Pre–Equilibrium and Equilibrium decays in Geant4

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1. Theoretical Driven Hadronic Models

- **G4PartonTransportModel**
  - Scatter()
  - GetWoundedNucleus()

- **G4PythiaAhInterface**
  - Scatter()
  - GetWoundedNucleus()

- **G4NhModel**
  - Scatter()
  - GetWoundedNucleus()

- **G4PythiaNInterface**
  - Scatter()
  - GetWoundedNucleus()

- **G4QuarkGluonStringModel**
  - GetStrings()
  - GetWoundedNucleus()
  - CreateDiffractiveString()
  - CreateHardString()
  - CreateSoftString()

- **G4FTFModel**
  - GetStrings()
  - GetWoundedNucleus()
  - Init()
  - ExciteParticipants()
  - BuildStrings()
  - GaussianPt()
  - ChooseX()

- **G4QMDModel**
  - GetWoundedNucleus()
  - CreateDiffractiveString()
  - CreateHardString()
  - CreateSoftString()

- **G4PartonStringModel**
  - Scatter()
  - GetWoundedNucleus()
  - Init()
  - GetStrings()
  - CorrectHadronMomenta()
  - SetThisPointer()

- **G4VintraNuclearTransportModel**
  - ApplyYourself()
  - Propagate()
  - theDeExcitation

- **G4VIntraNuclearTransportModel**
  - ApplyYourself()
  - Propagate()

- **G4HadronKineticModel**
  - SetTimeStep()
  - StopTimeLoop()
  - CheckPauliPrinciple()
  - FindFragments()
  - UpdateKineticTrack()
  - DoTimeStep()

- **G4HadronicCascade**
  - ApplyYourself()
  - Propagate()
  - FindInteraction()
  - DoReaction()
  - DoDecay()
  - TerminationCondition()
  - CheckPauliPrinciple()
  - FindClusters()

- **G4ExcitationHandler**
  - theEvaporation : G4VEvaporation
  - theMultiFragmentation : G4VMultiFragmentation
  - theFermiModel : G4VFermiBreakUp
  - BreakItUp()
2. **Pre–Equilibrium Decays**

- The responsibility of the Pre–Equilibrium domain is to decay excited nuclei with excitation energies $O(100 \text{ MeV})$.

- Pre–Equilibrium fills the gap between the arbitrary cutoff of the Intra–Nuclear cascade and equilibrium decays.

- It models the high energy continuum region of ejectile spectrum.

- The Griffin’s semiclassical Exciton Model has been used.

- In the Exciton Model, the composite nucleus states are characterized by the number of excitons $n$ (excited particles $p$ and holes $h$).

- Successive two–body interactions give rise to an intranuclear cascade which eventually leads to a fully equilibrated nucleus.
At each stage of this equilibrium process there is a competition between two decay modes:

- Emission of particles into the continuum.
- Exciton–Exciton interaction to more complex configurations. Selection rules: \( \Delta n = 0, \pm 2, \Delta p = 0, \pm 1, \Delta h = 0, \pm 1 \)

The transition rate between two states \( n \) and \( n' \) is:

\[
\lambda_{nn'} = \frac{2\pi}{h} |M|^2 \rho_n'(E^*)
\]
2.1. Pre–Compound Fragments

Assuming equally spaced single–nucleon states with density \( g \), the state density becomes

\[
\rho_n(E^*) = \frac{g(gE^*)^{n-1}}{p!h!(n - 1)!}
\]

We have to distinguish between simple fragments (nucleons) and more complex fragments (ions).
2.1.1. Pre–Compound Nucleons

- In the decay rate we must include a factor that takes into account the condition for the exciton to be a proton or an neutron.
2.1.2. Pre–Compound Ions

- For ions, we have to consider the condensation probability of such fragment.
3. **Equilibrium Decays**

![Diagram](image)

- Compound nuclei are excited nuclei that have reached statistical equilibrium.
- **G4ExcitationHandler** manages 5 de-excitation mechanisms.
  - Evaporation is the main de-excitation mechanism.
  - Fission as an evaporation competitive channel for heavy nuclei.
  - Fermi Break-Up model for light nuclei.
  - Multifragmentation for very excited nuclei.
  - Photon evaporation as competitive channel in evaporation and for residual excitation energies.
4. Evaporation

- **G4Evaporation** implements the statistical Weisskopf–Ewing model.
- Channels are treated polymorphically through the abstract interface **G4VEvaporationChannel**.
- By default there are 8 evaporation channels:
  - p, n, deuteron, triton, $^3\text{He}$, alpha
  - Photon
  - Fission
4.1. Evaporation Channels

- **G4EvaporationChannel** implements those channels that always result in emission of nucleons or light ions.
- The most important “ingredients” are abstracted out:
  - Coulomb Barrier
  - Level Density Parameter
  - Evaporation Probability

```plaintext
G4EvaporationChannel
  Initialize()
  BreakUp()
  EmissionProbability()
  SetEmissionStrategy()

G4CoulombBarrier
G4LevelDensityParameter
G4EmissionProbability

G4ProtonEvaporationChannel
G4NeutronEvaporationChannel
G4DeuteronEvaporationChannel
G4TritonEvaporationChannel
G4He3EvaporationChannel
G4AlphaEvaporationChannel
```
4.2. Level Density Parameters

