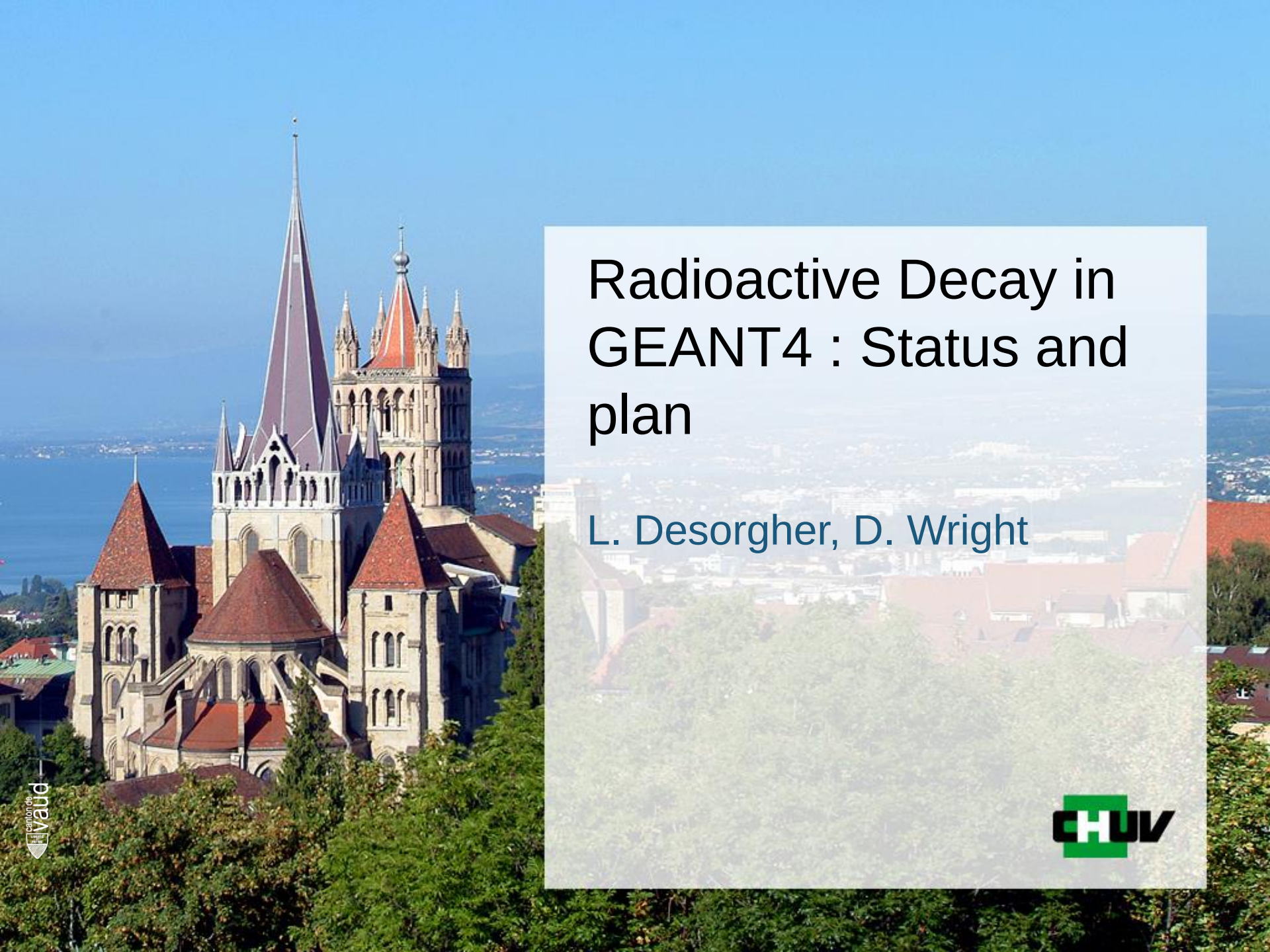


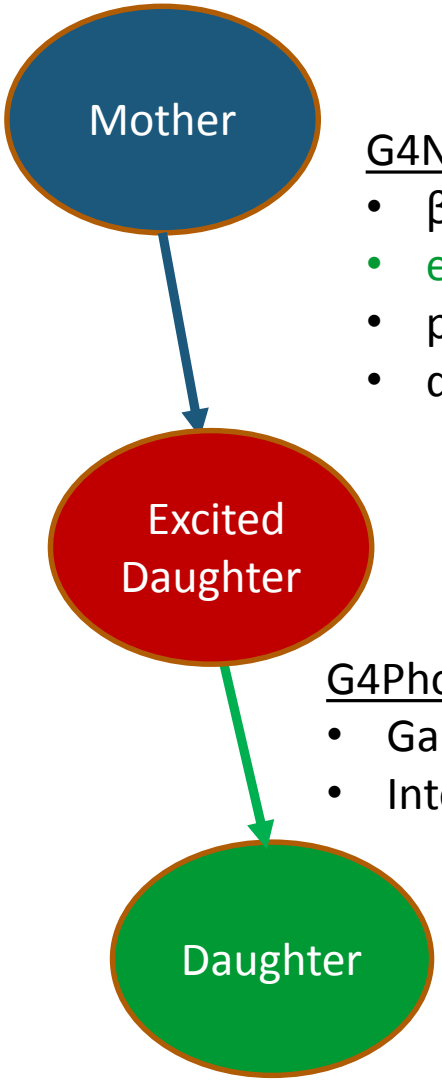
Radioactive Decay in GEANT4 : Status and plan

L. Desorgher, D. Wright

Outline

- Radioactive Decay in GEANT4
- Correction and validation of biasing mode
- Improvement of electron capture
- Status of database
- Validation
- Plan

Radioactive module in Geant4



G4NuclearDecay

- β^-,β^+, α
- e^- capture K,L, M, + N
