G4RadioactiveDecay

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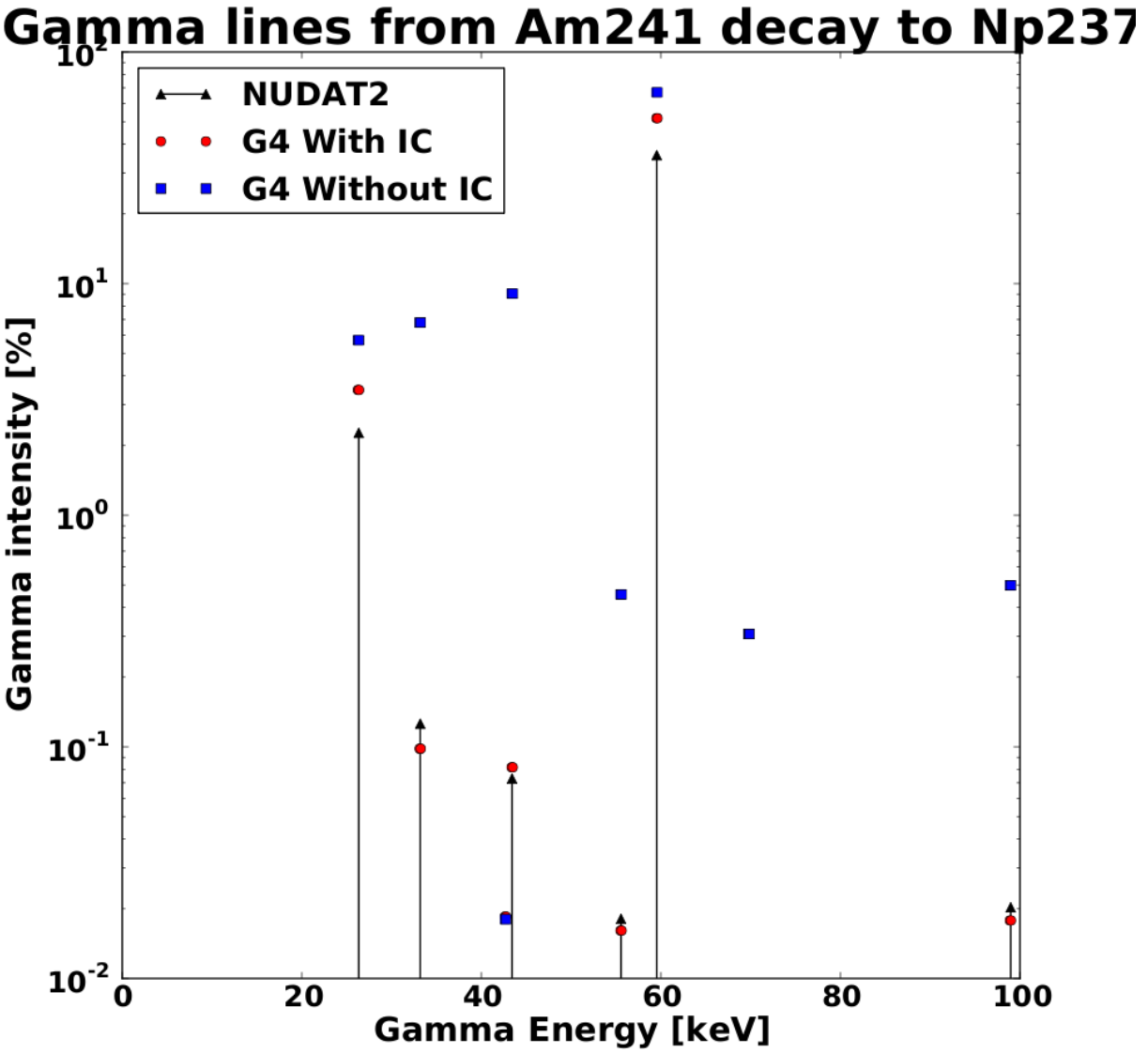
Outline

- **Improvement of internal conversion in photo-evaporation model**
  - **Building of new database based on nudat2 (ENSDF interface)**
  - **Test of G4RadiocativeDecay against nudat2 data**
- **Improvement of Beta decay spectrum shape (D. Wright)**
- **Extension of the use of the G4RadioactiveDecay module to Z>100**

Problem with Internal conversion in Decay of ^{241}Am

- ^{241}Am alpha decays to different energy levels of ^{237}Np
- Decays of ^{237}Np excited levels to ground state do not produce the expected gamma line intensity in G4
- Problem in modeling of electron internal conversion in the G4 photo-evaporation model



