L. Desorgher¹, D. Wright²
1.SpaceIT GmbH, Bern, Switzerland
2.SLAC
Outline

- Improvement of internal conversion in photo-evaporation model
  - Building of new database based on nudat2 (ENSDF interface)
  - Test of G4RadioactiveDecay 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 $^{241}\text{Am}$

$^{241}\text{Am}$ alpha decays to different energy levels of $^{237}\text{Np}$

- Decays of $^{237}\text{Np}$ 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

![Gamma lines from Am241 decay to Np237](image)
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 $\alpha = \frac{I_e}{I_{\gamma}}$ can be computed from programs as: BrICCC, XICC, ...

• In Geant4 the $\alpha$ 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)
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 focus only on gamma ray line intensity

- Other tests could be needed as the photo-evaporation process is used by different processes ???
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.
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
  • 1st, 2nd and 3rd 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 \( Z \leq 100 \) and \( A < 250 \) while the photo-evaporation model is limited to \( Z \leq 98 \)

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

- **New developments implemented to fulfill this user requirement:**
  - Allow the user to set the \( Z \) and \( A \) higher limits in G4RadDecay above the \( Z \leq 100 \) and \( A < 250 \) limits
  - Suppress the \( Z \leq 98 \) 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`
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
Acknowledgments

• Michel Maire, Vladimir Ivantchenko

• Fan Lei, Pete Truscott (QinetiQ)

• Giovanni Santin, Petteri Nieminen (ESA)

• All the users that have contributed to the G4UserForum and G4bugzilla system in reporting issues on the G4RadioactiveDecay module

• This work has been sponsored by the ESA/ESTEC Contract No. 4000102407