- p,n emission
- discrete β^- n delayed

G4PhotoEvaporation

- Gamma transition
- Internal conversion

G4AtomicRelaxation

- Xrays emission
- Auger emission

Two simulation modes

- Analog
- Biased

Contributors

- P. Truscott
- F. Lei
- D. wright
- L. Desorgher
- L. Sarmiento
- V. Ivanchenko
- M. Maire

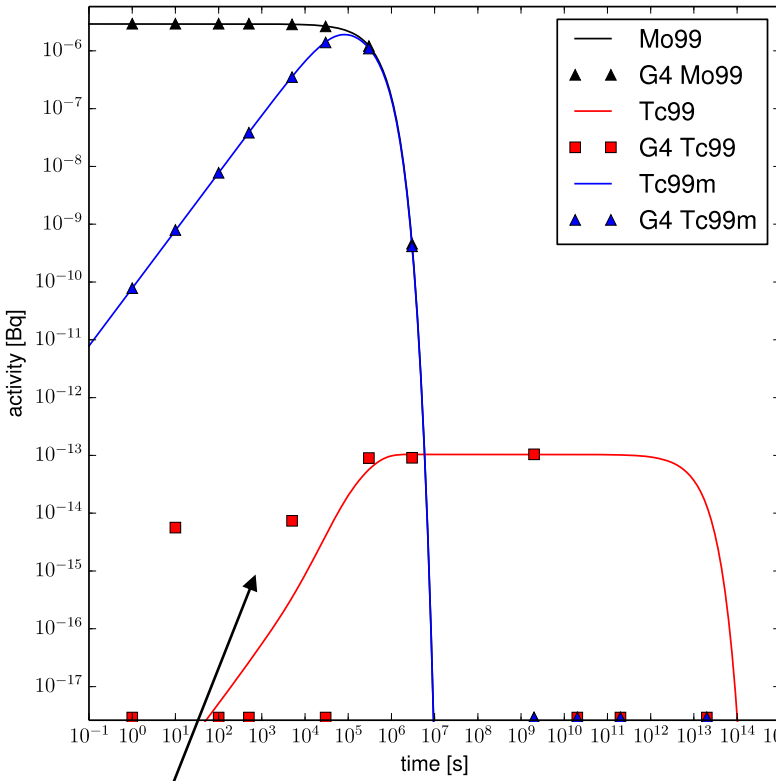
Correction of biased mode of G4RadioactiveDecay

