Pre–equilibrium and equilibrium decays in Geant4

Vicente Lara[1]*, Johannes Peter Wellisch*[1]

CERN, Genève 23, 1211 Geneva, Switzerland

Abstract

In order to allow extrapolation beyond the experimental data and to provide an alternative set of models at conventional energies, theory based hadronic shower models are being developed for the Geant4 simulation tool-kit. Here, for incoming particle energies below $O(100\mathrm{MeV})$, the precompound reaction mechanism is used to model the high energy continuum region of ejectile spectra and to fill the gap between the arbitrary cutoff of the Intra-Nuclear Cascade models and equilibrium evaporation decays. The behaviour of compound nuclei is then modeled by means of several equilibrium deexcitation models.

Our design follows the philosophy of hadronic models in Geant4, allowing for maximum of extendibility and customizability of the underlying physics by means of the use of abstract interfaces. We present the Object Oriented Design of a semiclassical exciton model for pre–equilibrium decays and the Weisskopf–Ewing evaporation model for equilibrium decays. We present extensions, based on Fermis break–up model for light nuclei and multifragmentation for very high excitation energies. Fission is treated as a evaporation competitive channel.

Keywords: Geant4,OO Design, Hadronic Shower, Simulation, De–excitation, Pre–equilibrium, Compound Nucleus

1 Introduction

Pre–equilibrium and Equilibrium decays are part of the set of theory driven models for hadronic inelastic scattering in the Geant4 Simulation Tool–kit. We present the Object Oriented design of these models, which provides a flexible and customizable framework allowing the user to extend or re–implement the models at several levels.

2 Pre–equilibrium decays.

The responsability of the pre–equilibrium domain is to treat particles in the low energy range, and to produce a set of secondaries that can be used by geometrical tracking. `G4VPreCompundModel` has a two–folded interface because there two use–cases: as a hadronic interaction model and as a back–end to models that work at higher energies. `G4VPreCompundModel` inherits the public interface to the processess as defined in `G4HadronicInteraction`. The Griffin's semiclassical exciton model[1, 2] is used to implement both interfaces in `G4PreCompoundModel`. As an example, detailed design of pre–equilibrium design is shown in figure 1

Given a composite nucleus, represented by `G4Fragment`, whose states are characterized by the number of excitons, succesive two–body interactions give rise to an intranuclear cascade which eventualy leads to a fully equilibrated residual nucleus. When the nucleus has reached the equilibrium, it is sent to `G4ExcitationHandler` for its clomplete deexcitation. At each stage of this equilibration process there is a competition between two decay modes. The decay by exciton–exciton interactions to more complex configurations is managed by `G4PreCompoundTransitions`.

This class calculates the rate at which a nucleus in a given state makes transitions to other states respecting the restrictions imposed by the selection rules.

A composite nucleus can also decay by emission of particles into the continuum. There is a set of six channels implemented and they are managed by `G4PreCompoundFragmentVector` in such a way that this is transparent for `G4PreCompoundModel`. Each channel have to be able to calculate its decay rate and to sample its kinetic energy. The channels are treated polymorphically through `G4VPreCompoundFragment`. We can distinguish between two kind of fragments. `G4VPreCompoundNucleon` is a specialization of `G4VPreCompoundFragment` that implements commonality between `G4PreCompoundProton` and `G4PreCompoundNeutron`. By the other hand, for more complex fragments, represented by `G4VPreCompoundIon`, we have to tak. into account the probability of formation of such fragments.

3 Equilibrium decays.

Compound nuclei are nuclear fragments produced in an interaction that have excitation energies and have reached a state of statistical equilibrium. The decay process of these fragments is managed by the `G4ExcitationHandler` class. Its responsability is to dispatch individual fragments to the models that perform the actual break up of the nucleus, based on ranges of applicability of the models and to return a list of particles with macroscopic path lenght, and nuclear fragments without excitation energies. `G4ExcitationHandler` manages five de–excitation models: `G4VEvaporation`, `G4VFission`, `G4VFermiBreakUp`, `G4VMultiFragmentation` and `G4VPhotonEvaporation`. These are abstract classes, so that the user can register alternative implementations. The statistical de–excitation classes are used as a default.

