Radioactive Decay in Geant4: Status and Plans

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Outline

- Summary of recent features of Geant4 radioactive decay
- Strengths and weaknesses of the models
- Improvements required or desired
- Plans/tasks and discussion
- Summary

G4RadioactiveDecay Redesigned

- Refactored
  - each decay type now its own class, with common base class
  - biasing and analog code separated → biased code is now a separate class derived from the analog base class

- 10 separate decay modes in seven separate classes
  - α
  - β^-, β^+
  - electron capture (from K, L, M, N shells)
  - isomeric transition
  - neutron emission
  - proton emission

Databases Improved

- RadioactiveDecay5.3 (ENSDF)
  - new channels added: proton emission, neutron emission
  - expanded format: floating levels +X, +Y, … of initial and final levels, where available (Xx999[Ex+X])
  - gamma levels now consistent with those in PhotonEvaporation

- PhotonEvaporation5.3 (ENSDF)
  - expanded format: floating levels, multipolarity, multipolarity mixing
  - all levels listed with an order number to speed up calculations
    - all daughter levels now grouped and ordered underneath their mother level

Modeling Improvements

- Improved physics
  - better electron, neutrino spectrum shapes from beta decay
  - correlated gamma emission for IT decays
  - more electron capture channels
  - improved atomic relaxation
  - new decay modes

- Paid more attention to energy conservation
  - use atomic masses instead of nuclear masses
  - improved atomic relaxation also helped

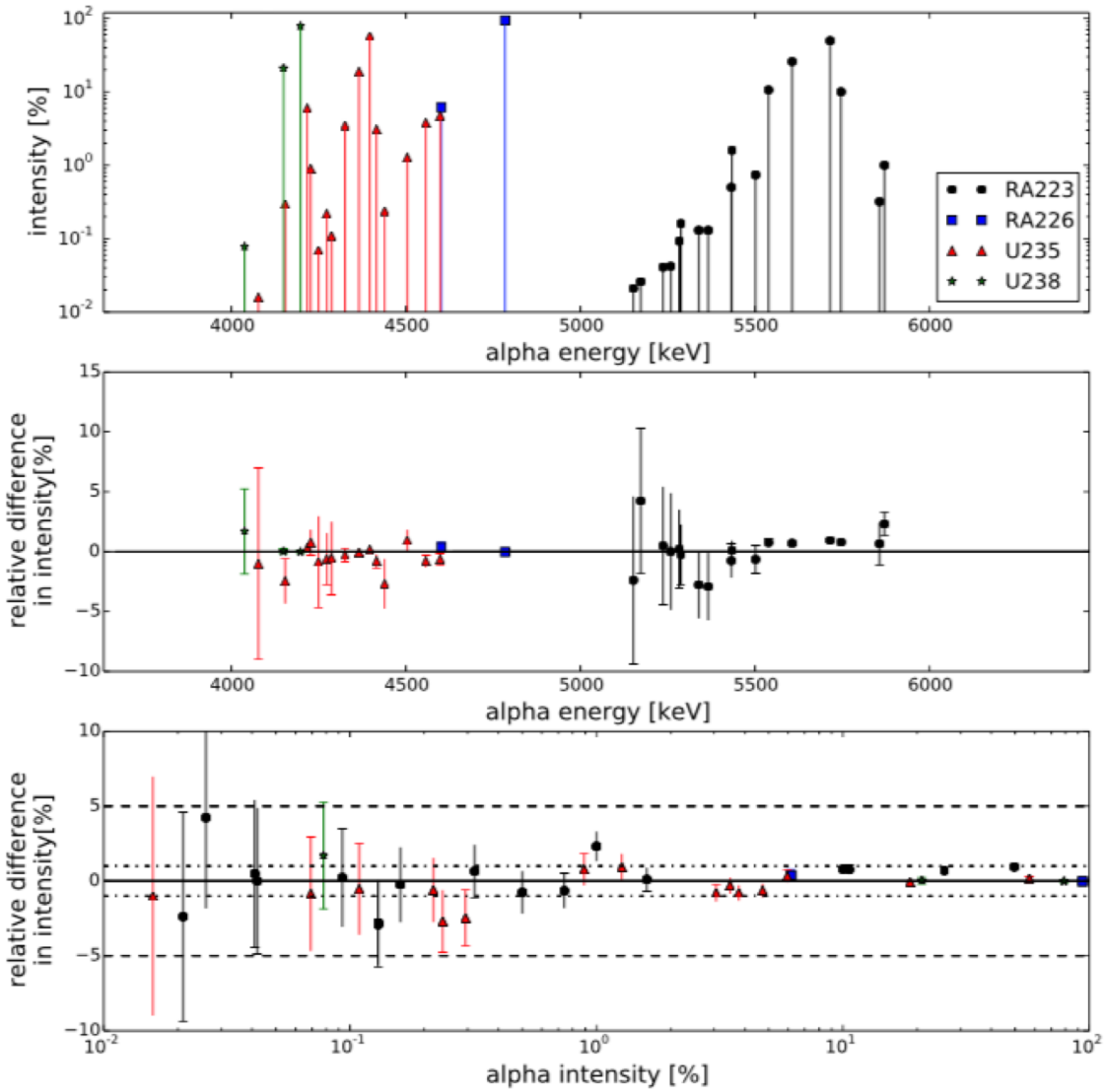
- Activation calculations refactored and cleaned up
  - led to fix of long-standing bug