Internal conversion process

- **Two possible mechanisms for the deexcitation of a nuclear level:**
  - **Gamma emission**
  - **Internal conversion where an atomic e- is extracted from an atomic shell**

- **Conversion coefficient $\alpha = I_e / I_{gamma}$ can be computed from programs as : BrICC, XICC, ...**

- **In Geant4 the α coefficients are pre-computed and tabulated in the photo-evaporation database**

Internal conversion in Geant4

- **The G4 photo evaporation model samples correctly the rate of e- conversion and gamma decay from the α coefficients provided in the evaporation database**

- **In former photo-evaporation database the conversion coefficients were computed by XICC and HICC programs (QinetiQ)**

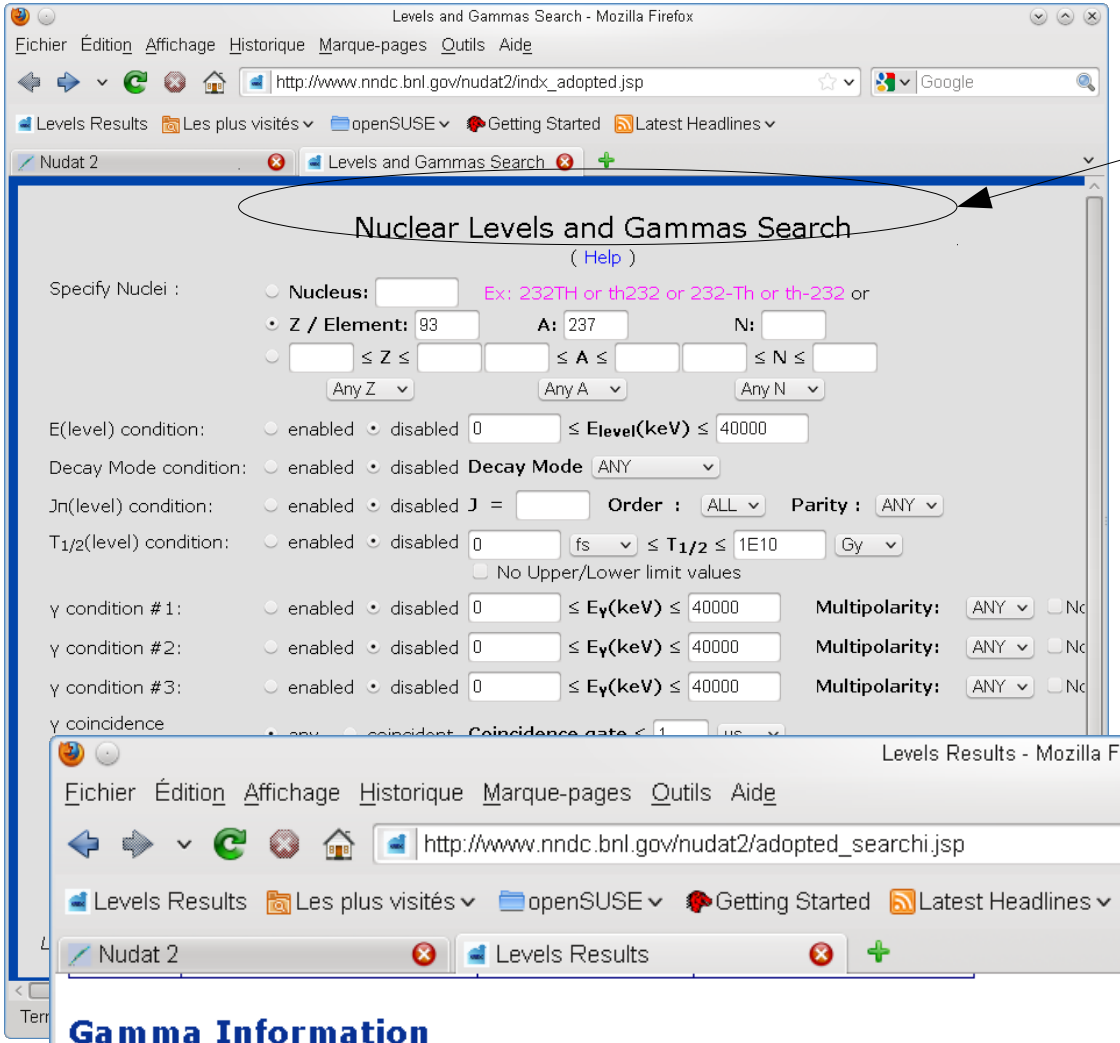
- **Ok for most of the nuclei where the theory agrees within few % with the measurements**