Dennis wright

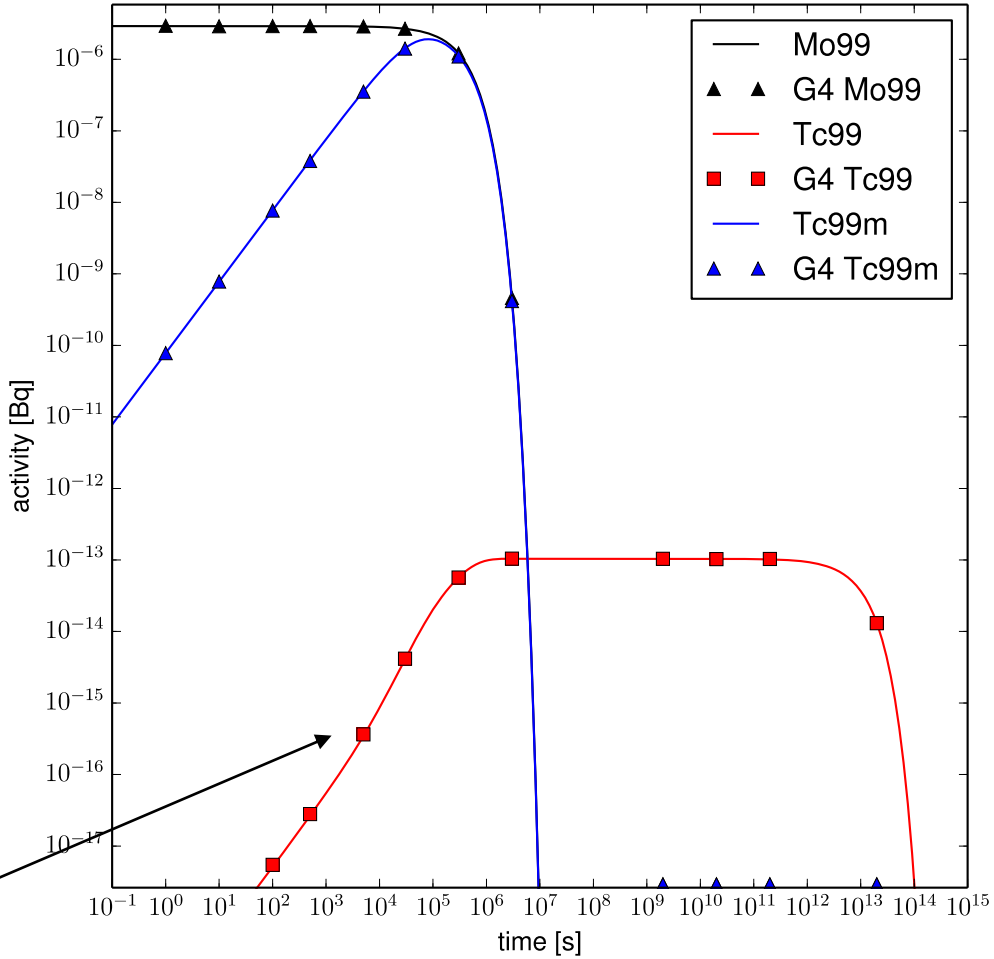
- GEANT4 biasing mode capability:
  - Compute radioactive decay products and activity of isotopes in user defined time window
  - Convolution of MC results with time beam profile
  - Solving of Bateman equations

- Issue in computation of weight