Alpha Decay

- Already quite good
  - simple two-body decay
  - excellent energy conservation (~ fraction of eV)
  - MC relative intensities often within 5% of theory

- Currently no atomic rearrangement as part of decay
  - is there a model for throwing away two electrons?

α Decay (Geant4 vs. DDEP calculation)



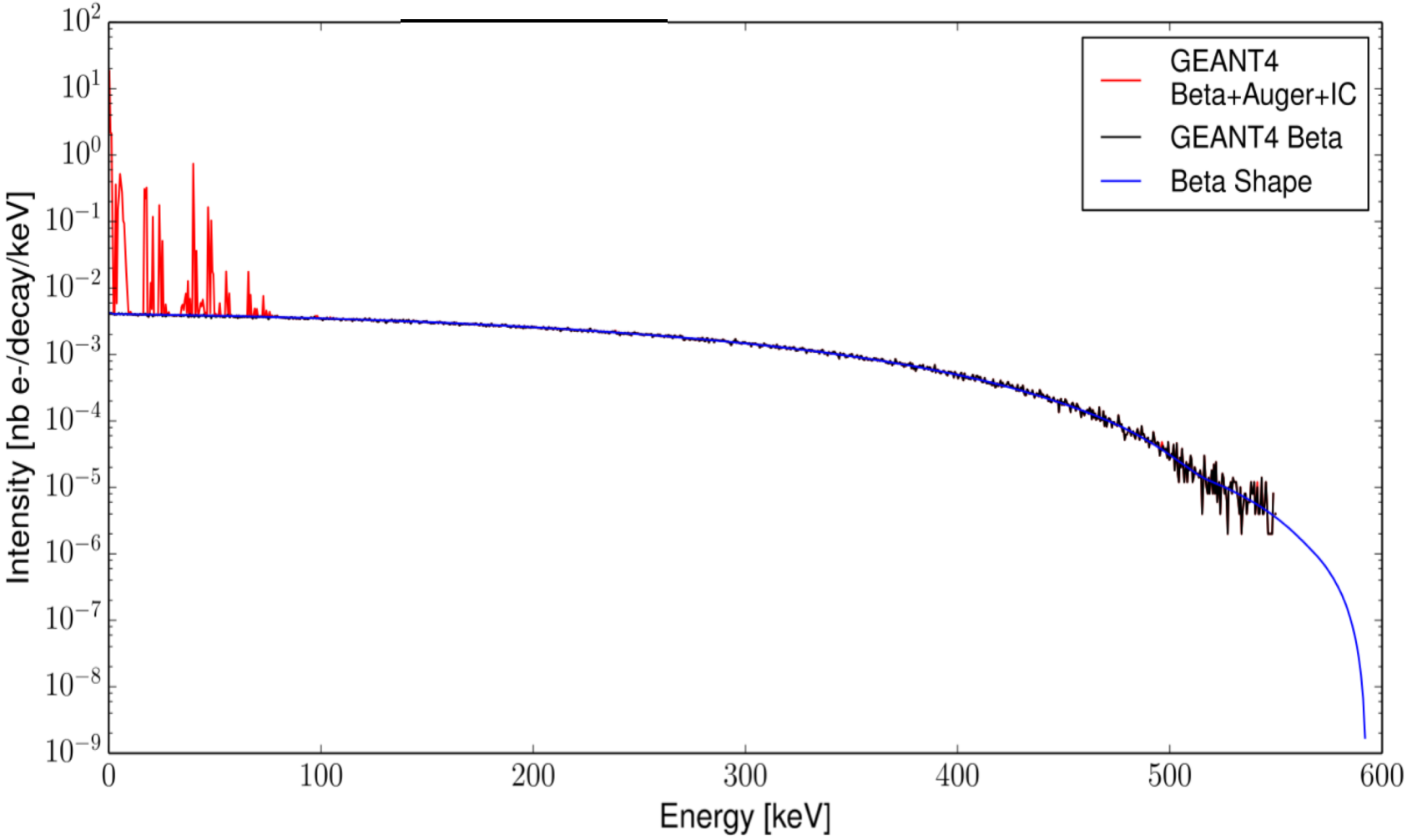
Beta Decay

- e^+/e^- spectra look good for allowed transitions
  - also have good theoretical shape corrections for unique first, second and third forbidden transitions

- Only one case (^{210}Pb) for which we have a non-unique forbidden shape in Geant4
  - it takes many parameters to describe these
  - would need to extend both database and code to add these

- No atomic relaxation as part of decay
  - need to pick up or throw away one electron

β^- Decay (^{161}Tb) (Geant4 vs. theory)