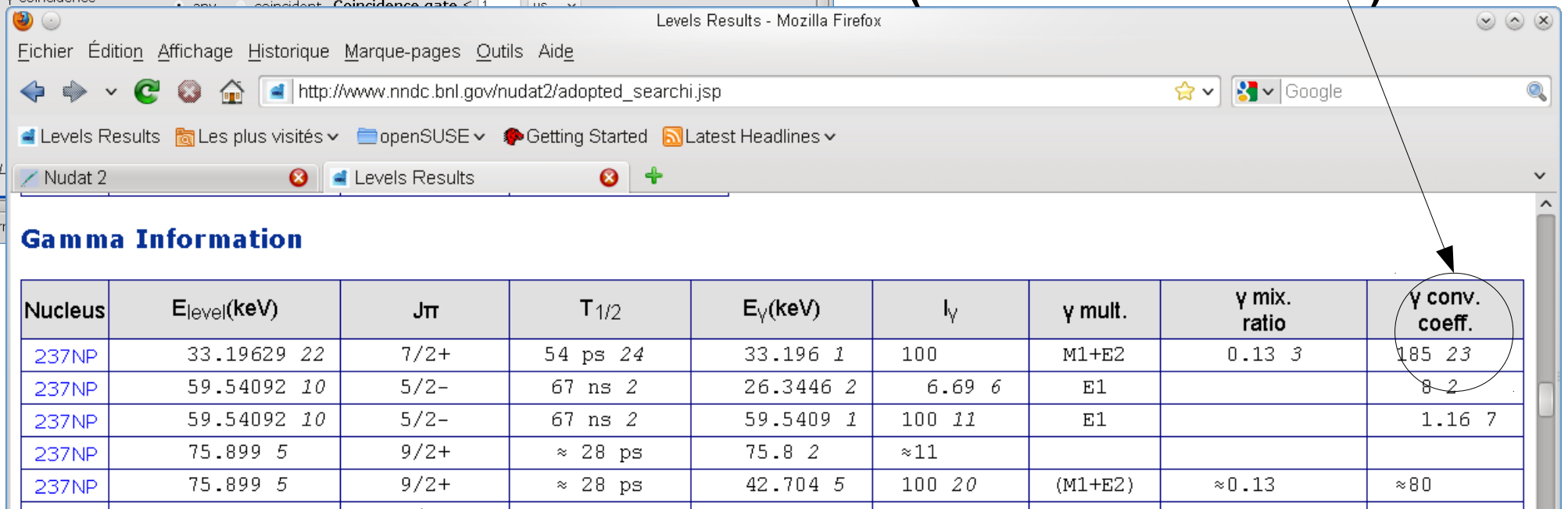
- **But in some rare cases as Np237 theoretical α differs significantly from experiment**

- **Need of rebuilding of the photo-evaporation database with use of α from ENSDF datafile when available**

Automatic rebuilding of the evaporation database with PYTHON from Nudat2 and BrICC

- **Automatic download of nuclear level and gamma data from nudat2 by using the mechanize PYTHON library**
- **Total conversion coefficients taken from nudat2 if available otherwise computed with BrICC**
- **Partial coefficients for the e-shell computed with BrICC (reference for ENSDF)**





Nucleus	E_{level}(keV)	Jπ	$T_{1/2}$	E_γ(keV)	I_γ	γ mult.	γ mix. ratio	γ conv. coeff.
237NP	33.19629 *22*	7/2+	54 ps *24*	33.196 *1*	100	M1+E2	0.13 *3*	185 *23*
237NP	59.54092 *10*	5/2-	67 ns *2*	26.3446 *2*	6.69 *6*	E1		8 *2*
237NP	59.54092 *10*	5/2-	67 ns *2*	59.5409 *1*	100 *11*	E1		1.16 7
237NP	75.899 *5*	9/2+	≈ 28 ps	75.8 *2*	≈11			
237NP	75.899 *5*	9/2+	≈ 28 ps	42.704 *5*	100 *20*	(M1+E2)	≈0.13	≈80

