$A_{KXY}/A_K$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.6E-07</td>
<td>0</td>
<td></td>
<td></td>
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<td>2.0E-04</td>
</tr>
<tr>
<td>$K_{\alpha}/K$</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>
Measurement transfer function

AB, BC, AC

T
kB
\( \frac{dE}{dx} \)

Energy spectrum, \( S(E) \)

Numerical algorithm

Activity

Combination of standard deviations?
1. Numerical evaluation of sensitivity coefficients
2. Monte Carlo evaluation
1 Sensitivity coefficients, partial derivatives

$$\frac{\partial F(x_1, x_2, \ldots, x_n)}{\partial x_i} = \frac{F(x_1, \ldots, x_i + h, \ldots x_n) - F(x_1, \ldots, x_i - h, \ldots, x_n)}{2h}$$

• If $\varepsilon_F$ is the relative bias of the evaluation of $F$ around $x_i$
• If $h$ is optimal
  • Then the relative bias of the derivative is about $(\varepsilon_F)^{2/3}$

In practice, from 6 to 12 calculations of $F$ are necessary to calculate the derivative (Numerical recipes, Press et al.)
2 Monte Carlo method

- Mean value of each parameter
- Covariance matrix
- Probability distribution of each parameter
- Random generator

$n$ sets of input data

\[\begin{align*}
&AB_1 \\
&BC_1 \\
&AC_1 \\
&T_1 \\
&kB_1 \\
&S(E)_1 \\
&\text{etc.}
\end{align*}\]

\[\begin{align*}
&AB_2 \\
&BC_2 \\
&AC_2 \\
&T_2 \\
&kB_2 \\
&S(E)_2 \\
&\text{etc.}
\end{align*}\]

\[\begin{align*}
&AB_3 \\
&BC_3 \\
&AC_3 \\
&T_3 \\
&kB_3 \\
&S(E)_3 \\
&\text{etc.}
\end{align*}\]

\[\begin{align*}
&AB_n \\
&BC_n \\
&AC_n \\
&T_n \\
&kB_n \\
&S(E)_n \\
&\text{etc.}
\end{align*}\]

$n$ calculations

Numerical model

$n$ results

- mean

Probability distribution of the results?

- Standard deviation
How to calculate input data sets?

*Experimental data : AB, BC, AC, T*

The measurement is repeated \( m \) times (ex : \( m=10 \)) to get \( m \) values of \((AB, BC, AC, T)\)

1\(^{st}\) method:
- calculation of the means \( M_{AB}, M_{BC}, M_{AC}, M_T \) and experimental standard deviations \( s_{AB}, s_{BC}, s_{AC} \) and \( s_T \)
- Gaussian (or other) probability distribution of the values is assumed
- a random generator is used to produce an arbitrary number \( n \) of data sets \((AB_1, BC_1, AC_1, T_1), (AB_2, BC_2, AC_2, T_2), \ldots\)
How to calculate input data sets?

2\textsuperscript{nd} method (bootstrap):
• random sort of a data set in the \(m\) sets \((AB_x, BC_x, AC_x, T_x)\)
• repeat the procedure and get another (or the same) data set \((AB_y, BC_y, AC_y, T_y)\).
• repeat the procedure \(n\) times to get \(n\) data sets \((AB_1, BC_1, AC_1, T_1), (AB_2, BC_2, AC_2, T_2),...\)
Input data set

Parameters and theoretical values: $kB$, $dE/dx$, decay scheme parameters...

• If an evaluation of the mean $M$ and the standard deviation $s$ of the parameter is available → calculate $n$ Gaussian fluctuations of the parameter: $G(M,s)$

• If an estimation of the realistic interval of the values of the parameter $[a, b]$ is available → calculate $n$ uniform fluctuations of the parameter: $U[a,b]$  

• If there are good reasons to consider another probability distribution of the parameter, an ad-hoc random generator is used…(cf. § 6.4.1 supplement 1)
Tool box

- Random number generators
- Fitting algorithms
- Various calculation algorithms

- Advantage: models, algorithms and programs are explicit... no black box effect.

- Drawback: this needs more effort to use than « user-friendly-magical-do-everything » software packages...
Random number generators

**Uniform**: example « Ran » from Numerical recipes, pseudo-random, period $\sim 3.10^{57}$

```cpp
struct Ran {
    Ullong u,v,w;
    Ran(Ullong j) : v(4101842887655102017LL), w(1) {
        u = j ^ v; int64();
        v = u; int64();
        w = v; int64();
    }
    inline Ullong int64() {
        u = u * 2862933555777941757LL + 7046029254386353087LL;
        v ^= v >> 17; v ^= v << 31; v ^= v >> 8;
        w = 4294957665U*(w & 0xffffffff) + (w >> 32);
        Ullong x = u ^ (u << 21); x ^= x >> 35; x ^= x << 4;
        return (x + v) ^ w;
    }
    inline Doub doub() { return 5.42101086242752217E-20 * int64(); }
    inline Uint int32() { return (Uint)int64(); }
};
```