  - Issue with weight correction factor $1 - \exp(x) \quad (x\ small)$
  - Accumulation of weight errors give negative weights
  - Correction by using more precise exponential computation expm1 C++11 function

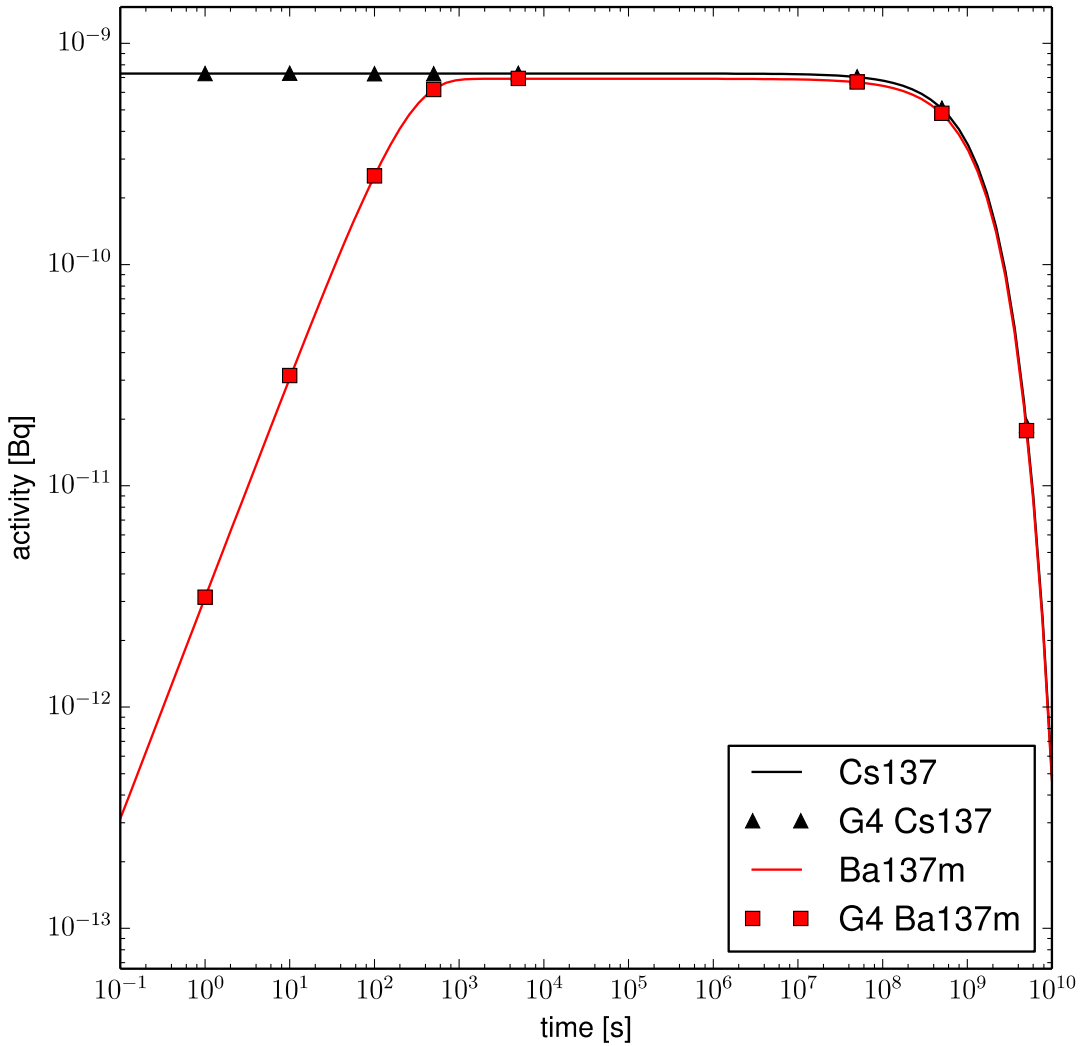
Validation of biased mode of G4RadioactiveDecay