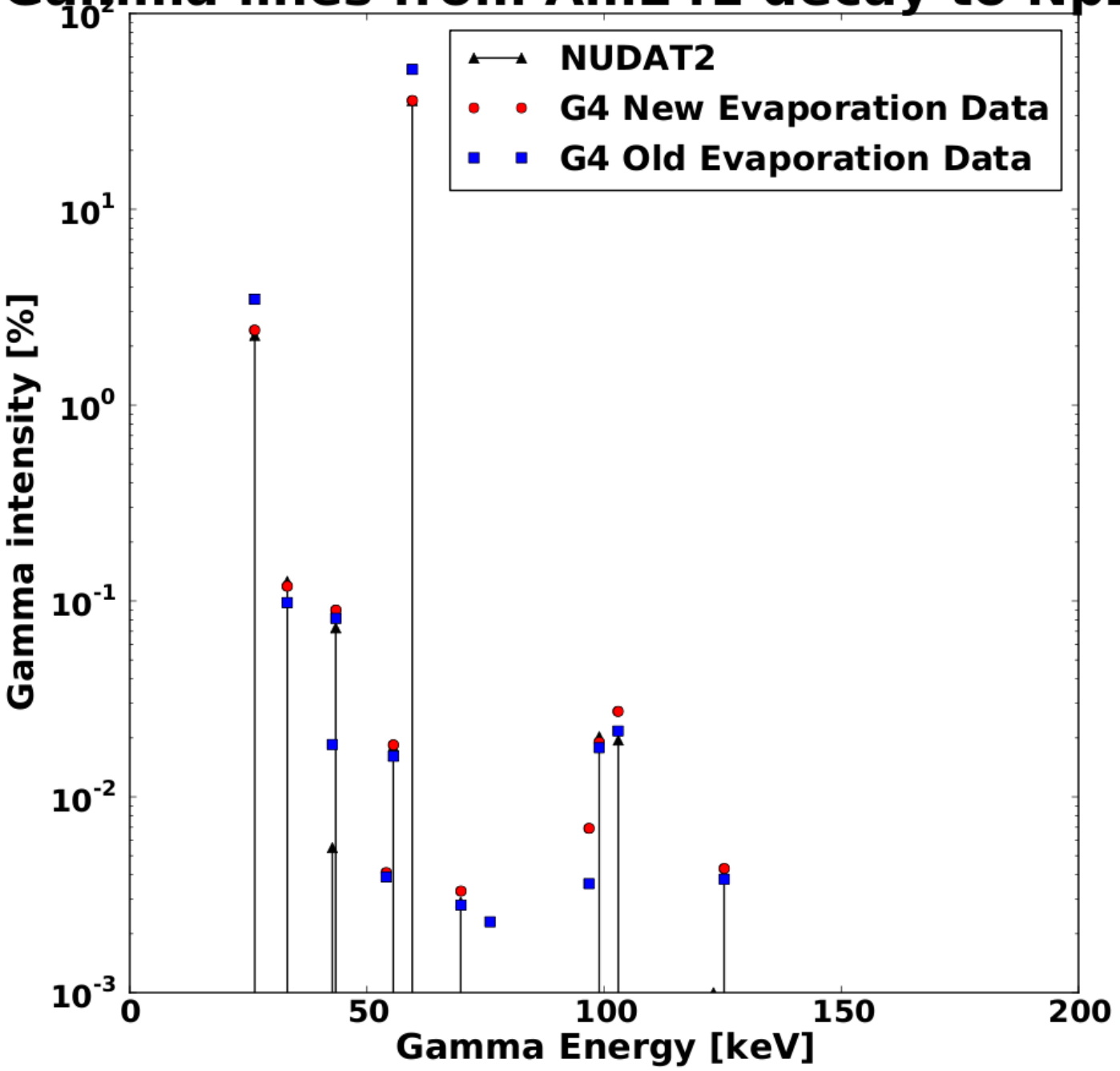
Test of G4RadioactiveDecay gamma line production against nudat2

- Development of a test suite for the G4RadioactiveDecay module
- Automatic download of decay product files from nudat2 with PYTHON code
- Comparison of G4RadDecay gamma line output with nudat2 data. Use of PYTHON/ROOT and PYTHON/PYLAB. This could be automatized.
- Switch-off atomic relaxation in G4RadDecay to focuse only on gamma ray line intensity
- Other tests could be needed as the photo-evporation process is used by different processes ???