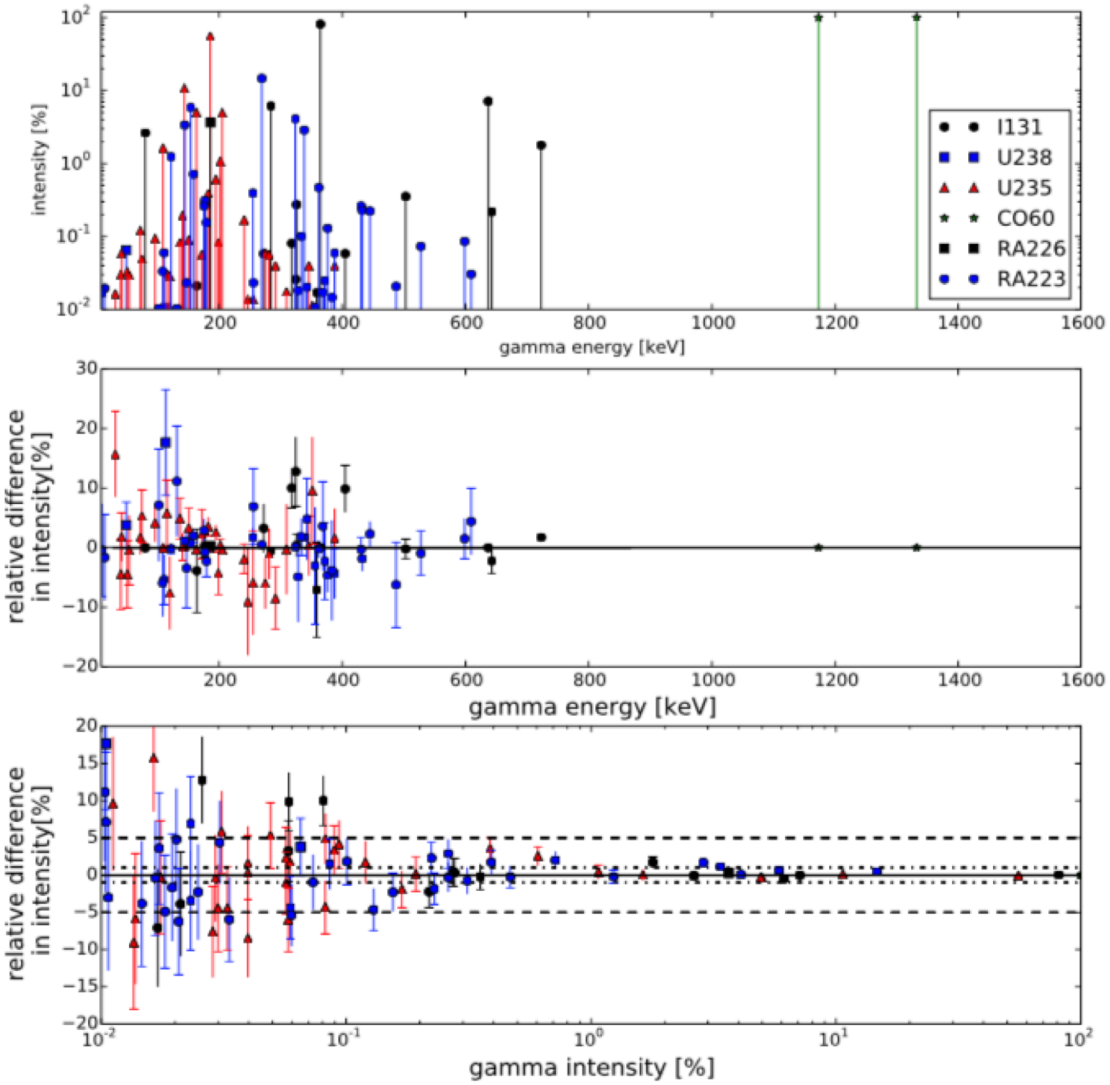
Electron Capture

- Very good now that up to N-shell process is included
  - probably don't need to go to O-shell
- Energy conservation is ad hoc
  - currently add a dummy electron to make up deficit between the binding energy and the kinetic energy given by the relaxation code
- Electron binding energies themselves are also a concern
  - use experimental or theoretical?
  - new set available using experimental values wherever possible

Gamma Transitions (IT)

- Uses G4PhotonEvaporation from Geant4 deexcitation module
  - → consistency between radioactive decay and nuclear deexcitation
  - internal conversion included
  - radioactive decay can use all the extra physics of deexcitation
    - fluorescence, Auger
- Correlated gamma emission added
  - gamma angular distributions now depend on multipolarity of transition, if included in database
  - however, very time-consuming if high multipolarity
    - currently turned off by default

IT Decay (Geant4 vs. DDEP calculation)



Gamma Transitions (IT)

- Energy conservation is ad hoc
  - same situation as for EC
- Binding energies
  - same situation as EC

- Because radioactive decay uses same gamma deexcitation module used in nuclear de-excitation, some tension in how the interface is used
  - radioactive decay always uses single gamma decay, while general de-excitation module uses single, multiple and continuous gamma emission
  - different initialization options for BuildPhysicsTable
  - different CPU efficiency options

Neutron and Proton Emission

- A nucleus with excess of neutrons (or deficit of protons) can decay by neutron emission (below the neutron drip line)