After correction



Validation biasing mode of G4RadioactiveDecay ^{137}Cs



Improvment of electron capture

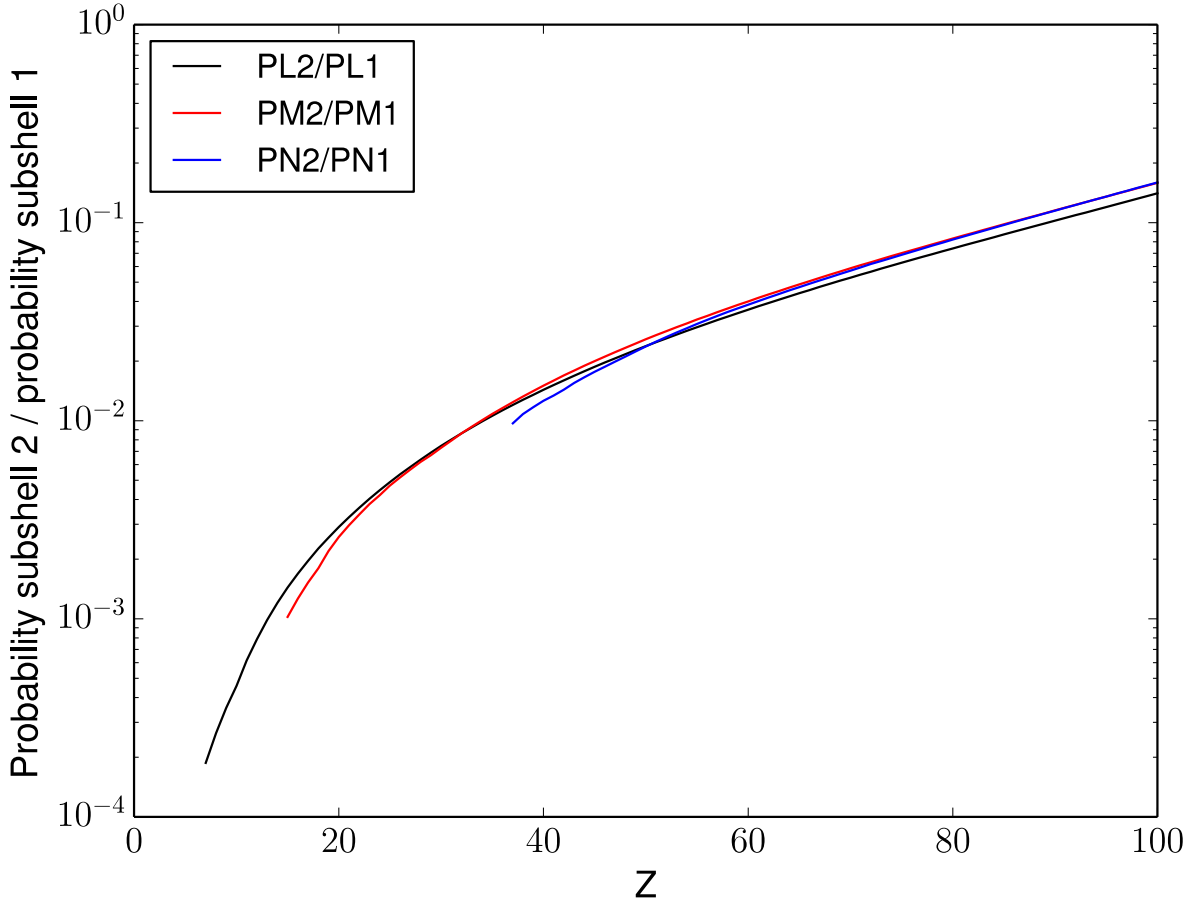
L. Desorgher

Extension of G4ECapture to the N Shell

```
# 125I ( 59.400 D )
# Excitation flag Halflife Mode Daughter Ex flag Intensity Q
P 0 - 5132765
        MshellEC 0 0.0349
        KshellEC 0 0.8011
        LshellEC 0 0.1561
        NshellEC 0 0.0079
        MshellEC 35.4925 - 3.49 150.2775
        KshellEC 35.4925 - 80.11 150.2775
        LshellEC 35.4925 - 15.61 150.2775
        NshellEC 35.4925 - 0.079 150.2775
P 2350.52 - 1.6e-09
        IT 0 1
```

Improvment of electron capture

- Improve the probability of partial probability of capture from subshell
  - Probability to L3,M3,N3 and above is 0
  - Valid for allowed transition
  - PL2/PL1 PM2/PM1 and PN2/PN1 taken from Bambynek et al. 1971



Minor updates of the databases

RadioactiveDecay5.3
Few nuclei corrected

PhotoEvaporation 5.3
Few nuclei corrected

G4ENSDFSTATE2.2
No changes

Validation work

- Analyse of all secondaries in function of decay type
  β, α, γ, INC e-, Xrays, Auger

- Add decay mode as model index to the secondary

- Comparison against:
  - Decay Data Evaluation Project (DDEP)
  - Nudat2 if no data in DDEP
  - Code Beta shape for the β electron spectrum (X. Mougeot @ CEA)

DDEP Table ^{55}Fe

LNE – LNHB/CEA **Table de Radionucléides**

$^{55}_{26}$Fe$_{29}$

$^{55}_{26}$Fe$_{29}$

1 Decay Scheme

Fe-55 disintegrates by electron capture. A gamma transition with a small probability ($1{,}3 \times 10^{-7}$ %) has been observed. A background radiation, due to an inner-bremsstrahlung, with an intensity relative to K capture of $3{,}24(6) \times 10^{-5}$ photons produces a continuous spectrum up to 231,21 keV.

Le Fe-55 se désintègre par capture électronique. Une transition gamma de faible probabilité a été observée. Un rayonnement de freinage interne produit une émission radiative, dont la probabilité relative à la capture électronique K est de $3{,}24(6) \times 10^{-5}$.

2 Nuclear Data

$T_{1/2}(^{55}\mathrm{Fe})$	:	2,747	(8)	a
$Q^{+}(^{55}\mathrm{Fe})$	:	231,21	(18)	keV

2.1 Electron Capture Transitions

	Energy keV	Probability × 100	Nature	lg ft	P_K	P_L	P_{M+}
$\epsilon_{0,1}$	105,26 (18)	0,00000013 (1)	2nd Forbidden	14,2			
$\epsilon_{0,0}$	231,21 (18)	100	Allowed	6	0,8853 (16)	0,0983 (13)	0,0163 (8)

3 Atomic Data

3.1 Mn

ω_K	:	0,321	(7)
$\bar{\omega}_L$	:	0,0047	(7)
$\bar{\omega}_M$	:	0,000027	(2)
n_{KL}	:	1,478	(4)
$\bar{n}_{LM}$	:	1,996	(8)