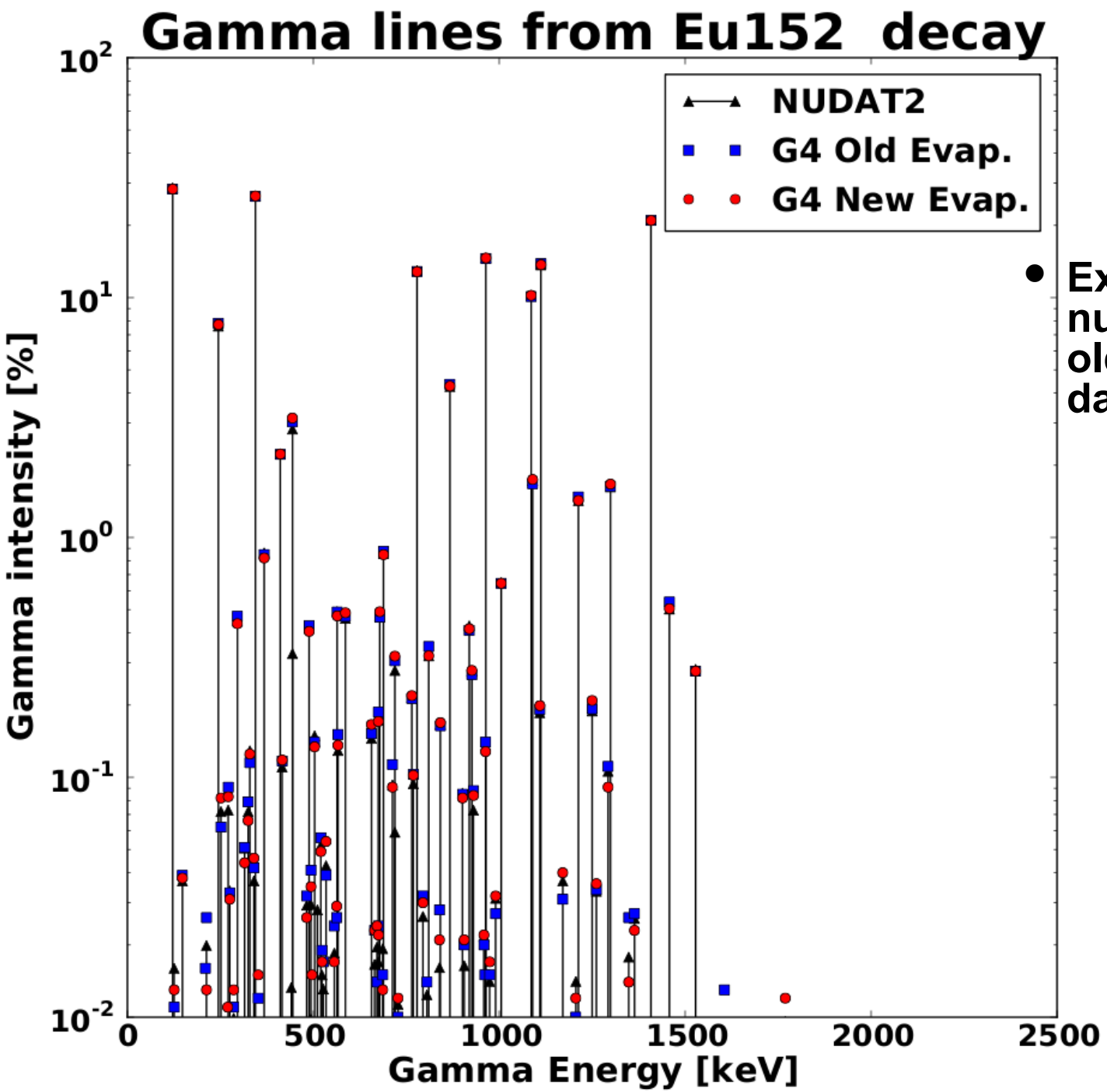
Gamma and X-ray radiation:

	Energy (keV)	Intensity (%)	Dos (MeV/E
XR l	13.9	37 % *3*	0.005
	26.3446 *2*	2.27 % *12*	6.0E-
	33.196 *1*	0.126 % *3*	4.18E-
	42.704 *5*	0.0055 % *11*	2.3E-
	43.420 *3*	0.073 % *8*	3.2E-
	51.01 *3* S	2.6E-5 % *12*	1.3E-
	55.56 *2*	0.0181 % *18*	1.01E-
	59.5409 *1*	35.9 % *4*	0.021
	64.83 *2* S	1.45E-4 % *18*	9.4E-
	67.45 *5*	4.2E-4 % *10*	2.8E-
	69.76 *3*	0.0029 % *4*	2.0E-
	75.8 *2*	5.9E-4 % *6*	4.5E-
XR kα2	97.069	0.00114 % *4*	1.10E-
	98.97 *2*	0.0203 % *4*	2.01E-
XR kα1	101.059	0.00181 % *6*	1.83E-
	102.98 *2*	0.0195 % *4*	2.01E-
	109.70 7	4.90E-6 %	5.38E-
XR kβ3	113.303	2.27E-4 % 7	2.57E-
XR kβ1	114.234	4.30E-4 % *14*	4.91E-
XR kβ2	117.463	1.68E-4 % *5*	1.97E-