You can find better ones… and probably a lot worse!
Random number generators

Other distributions, transformation method

From a uniform random number $x$, calculate a random number $y$, with a probability density function $p(y)dy$

$$p(y(x)) = p(x)\left.\frac{dx}{dy}\right|$$

Sort $x \sim U[0,1]$

Get $y$ with a $p(y)$ distribution
Random numbers generator

Other distributions, rejection method

Choose $f(y)$ for $f(y) > p(y)$ and calculate $\int_{0}^{y} f(y)dy$

Sort $x \sim U[0,1]$

Get $y$

Sort $z \sim U[0,f(y)]$

If $z < p(y)$ keep $z$

Si $z > p(y)$ discard $z$
Random numbers generators

Other distributions, method of the ratio of uniform distributions

- Build in the $x,y$ plane a domain bounded by $0 \leq x \leq [p(y/x)]^{1/2}$
- Sort uniform random numbers $x$ and $y$ in this domain
- $y/x$ is a random number with a distribution $p$

Example: Gaussian distribution

Program Normaldev, Numerical Recipes
Difficulties: correlated data

Example: $AB$ and $T$

1\textsuperscript{st} method : uncorrelate data by considering $(AB-T)$ and $T$

2\textsuperscript{nd} method : use a multivariate Gaussian random number generator
Correlated parameters

Example $P_K$, $P_L$ et $P_M$

$$\sum_i P_i = 1$$

Consider than $P_K$ and $P_L$ are not correlated and calculate

$$P_M = 1 - (P_K + P_L)$$

A strict calculation requires the covariance matrix… which is not given in the decay data evaluation files
Practical considerations

*Monte Carlo does not mean brute force extensive calculation...*

It is useful to first try a short sensitivity study to evaluate the weight of the parameter in the final result.

**Example, parameter $\alpha$:**

Make 2 calculations with $\alpha_{\text{min}}$ and $\alpha_{\text{max}}$ keeping constant all the others parameters and observe the result variation. If this variation is small (compared to the order of magnitude of the required final uncertainty), do not vary $\alpha$ in the MC procedure.
Going back to $^{55}\text{Fe}$

Activity $A = \frac{N}{R}$

Counting uncertainty is negligibly small behind the uncertainty of the calculated detection efficiency. This is good news because this justify to only consider the uncertainty of the detection efficiency (and simplifies a lot the problem as detection efficiency is a function of $T/D$, so is correlated with counting rates)

MC procedure using Gaussian and uniform distributions
55Fe, Gaussian input parameters

Fe-55 Gaussian fluctuations n=1E4

Detection efficiency (D)

Frequency

$\varepsilon_D = 0.5219 \pm 0.0008$
$^{55}$Fe, Gaussian input parameters

![Gaussian fluctuations n=1000](image)
$^{55}\text{Fe}$, uniform input parameters

$$\varepsilon_D = 0.5222 \pm 0.0012$$
$^{55}$Fe, uniform input parameters

![Graph showing Uniform fluctuations n=1000](image)

Detection efficiency (D) vs Frequency plot.
Comments on the PDF’s of input data

Selection rules:
• physical
• best estimate (maximum of entropy, guesswork)

For $^{55}\text{Fe}$ a posteriori analysis shows that 2 parameters are the dominant contributors to the uncertainty, so:
• uniform PDF’s give triangular PDF of the results
• Gaussian PDF’s give Gaussian PDF of the results

The PDF of the results is, in this case, a direct consequence of the PDF’s of the input data. As the choice of the PDF of the input data is questionable, it may be useful to ask ourselves if the knowledge of the PDF of the results gives any additional information on the uncertainty of the measurement...
Conclusions

When the measurement function is not explicit, the MC uncertainty evaluation procedure is the best (and sometimes only) possible approach. As shown in supplement 1, the MC procedure is fully compatible with the GUM philosophy.

**Advantages:**
- Simple numerical methods which could be easily implemented in the program used for the calculation of detection efficiency
- Input data or parameter could have large fluctuations (uncertainties)
- The measurement function can be non-linear

**But:**
- The evaluation of input parameters uncertainties and covariance is not trivial. Simplifications are often necessary…
- The PDF of the results is often an image of the PDF’s of the input data… or is just a good illustration of the central limit theorem!
My personal conclusion 1

Uncertainties are generally evaluated from (more or less) known data, parameters and models and subjective considerations are sometimes necessary. It is generally admitted that the relative uncertainty of the uncertainty is about 30 % (for a serious evaluation) ...and we can live with this in most cases.

This must encourage pragmatic approach, allow the use of simplifications and give some good arguments to avoid endless discussions on the performance of random generators...

Uncertainty is just an expression of the doubt on the result. The main point is to express this doubt in a way that is understood by everybody (i.e. using the GUM concepts)...
My personal conclusion 2

I am not sure that the PDF of the result evaluated by a MC method gives much more information on the uncertainty than the value of its mean and standard deviation… The shape of this PDF is just a direct consequence of the PDF’s of the input data, which are surely not univocal. You just get what you deserve!

Moreover, I think that it would be dangerous to extend the uncertainty concept to the PDF of the result because it would ruin all the efforts done during the last 20 years to uniform uncertainty evaluation in metrology.

Uncertainty evaluation is too important to be left to statisticians!