4 Electron Emissions

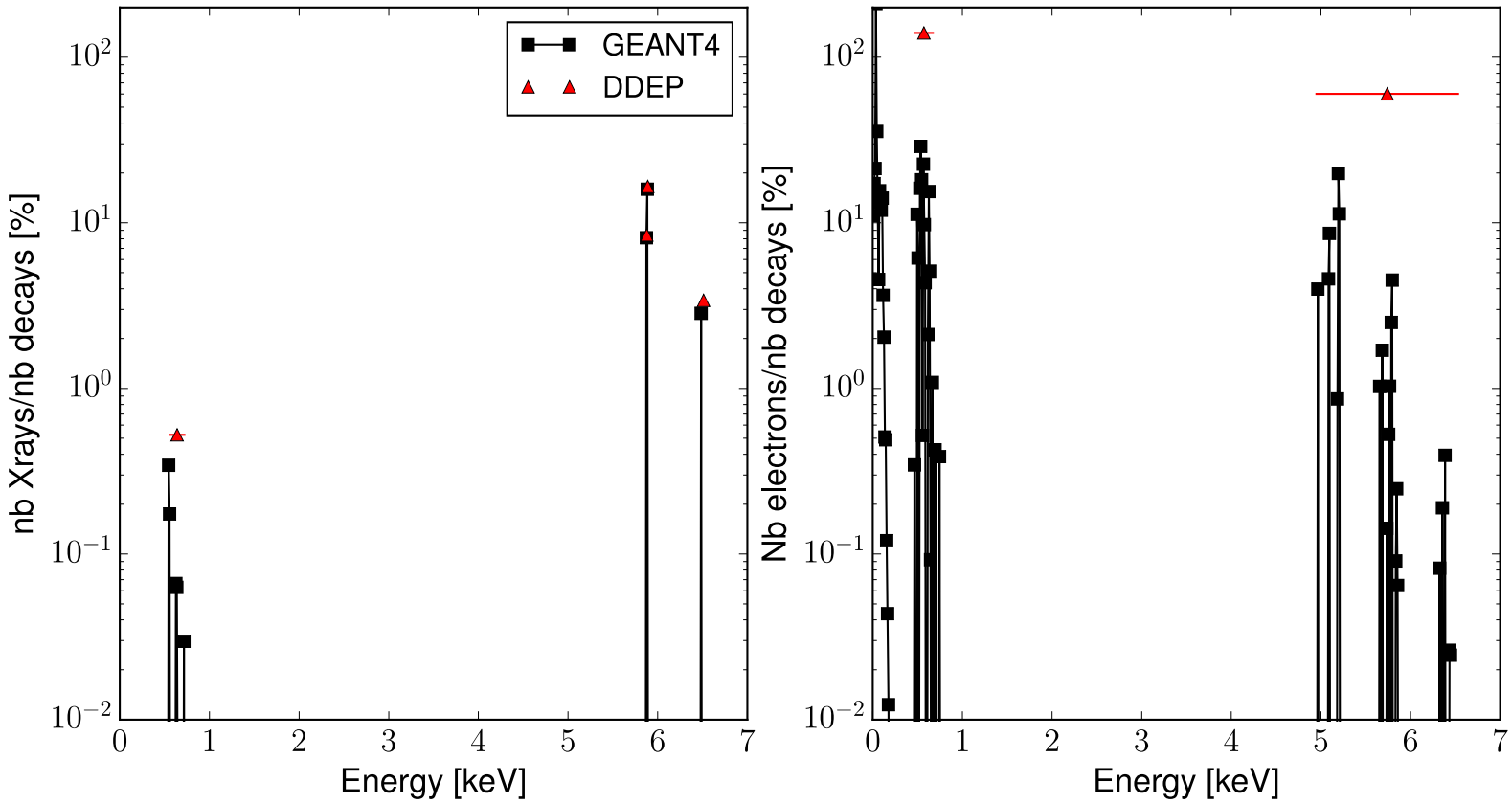
		Energy keV		Electrons per 100 disint.
e_{AL}	(Mn)	0,47 - 0,67		140,2 (8)
e_{AK}	(Mn)			60,1 (5)
	KLL	4,953 - 5,210	}	
	KLX	5,671 - 5,895	}	
	KXY	6,370 - 6,532	}	

5 Photon Emissions

5.1 X-Ray Emissions

		Energy keV		Photons per 100 disint.	
XL	(Mn)	0,556 — 0,721		0,524 (21)	
XKα_2	(Mn)	5,88765		8,45 (14)	} Kα
XKα_1	(Mn)	5,89875		16,57 (27)	}
XKβ_3	(Mn)	6,49045	}		
XKβ_1	(Mn)		}	3,40 (7)	K$'\beta_1$
XKβ_5''	(Mn)	6,5352	}		
XKβ_4	(Mn)		}		K$'\beta_2$