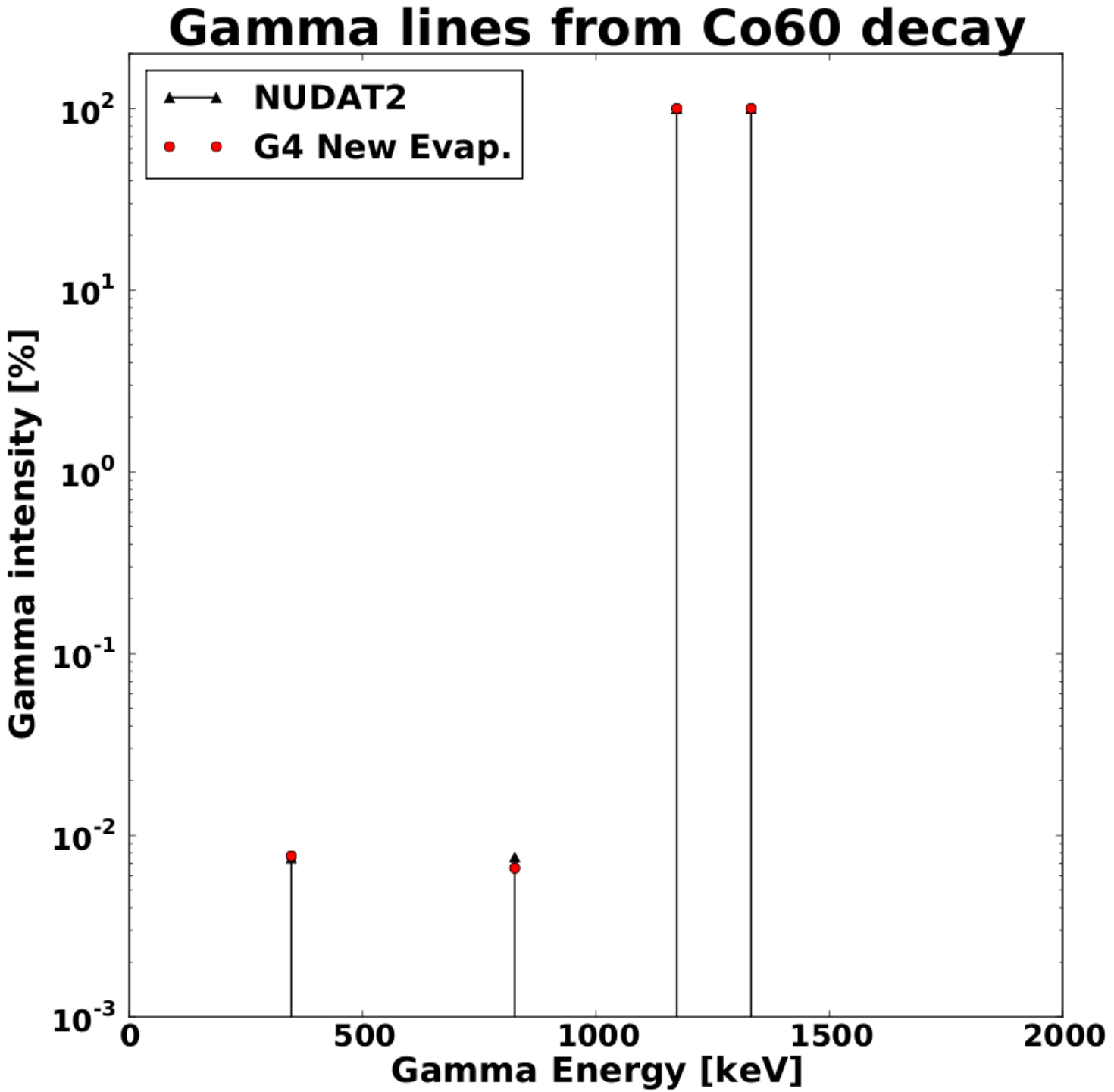
Gamma lines from Am241 decay to Np237



- Much better gamma ray line intensities with new database



- Excellent agreement G4 vs nudat2 for simulations with old and new evaporation database


Gamma lines from Co60 decay
NUDAT2
G4 New Evap.
Gamma intensity [%]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
0
500
1000
1500
2000
Gamma Energy [keV]

Bug in Geant4 when Internal conversion is switched off

- When the Internal conversion model is switched off by the user the conversion coefficients are set to 0
- gammas are always emitted during a nucleus deexitation
- The intensity of emitted gammas is overestimated
- The atomic relaxation is not considered
- Solution under discussions
  - Remove the ICM off option
  - Correct the weight of the emitted gamma by the factor $1/(1+\alpha)$
  - Compute the conversion e- but kill it before emission