3.1 Evaporation phase.

`G4Evaporation` implements the statistical Weiskopf–Ewing's model[3] and inherit from the interface expected by the excitation handler class. `G4Evaporation` has a default set of eight competitive evaporation channels that are treated polymorphically through `G4VEvaporationChannel`. The number of evaporation channels can be changed at initialization time by the user. Those evaporation channels that always result in evaporation of nucleons or light ions are modelled in the `G4EvaporationChannel` class. Here the evaporation probability, the Coulomb barrier and the level density parameter are abstracted out for code re–use and to provide the user with the possibility to implement separate strategies. `G4VLevelDensityParameter` is the abstract interface and it is implemented in `G4EvaporationLevelDensityParameter` allowing the user to implement his own model. With respect to the Coulomb barrier, the abstract interface is defined in `G4VCoulombBarrier` while `G4CoulombBarrier` implements commonality for Coulomb barriers calculation. There exist specific classes for each kind of default fragments (n, p, ^{2}H, ^{3}H, ^{3}He and ^{4}He) that implement particularities for Coulomb barriers calculation like barrier penetration factors and serves to initialize properly the particular channel moving out of `G4Evaporation` the knowledge needed to instantiate the channels. The same schema is followed in the probability calculation. Here `G4VEmissionProbability` is the abstract interface and the implementation of that interface is done in the `G4EvaporationProbability` class. Particular classes are also responsibles for the right initialization and storing all the data needed in the probability classes. Finally, a set of subclasses, for instance `G4DeuteronEvaporationChannel` for ^{2}H, instantiate the channels mentioned above.

An important channel of de–excitation of heavy nuclei is fission. This process competes with evaporation particle emission and therefore it is implemented like a evaporation channel by using the abstract interface `G4VEvaporationChannel`. The implementation is done following

the Bohr–Wheeler statistical approach in the G4CompetitiveFission class. Again we have abstracted out the probability, level density parameter and fission barrier calculations re–using the already defined G4VLevelDensityParameter and G4VEmissionProbabiliy abstract classes. The probability calculation is implemented now by means of the class G4FissionProbability and calculation of level density parameter is done in G4FissionLevelDensityParameter class which uses G4EvaporationLevelDensityParameter. The new abstract interface defined is G4VFissionBarrier and the height of the fission barrier is worked out in the G4FissionBarrier class.

3.2 Explosive decays.

At very high excitation energies (> 3 MeV/nucleon) the secuential decays like the evaporation process are not valid any more. In this case we should expect a continuous flux of nucleons and light clusters from the decaying nucleus or even an explosion-like process leading to the total disintegration of the nucleus and the multiple emission of nuclear fragments of different masses for excitation energies comparable with the total binding energy. This fast process is the so called multifragmentation[5].

The G4StatMF implements the interface expected by excitation handler. We have implemented two ensembles defined by the common interface G4VStatMFEnsemble. In the microcanonical ensemble (G4StatMFMicroCanonical) all microscopic states obey strictly the conservation laws. All such states are considered to be equaly probable and the statistical weights of a break–up partition, implemented in the G4StatMFMicroPartition class, are determined by their entropy. The probability of each partition is calculated by G4StatMFMicroManager. In the macrocanonical ensemble G4StatMFMacroCanonical we have only constraints on the average mass and charge of the system. The distribution of partitions probabilities is given by a thermodynamical potential which depends on two chemical potentials and the free energy of the system. The temperature is fixed by the energy balance equation. Al these quantities and some other like the mean multiplicity are calculated by solving a set of coupled equations through the classes G4StatMFMacroTemperature, G4StatMFMacroChemicalPotential and G4StatMFMacroMultiplicity. In order to re–used the zero finding algorithm the parenthesis operator of those clases has been overloaded and the G4Solver template class is responsible to solve equations. Due to the fact that liquid–drop description is meaningless for the lightest clusters, we have created an interface G4VStatMFMacroCluster for clusters implementing in G4StatMFMacroMultiNucleon the characteristics of clusters with more than four nucleons and particular classes for clusters with one to four nucleons.

When a partition has been selected the excitation energy of each fragment is calculated. The fragment momenta the chaotical thermal motion is generated and the collective flow included. The kinetics energies obey the Boltzmann–Maxwell distribution with the common temperature. After the break–up fragments fly away from each other under the influence of the mutual Coulomb field leading to redistribution of fragment energies. All those processes are achieved with the help of G4StatMFChannel which, of course, manages a set of G4StatMFFragments.