Comparison Geant4 and DDEP data for ^{55}Fe



Comparison Geant4 and DDEP data for ^{55}Fe

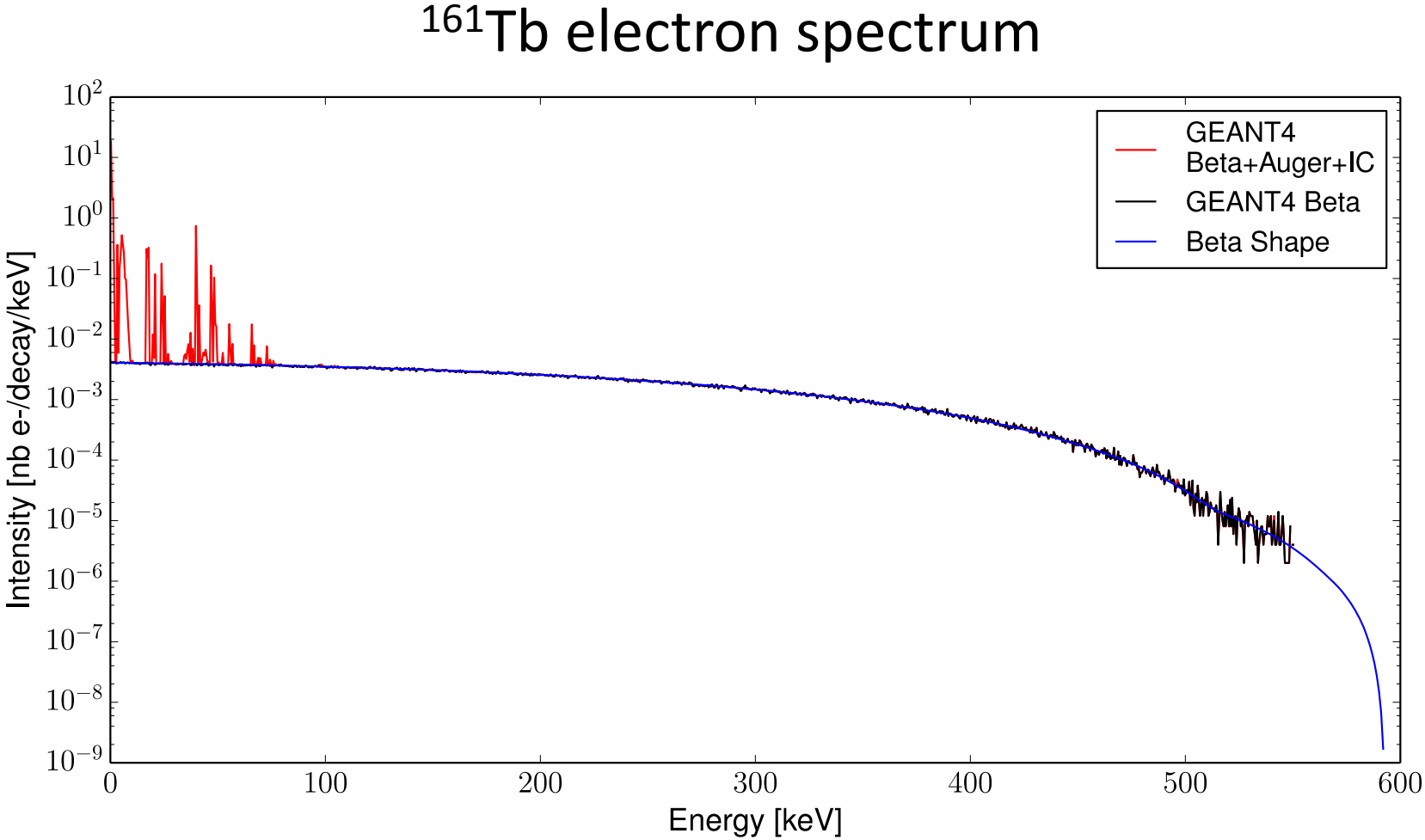
Emission type	Geant4 AtomicRelax default %	Geant4 AtomicRelax modified %	DEEP %
Xrays $K\alpha_1$	15.93	16.57	16.57
Xrays $K\alpha_2$	8.12	8.46	8.45
Xrays $K\beta$	2.89	3.4	3.4
Xrays L	0.65	0.527	0.524
Auger K	61.59	60.1	60.1
Auger L	143.17	141.6	140.2

Need to change atomic relaxation data in GEANT4 to have same emission probability than in DDEP