◆ This parameter plays a major role in the level density models.
◆ We use the functional form proposed by Ignatyuk:

\[ a(A, Z, U) = a_0(A) \left[ 1 + \Delta_{\text{shell}}(A, Z) \frac{f(U - \Delta_{\text{pair}})}{U - \Delta_{\text{pair}}} \right] \]

There are other possible equations.
◆ \( a_0(A) = \alpha A + \beta A^{2/3} B_s \) is the Fermi–gas value of \( a \) at high excitation energies.
◆ There are several choices for the parameters values . . .
4.3. **Coulomb Barriers**

- Coulomb barriers are calculated according to:

\[
V = K \frac{Z_f Z_{\text{res}} e^2}{R_{\text{comp}}(A_f^{1/3} + A_{\text{res}}^{1/3})}
\]

- \(K\) is a barrier penetration factor that depends on the kind of particle.
4.4. Emission Probabilities

◆ Weisskopf’s expression for the probability per unit time for the emission of a particle $f$:

\[
W_f = \int_0^{T_{\text{max}}} \frac{(2s_f + 1)m_f}{\pi^2\hbar^3} \sigma_f(T) \frac{\rho(U_f - T)}{\rho(U_{\text{res}})} dT
\]

◆ Empirical equations for Inverse Reaction Cross Sections:

✦ For neutrons $\sigma_c(A, T) = (\alpha(A) + \beta(A)/T)\sigma_g$
✦ For charged particles $\sigma_c(Z, T) = (1 + C(Z))(1 - V/T)\sigma_g$
4.5. An example: Proton Evaporation Channel

- Particular classes like, for example, `G4ProtonEvaporationChannel`, are responsible for the proper initialization of channels.

- They provide data: $A, Z, \ldots$

- They instantiate the right:
  - Coulomb Barrier: `G4ProtonCoulombBarrier`
  - Evaporation Probability: `G4ProtonEvaporationProbability`
5. Fission

- Fission is an important channel of de–excitation of heavy nuclei \((A > 200)\).

- \textit{G4CompetitiveChannel} follows the Bohr–Wheeler statistical approach.

- Fission probability is proportional to the level density at the saddle point:
  \[
  W_{\text{fis}} = \frac{1}{2\pi \rho_{\text{comp}}(U)} \int_{0}^{U-B_{\text{fis}}} \rho_{\text{sp}}(E^* - \Delta_{\text{fis}} - B_{\text{fis}} - T) dT
  \]

- The height of fission barrier is defined as the difference between the saddle point and ground state masses. It is approximated as
  \[
  B_{\text{fis}} = B_{\text{fis}}^0 + \Delta_{\text{shell}} + \Delta_{\text{sp}}
  \]

- Fission fragments mass distribution consists of a symmetric and an asymmetric components:
  \[
  F(A_{\text{fis}}) = F_{\text{sym}}(A_{\text{fis}}) + w(U, A, Z)F_{\text{asym}}(A_{\text{fis}})
  \]
  and \(w(U, A, Z)\) is the relative contribution of each component.
6. Multifragmentation

- At very high excitation energies (> 3 MeV/nucleon) we have an explosion–like de–excitation process.
- G4StatMF implements an statistical mechanism based on the Copenhagen Model.
- Due to the huge number of open channels, we have to use two approaches.

![Diagram of multifragmentation processes]
6.1. Microcanonical Ensemble

- In the microcanonical ensemble all microscopic states of the system obey strictly the conservation laws.
- The statistical weights of a break-up partition are determined by its entropy.

\[ W_{f}^{\text{mic}} \sim \exp(S_f(E_0, V, A_0, Z_0)) \]

- We calculate all possible partitions with multiplicity less than \( M_0 \).
- We calculate the mean multiplicity \( \langle M \rangle \).
- If \( \langle M \rangle \ < \ M_1 \) one of these partitions is randomly selected according with their statistical weights.
6.2. Macrocanonical Ensemble

In the macrocanonical ensemble, we have only constraints on the average mass and charge of the system.

The distribution of partition probabilities in the macrocanonical approximation is given by

\[ W_{f}^{\text{mac}} \sim \exp(-\Omega_f(T, V, \mu, \nu)/T) \]

We have to solve for \( T, \mu, \nu \), in order to find out \( \langle N_{AZ} \rangle \), \( \langle N_A \rangle \) and \( N(Z) \).
6.2.1. Macrocanonical Clusters

◆ For clusters with more than 4 nucleons we can use the liquid drop model.

◆ But this approach is not valid for light clusters.
7. Fermi Break–Up

- For light nuclei ($A \leq 16$) even small excitation energies are comparable to their total binding energies.
- The Fermi model is analogous to the statistical multifragmentation.
- Due to the small size of nuclei, we can use only the microcanonical approach.
7.1. Fermi Breal-Up Channels

- Coulomb expansion is not considered explicitly, but momentum distributions are obtained sampling over the accessible phase space.

- Long-lived unstable nuclei will decay at the end of the expansion.
8. Results

8.1. Differential cross sections.
8.2. Angular distributions.
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\[ \text{Zr}(p,n) \quad 45 \text{ MeV} \quad \theta = 20^\circ \]
\[ \text{Zr}(p,n) \quad 45 \text{ MeV} \quad \theta = 60^\circ \]
\[ \text{Zr}(p,n) \quad 45 \text{ MeV} \quad \theta = 120^\circ \]
\[ \text{Zr}(p,n) \quad 45 \text{ MeV} \quad \theta = 160^\circ \]
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