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**OBJECT ORIENTED DESIGN AND IMPLEMENTATION OF AN
INTRA-NUCLEAR TRANSPORT MODEL**

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Abstract

The Hadron Kinetic Model is part of the Geant4 Simulation Toolkit; it covers the simulation of hadronic interactions in the intermediate energy range. Its role in the context of Geant4 hadronic models is outlined with emphasis on the physics content, and its Object Oriented design is illustrated.

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1 Introduction

The Geant4 Toolkit provides an ample set of physics models for the simulation of hadronic interactions. The models follow three different basic approaches: data-driven, parameterisation-driven and theory-driven modelling; in the overall framework Geant4 offers both complementary and alternative models. The hadronic models all follow the basic approach adopted through Geant4, that consists in exposing the physics to the users through the object oriented design, thus contributing to the transparency required for the validation of experimental results.

In the theory-driven approach parton string models cover the high energy ($E_{cm} > 5\text{GeV}$) domain; intra-nuclear transport models cover the intermediate energy régime down to energies of the order of 100 MeV; pre-compound models are provided for the lower energy end and a variety of nuclear deexcitation models cover the evaporation phase.

The Hadron Kinetic Model is part of the set of theory driven models for intra-nuclear transport [1] in the Geant4 Simulation Toolkit [2]. It can satisfy two use cases for intranuclear transport, both as a hadronic interaction model to be used by the physics processes, and as a back-end to higher energy models.

Object Oriented technologies play a fundamental role to address the complex physics domain described by this model. The Object Oriented design also provides the basis for extensive code reuse by other models, such as cascade models or quantum molecular dynamics models; it also provides the means for easy extension or evolution of the system.

2 The physics of the Hadron Kinetic Model

Geant4 Hadron Kinetic Model implements the physics describing meson-meson, meson-baryon, baryon-baryon interactions, involving resonance excitation and deexcitation and particle absorption, in the energy range O(100 MeV) to O(5 GeV); it includes a large set of exclusive channels.

Due to the complexity of the physics handled by the Hadron Kinetic Model, only a few main features are outlined in this paper; a more detailed description is available in reference [6].

2.1 The Kinetic Algorithm

The novelty of the model consists in introducing the concept of time development into the traditional approach of intra-nuclear cascade. The Kinetic Algorithm can be considered

a step by step updating of a particle vector; its implementation is performed according to the following scheme.

1. Create a vector of particles: assign initial particle types, their coordinates and momenta etc.; assign initial value for the time evolution parameter.
2. For a given step of the time evolution parameter find pairs of particles, according to a collision criterion, which are assumed to collide and particles which, according to their lifetimes, are assumed to decay.
3. Perform particle collisions and particle decays, determining the generation of outgoing particles; during this step particle coordinates and momenta are updated (particle propagation).
4. Starting from 2, perform the next step.

2.2 The scattering: cross sections and final states

The Hadron Kinetic Model handles two-body hadron elastic and inelastic scattering, including resonance excitation and deexcitation. The processes implemented cover baryon-baryon interactions (including baryon resonances), baryon-antibaryon annihilation, meson-baryon and meson-meson interactions. They include exclusive two-body processes for the following categories of interactions (where N indicates a nucleon, proton or neutron):

- proton-proton and neutron-neutron
- proton-neutron
- $N - \Delta$
- $N - N^*$
- $N - \Delta^*$
- $N^* - \Delta$
- $\Delta - \Delta^*$
- $N^* - N^*$, $\Delta^* - \Delta^*$ and $N^* - \Delta^*$
- $\Delta - \Delta$
- generic baryon-baryon

- baryon-antibaryon
- meson-baryon
- meson-meson

The cross sections are functions of the incoming and outgoing particle types, their internal quantum numbers, like isospin, and their momenta. The overall physics approach of the Hadron Kinetic Model in this domain closely follows the one adopted by the UrQMD model [4]. The cross sections are calculated through various methods: from tabulations of experimental data, from parameterisations according to an algebraic function or from other cross sections via general principles, such as detailed balance [3], [4] or the additive quark model [5].

The angular distributions for all the relevant two-body processes are assumed to be similar and are determined according to the procedure described in reference [4].

Resonance decay channels are sampled according to the partial decay widths, which depend on the mass of the resonance.

Hadron-nucleus or nucleus-nucleus processes involve hadron-hadron collisions in high density nuclear matter. Under these extreme conditions the Pauli-blocking, which modifies the process vacuum behaviour, reducing a free particle cross section or decay width to an effective one due to Fermi statistics, must be taken into account. Each possible collision or decay is validated by checking the phase space fermion density, since a process can occur only if there is enough room (according to the Pauli principle) to accommodate the final state fermions. This effect is implemented treating fermions as gaussian shaped density distributions in the phase space. For each new fermion, produced by a possible collision or decay, a phase space overlapping density function is calculated and used to simulate Pauli-blocking. A detailed description of the used procedure is available in reference [6].