Improvement of Beta Decay Shapes in G4RadioactiveDecay (D. Wright)

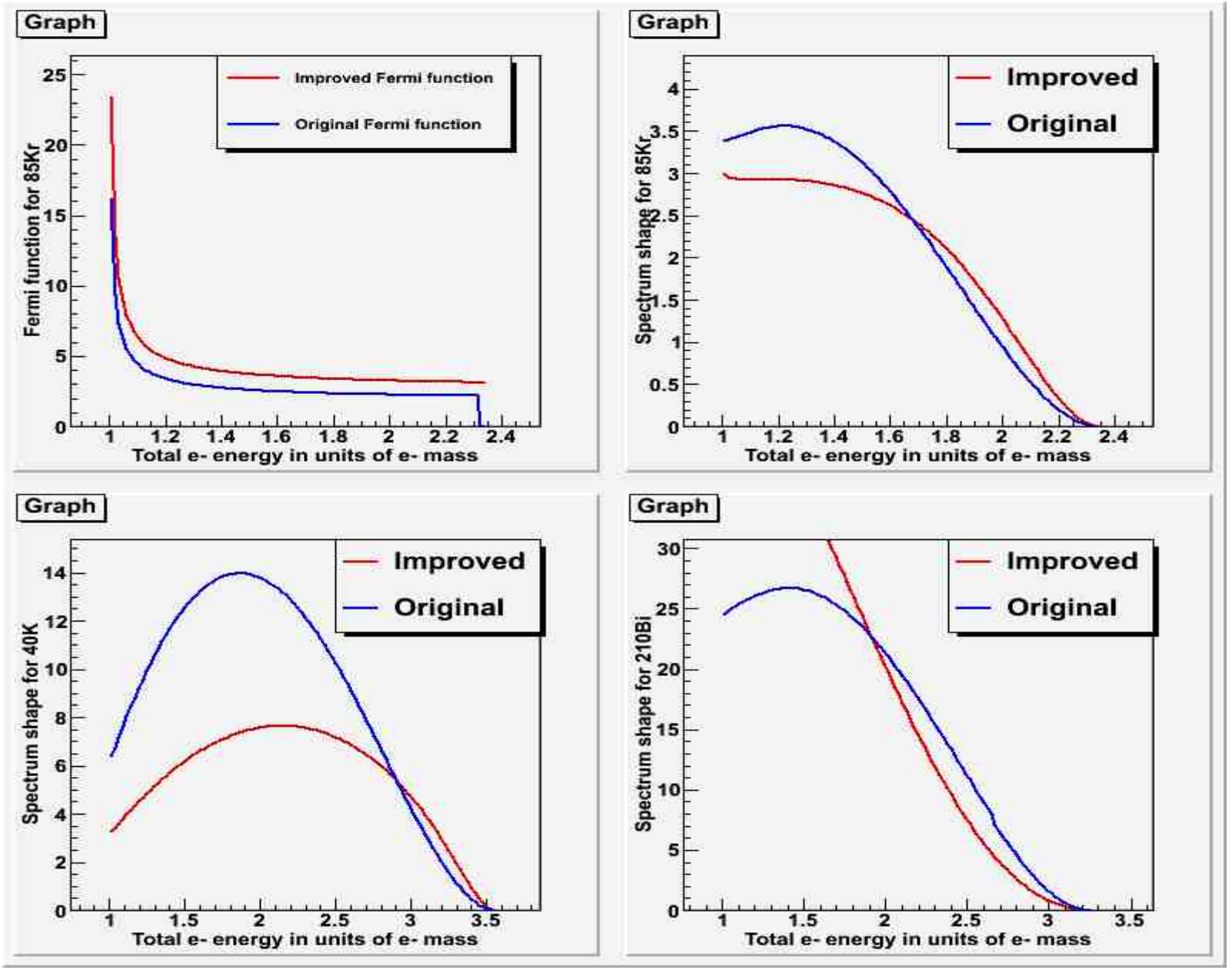
- **Until now, only the so-called allowed transitions of beta decay were implemented in G4RadioactiveDecay**

- **Now, "forbidden" decay shapes have been added**
  - **1^{st}, 2^{nd} and 3^{rd} unique forbidden transitions include nuclear size information, take into account angular momentum of nuclear states**
  - **Unique forbidden transitions have a different energy dependence which shifts the mean beta energy upward compared to simple allowed transitions**
  - **One special case added for non-unique forbidden (210Bi)**