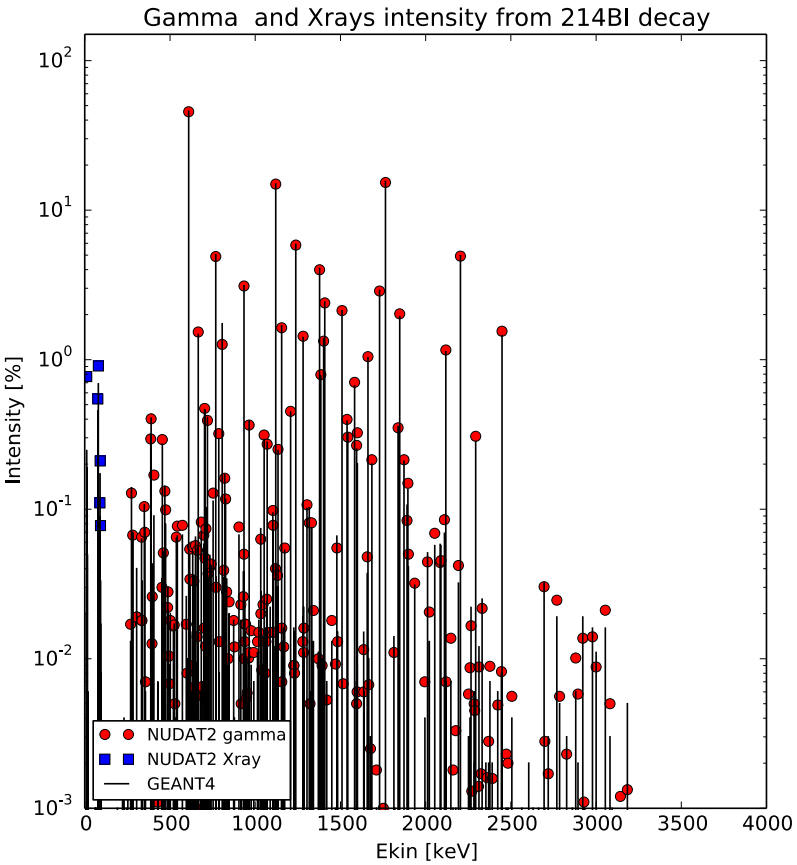
Comparison Geant4 and DDEP data for ^{54}Mn

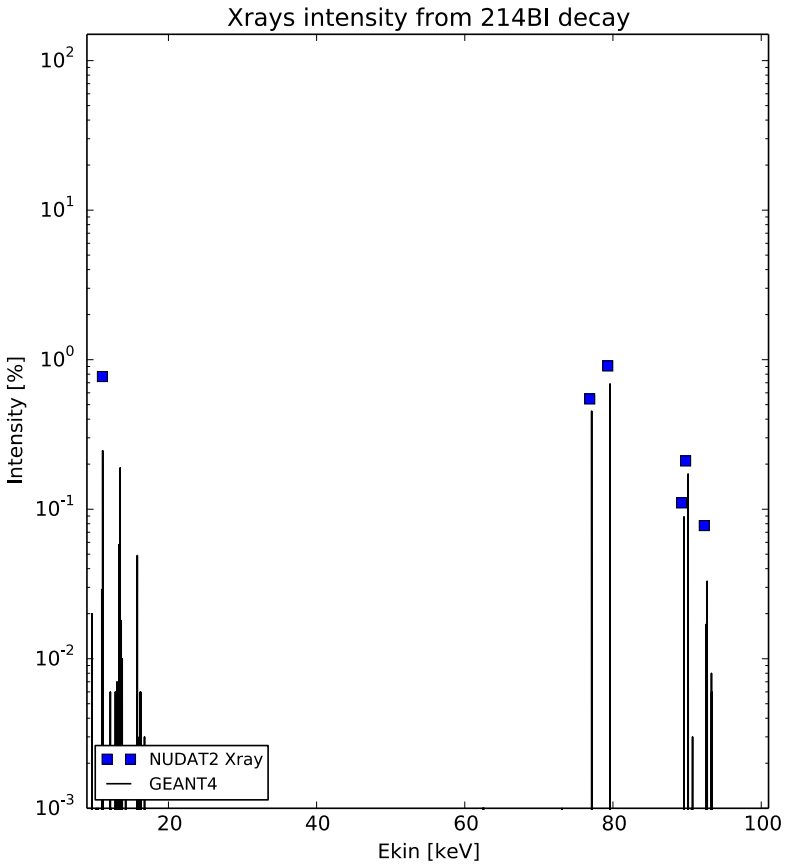
Emission type	Geant4 modified %	DEEP %
γ 834.848 keV	99.977	99.975
Xrays $K\alpha_1$	15.04	15.02
Xrays $K\alpha_2$	7.63	7.65
Xrays $K\beta$	3.03	3.05
Xrays *L*	0.65	0.65
Auger *K*	63.3	63.3
Auger *L*	144.6	143
IC e- K	0.021	0.022
IC e- L	0.0015	0.002

Validation beta spectrum



^{214}Bi vs Nudat2





G4RadioactiveDecay Status and Plan

GEANT4.10.5

- RDM biasing improvements D. Wright
- Improvments Electron Capture L. Desorgher
- Maintenance of the RDM & PhotoEvaporation data-sets L. Desorgher
- Declare Radecay Mode as Creator Model Index to secondary Track

FUTURE

- Beta-delayed neutron emission, Super Heavy Elements L. Sarmiento
- Publication
- Validation plots D. Wright, L.Desorgher
- Continue validation of electron spectrum