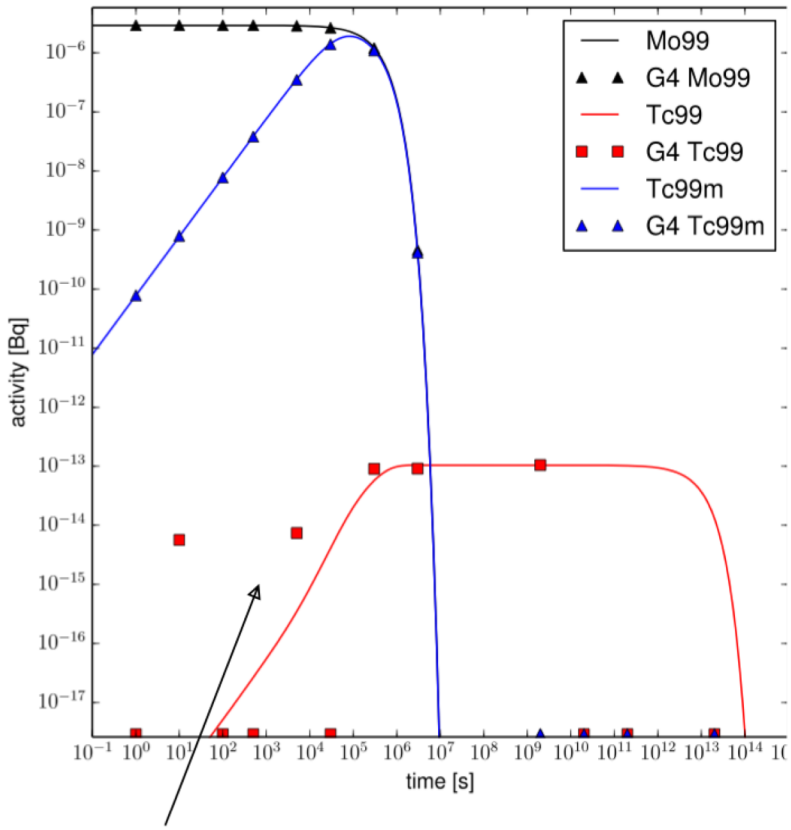
- A nucleus with excess of protons (or deficit of neutrons) can decay by proton emission (above the neutron drip line)