For light fragments (with $A < 17$) even a realtively small excitation energy may be comparable with their total binding energy. In this case we assume that the main mechanism of de–excitation is the explosive decay of the excited nucleus into several smaller clusters. To describe this process we use the Fermi model[6].

Fermis model is analogous to the statistical multifragmentation model, but final states are assumed to be in their ground state. Due to the limitation to deal with light nuclei, we use only the microcanonical approach beacuse the number of avalaible channels is smaller. G4FermiBreakUp has a configuration list. G4FermiConfigurationList creates all possible configurations for a

given nucleus. Each `G4FermiConfiguration` contains a list of fragments chosen between 100 available fragments. The interface `G4VFermiFragment` is implemented for two kinds of fragments: `G4StableFermiFragment` and `G4UnStableFermiFragment` that will decay into stable fragments. The last class has four spezialised classes for ^{5}He, ^{5}Li, ^{8}Be and ^{9}Be which know how to decay those unstable ions. When a configuration has been chosen it is given to `G4FermiFragment` and the momenta distribution is obtained by random generation over the whole accesible phase space instead of consider explicitly the Coulomb expansion.

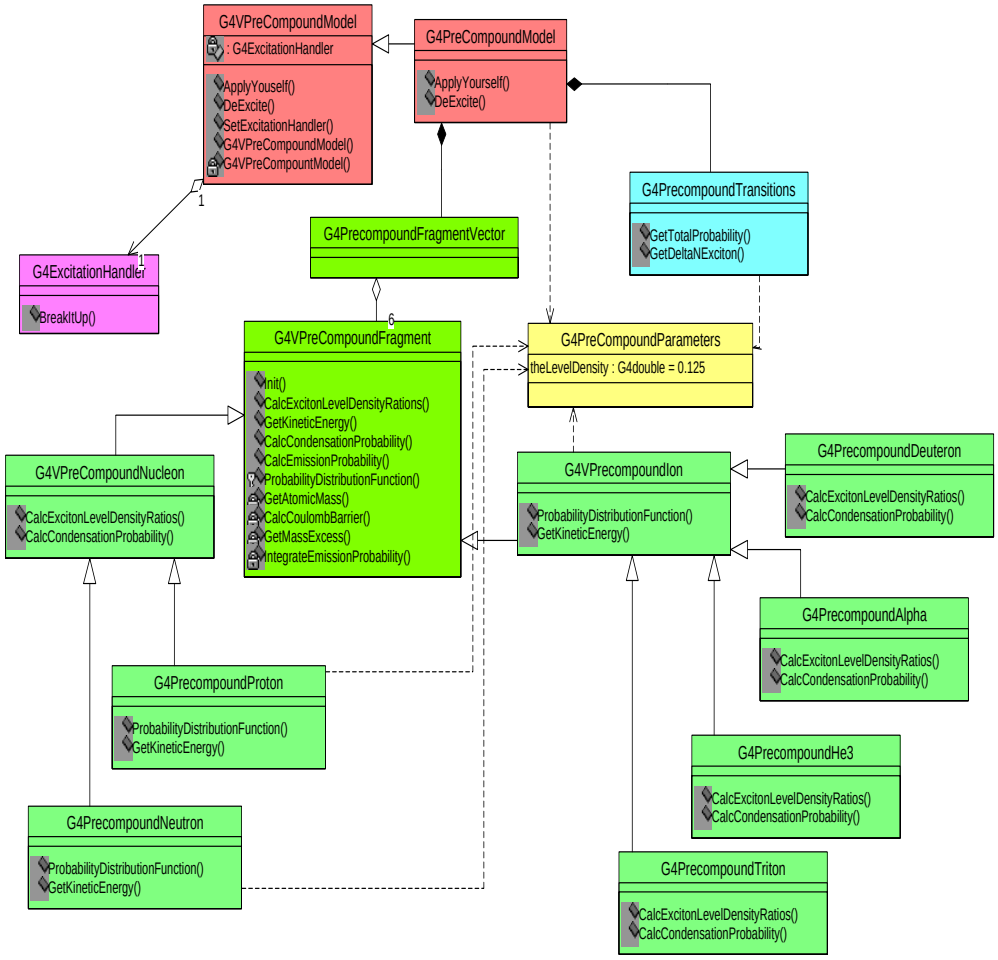

Figure 1: Detailed object oriented design of Pre–equilibrium category

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