- **Radioactive decay database must also be modified to indicate which levels are forbidden**

- **More precise Fermi function added (now good to < 0.1%)**

Improvements of Beta decay spectrum shapes (forbidden shapes included)



Extension of G4RadioactiveDecay to nuclei with Z>100

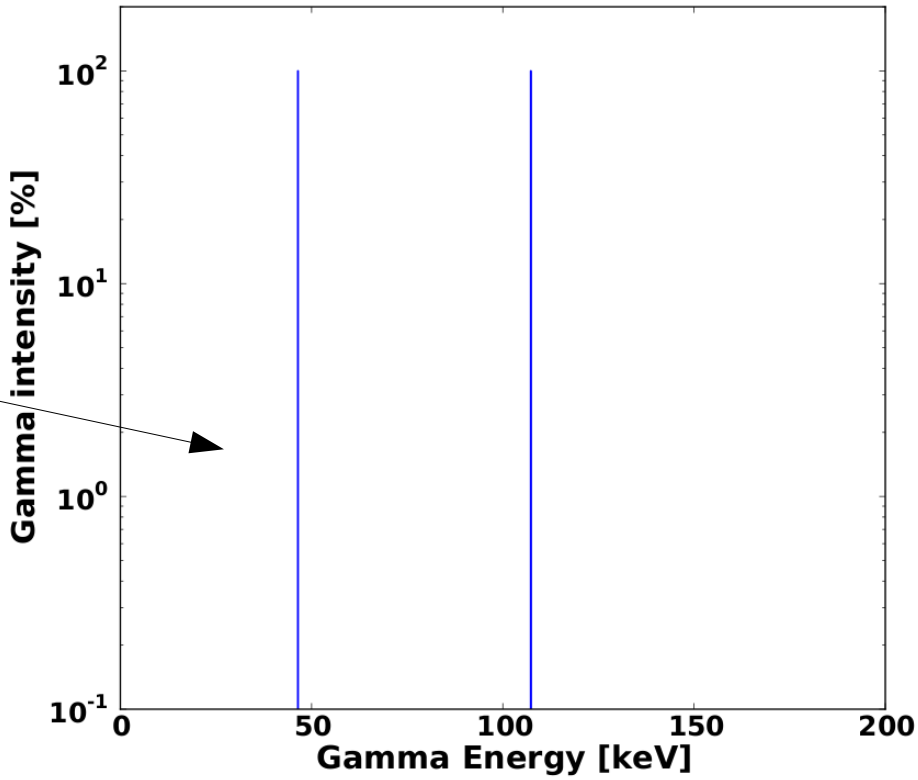
- **Until now the use of G4RadioactiveDecay module is limited to Z<=100 and A<250 while the photo-evaporation model is limited to Z<=98**

- **Some users have requested the possibility to simulate radioactive decays of nuclei with Z>100**

- **New developments implemented to fullfill this user requirement:**
  - **Allow the user to set the Z and A higher limits in G4RadDecay above the Z<=100 and A<250 limits**
  - **Suppress the Z<=98 limit in the photoevaporation model**
  - **Give the possibility to the user to define its own radioactive decay and photo-evaporation datafile for selected nuclei**
    - **/grdm/setRadioactiveDecayFile Z A file_name**
    - **/grdm/setPhotoEvaporationFile Z A file_name**

Test simulation of nuclear de-excitation of No252 Z=102

- **Decay of No252[153.7keV] to No252 ground state,**
  - **only gamma de-excitation**
  - **simulation works fine**



- **Decay of No252[320.7keV] to No252 ground state**
  - **In decay from [320.7keV] to [153.7keV] level the internal conversion process is dominant**
  - **Simulation fails → G4AtomicShells::GetBindingEnergy() does not work for Z>100**
  - **Need to add data for Z>100 in G4AtomicShells**

Conclusions

- **PYTHON codes have been developed:**
  - **to rebuild automatically the photo-evaporation database from nudat2 data**
  - **to validate production of gamma ray line from G4Radioactive Decay against nudat2 data**
  - **If needed conversion coefficient for shell >M could be added**

- **This work could be extended for other validation of the G4Radioactive decay and for direct use of ENSDF data instead of nudat2**

- **Beta Decay Shapes in G4RadioactiveDecay has been improved**
  - **Extension to forbidden transitions**
  - **Better Fermi function**

- **Possibility for the user to force the use of his data files for selected nuclei and to extend the radioactive decay for nuclei with Z>100 has been added**
  - **Need to add data for Z>100 in G4AtomicShells**

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