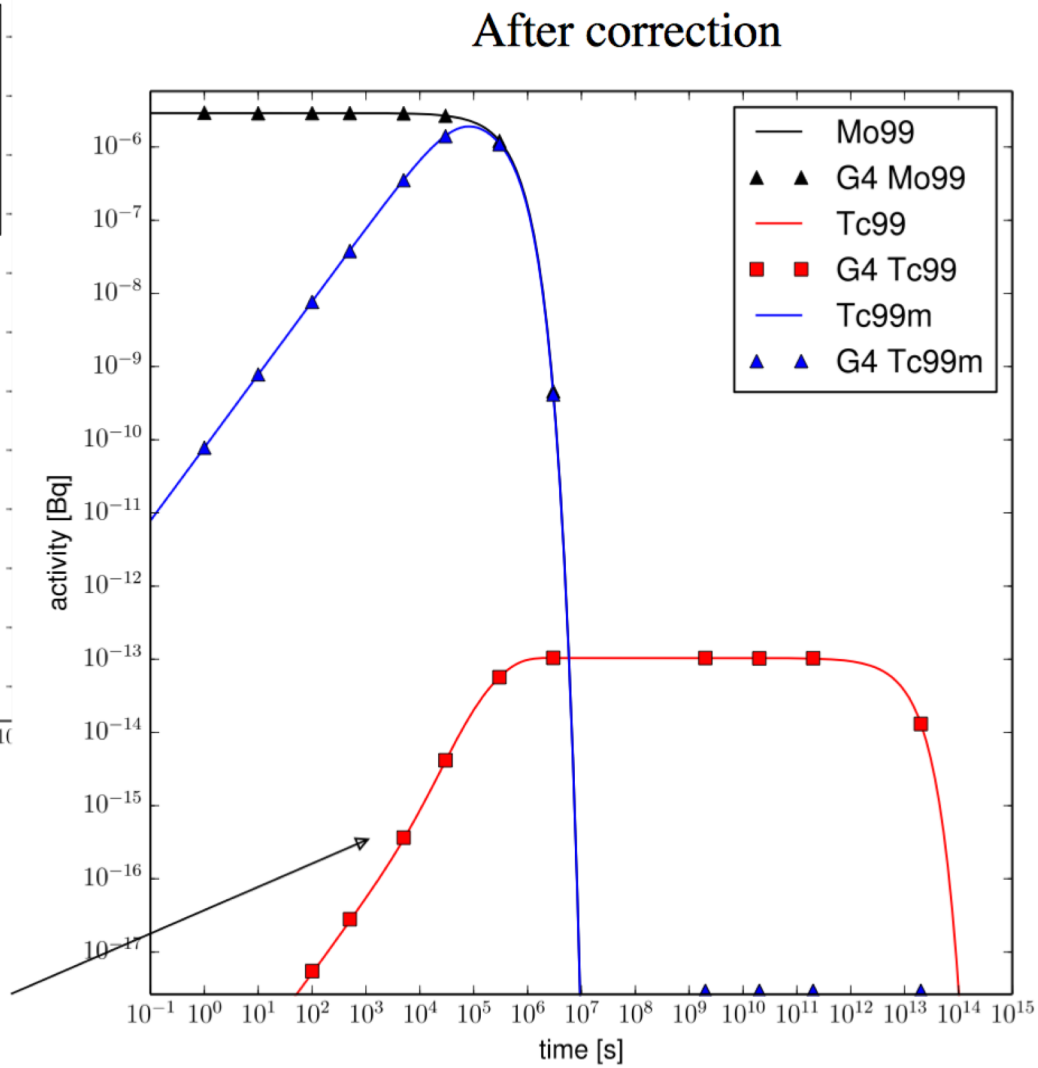
- Both coded the same as α decay → two-body final state
  - also no atomic re-arrangement after these decays

Activation

- Generalized Bateman equations for activation
  - multiple decay chains, multiple sources, feeding
  - source and detector time convolution
  - designed to decay one parent nucleus through all its decay chains, to stable products
  - all decays and products generated in a single track
    - secondaries from all generations of decay collected into final state
    - weights attached based on branching ratios, source and detector time convolution
    - collected for dose calculations
- Many biasing options available to speed up calculation (see later slide)

Activation


Mo99
G4 Mo99
Tc99
G4 Tc99
Tc99m
G4 Tc99m
activity [Bq]
time [s]


After correction
Mo99
G4 Mo99
Tc99
G4 Tc99
Tc99m
G4 Tc99m
activity [Bq]
time [s]

Biased Decay

- Activation was originally a fully integrated part of RDM
  - more like an application than a process → separate it from RDM
  - use base class like a process, then add biasing
- Biasing options
  - nucleus duplication (splitting)
  - branching ratio biasing (make all branches equal)
  - source time convolution
  - detector time convolution
  - directional biasing (in both activation and base)
  - set nucleus limits (in both activation and base)

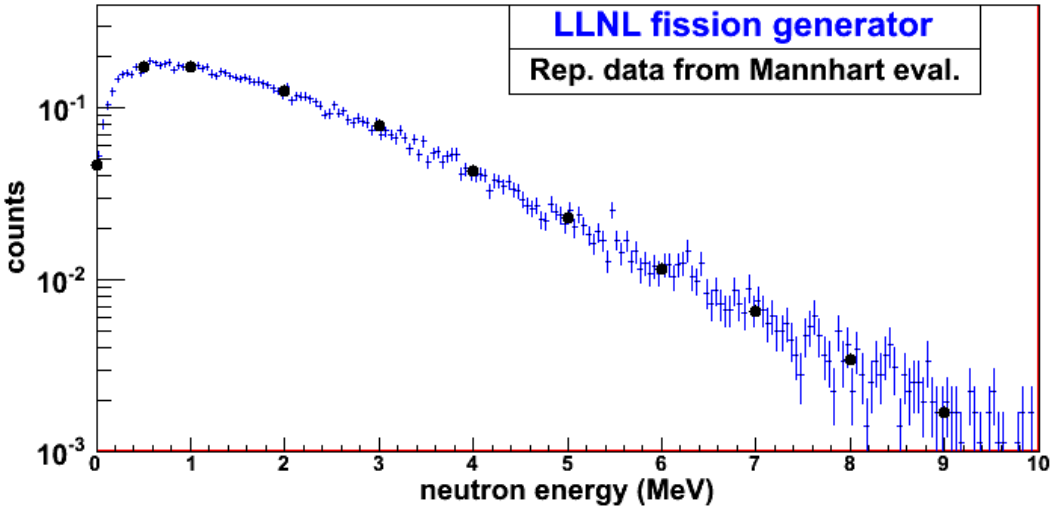
Biased Decay

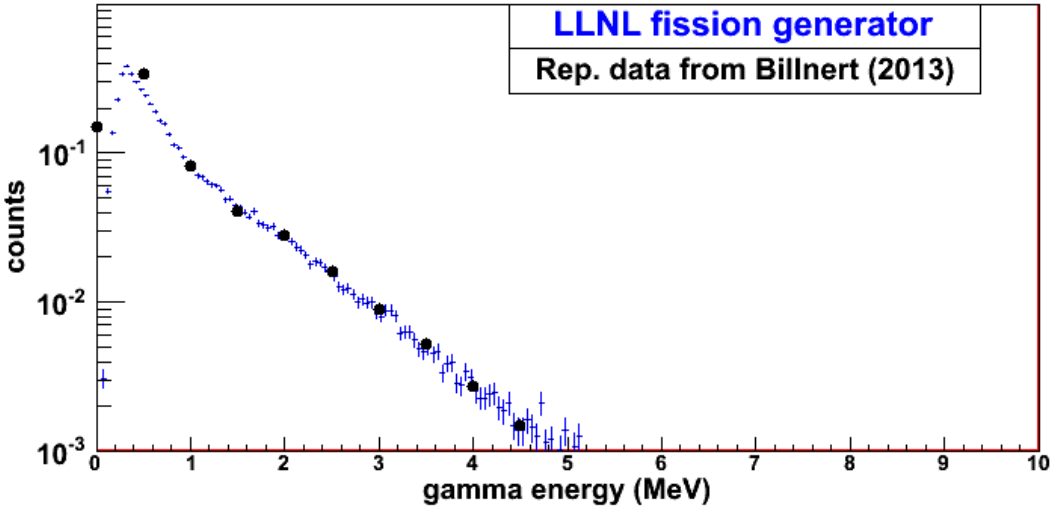
- Further development somewhat restricted by maintaining interface with G4GeneralParticleSource
  - some radioactive decay methods may be obsolete → can we delete?
- Cannot currently apply bias without running activation
  - may want to bias the decay in the base class
- Biasing options
  - no option to re-weight a single decay channel (currently can only choose all channels equal)
  - conform more to new Geant4 general biasing?

New Decay Modes Requested

- Spontaneous fission
  - requested by SuperCDMS
  - recently committed to repository (ready for 10.6 beta)
  - uses Livermore fission model class G4fissionEvent
    - neutron energy spectrum sampled from function fitted to Mannhart evaluated data set
    - gamma spectrum from parameterization of data
    - no heavy fission fragments
  - can be used for several heavy isotopes, but mostly for ^{252}Cf
  - possible to generate fragments and let them decay by gamma emission to get detailed gamma spectrum

Spontaneous Fission of ^{252}Cf





New Decay Modes Requested

- Beta-delayed neutrons and protons
  - nucleus beta decays to a daughter far from drip line, then decays by neutron or proton emission
  - some of these decays already happen in normal chain
    - no coding required
  - complete implementation requires a model of beta decay to densely populated, highly excited level region
    - use native Geant4 nuclear deexcitation model to emit neutron (or proton) from this region?
  - arbitrary decision about where low excitation region ends and high excitation region begins

Beta-delayed Neutron Emission

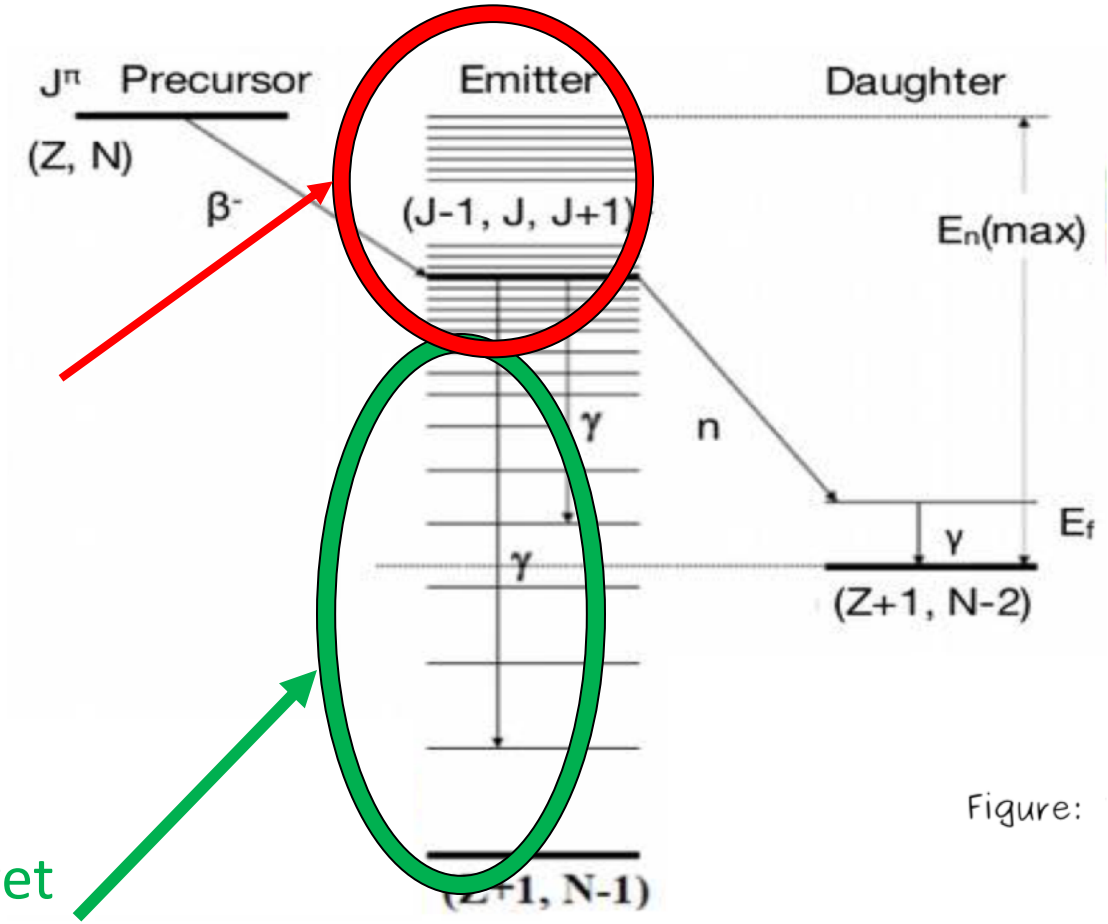


Figure:

These we don't

These we get already

New Decay Modes Requested

- Double beta decay
  - rare but important, requested by EXO and others
  - ordinary ($2\beta + 2\nu$)
  - could be implemented in Geant4
    - product of two beta decays
  - problem: very long decay times (~10^{21} years)
    - must treat otherwise stable nucleus as unstable
  - what about neutrino-less (>10^{25} years) ?

Validation

- Comparison to deterministic calculations
  - compare value generated by Geant4 to theoretical calculation
  - comparison may indicate missing physics in Geant4
- Comparison to data (ENSDF, DDEP)
  - very little of this done because we start from database
  - however, we must check that the code is OK → agreement must be very good
  - need to display this to users → validation suite

- In-flight vs. at-rest → never checked
- A number of tests in examples/extended/rdecay01, rdecay02

Plans and Improvements

- Implement spontaneous fission (nearly done)
- Add biasing to radioactive decay process (not activation)

- Implement full beta-delayed p, n emission
- Implement double beta decay

- Validate correlated gamma emission
- Check every test in extended examples

- RDM is a process, not a model → change this?

Plans and Improvements

- Almost no thought given to CPU optimization
  - are there any RDM applications that require high speed?
- If speed not important, go for more detail
  - better physics models
  - more decay branches
- Should we enable Geant4 to do equilibrium calculations?
- Develop a plan to handle handle transitions from floating to non-floating or vice versa

Summary

- Problems identified
  - very little CPU optimization
  - atomic relaxation is not always applied, and is not complete
  - much validation required
  - still room for improvement in several decay channels
  - still room for improvement in biasing

- Many improvements made
  - databases updated, expanded and re-formatted
  - new decay channels added
  - improved energy conservation
  - first steps made to separate activation from the RD process

- Message to Geant4 developers
  - consider more theory-based models
  - reach out to more nuclear physics users to determine their needs