2.3 The field propagation

At every step, before performing an interaction - i.e. particles collision or particle decay - coordinates and momenta of all particles travelling through the nucleus are updated from the values at the time of previous interaction to the current time. The transportation of these particles is done describing the particle-nucleus interaction using phenomenological mean-field potentials, the so called “optical potentials” [6].

The particle propagation can be operated either with the cascade approach, i.e. along a straight line trajectory, using potentials only to evaluate the final particle energy

at the end of the step, or with a numerical integration of the equations of motion, using the classical Runge-Kutta method.

3 The object oriented analysis and design of the model

The Hadron Kinetic Model is integrated in the framework of Geant4 Theory Driven Hadronic Models [7], that defines its design at the architectural level. An analysis and design process has been applied to define its detailed design.

The domain analysis has led to the identification of the main areas of responsibilities in the Model: the overall management, the handling of the scattering process and the propagation through the nuclear field. Additional utilities, such as the description of the nucleus and of the particles involved in the interactions, are common to the whole set of Geant4 hadronic models.

The Object Oriented Analysis and Design process has led to the class diagram of the Hadron Kinetic Model shown in figure 1; due to the complexity of the model, only the main features are listed - a more detailed design is available in reference [6].

The G4HadronKineticModel class inherits from the hadronic model base class G4VIntraNuclearTransportModel, that fullfills the role of providing to the intra-nuclear transport models an interface to the processes as well as the possibility to be used as a back-end to high energy models. G4HadronKineticModel class has the responsibility of managing the main functionality of the model, as described in section 2.1. It delegates the responsibility of the scattering and of the field transport to the G4VScatterer and G4VFieldPropagation classes respectively.

The concrete class G4Scatterer, inheriting from G4VScatterer, handles the scattering process. It manages the complex physics content of the scattering process in the energy domain of the intra-nuclear transport, including the resonance region, through a design based on a recurrent Composite Pattern [8]. The scattering channel classes inherit from the G4VCollision abstract base class; some of them are composed of sub-channels, modeled through the Composite Pattern (for instance, the “ExcitedNucleon-Nucleon” scattering channel consists of sub-channels such as N1440-p, N1520-n etc.). The Composite Pattern also handles the specialization of collisions into elastic (leaf) and inelastic (composite) ones. The Composite Pattern is also adopted to handle the cross section sector, mapping the availability of experimental data or theoretical cross section formulae for the collisions: for instance, the total cross section of a channel is represented by a leaf cross section whenever specific data or model are available and by a composite cross section (composed of single branch cross sections) when no measurements or models for it are available. Both leaf and composite cross sections are handled transparently by the

Collisions through the same abstract interface to `G4VCrossSectionSource`.

The Strategy Pattern [8] is used throughout the design to handle interchangeable algorithms, whenever alternative models or parameterisations for the same physics item are available.

A class diagram of the Scatterer is shown in figure 2.

This flexible design of the Scatterer allows for an easy extensibility of the set of scattering processes handled by the Hadron Kinetic Model, whenever new theoretical descriptions or experimental data become available to improve the overall precision of the physics of the model itself; at the same time, it makes alternative physics implementations for single scattering channels easily interchangeable, thus allowing to investigate and optimise the physics capabilities of the model. The clear separation between the cross section sector and the generation of final states further enhances the flexibility of the Scatterer to accommodate alternative modelling. The recurrent Composite Pattern contributes to improve the overall performance, by enabling to establish a logical hierarchy in the messaging of the physics components. The general design of the Scatterer makes it suitable to be used also by other hadronic simulation models (such as, for instance, the QMD Model or cascade models), as well as in other contexts of Geant4 physics simulation.

The field propagation is handled by the `G4VFieldPropagation` class, that is abstract to allow different strategies to be used. The concrete `G4RKFieldIntegrator` class derives from it, and performs the propagation of particles via a Runge-Kutta numerical integration. It uses classes for optical potentials (`G4VKMOpticalField`) and for their derivatives (`G4VKMOptical_EqRhs`) that are abstract in order to implement again a Strategy Pattern. `G4VKMOptical_EqRhs` inherits from the `G4Mag_EqRhs` class of the Geant4 geometry category; this allows to reuse in the Kinetic Model the code common to the Geometry-Transportation domain for the integration of the equations of motion.

The Hadron Kinetic Model makes use of other design components common to the Geant4 Hadronic Models, such as the classes responsible for the description of the nucleus and of the particles involved in the interactions.

The Object Oriented design allows to expose the physics of the model in a detailed way. The clear distinction between the calculation of cross sections and the generation of final states, the explicit use of units everywhere in the code, the absence of arbitrary parameters within formulae, the independence of the physics models from tracking contribute, together with the Object Oriented design, to the transparency of the physics, required for the validation of experimental results.

A spiral cyclic model of software process has been adopted throughout the whole development.

4 Conclusions

The Geant4 Hadron Kinetic Model represents a novel approach to intra-nuclear transport. Object Oriented methodologies have been a key factor to handle the complexity of the underlying physics and to ensure the future extensibility and maintenance of the model.

The Hadron Kinetic Model is meant to become part of Geant4 public release, following the completion of the testing phase.

5 Acknowledgements

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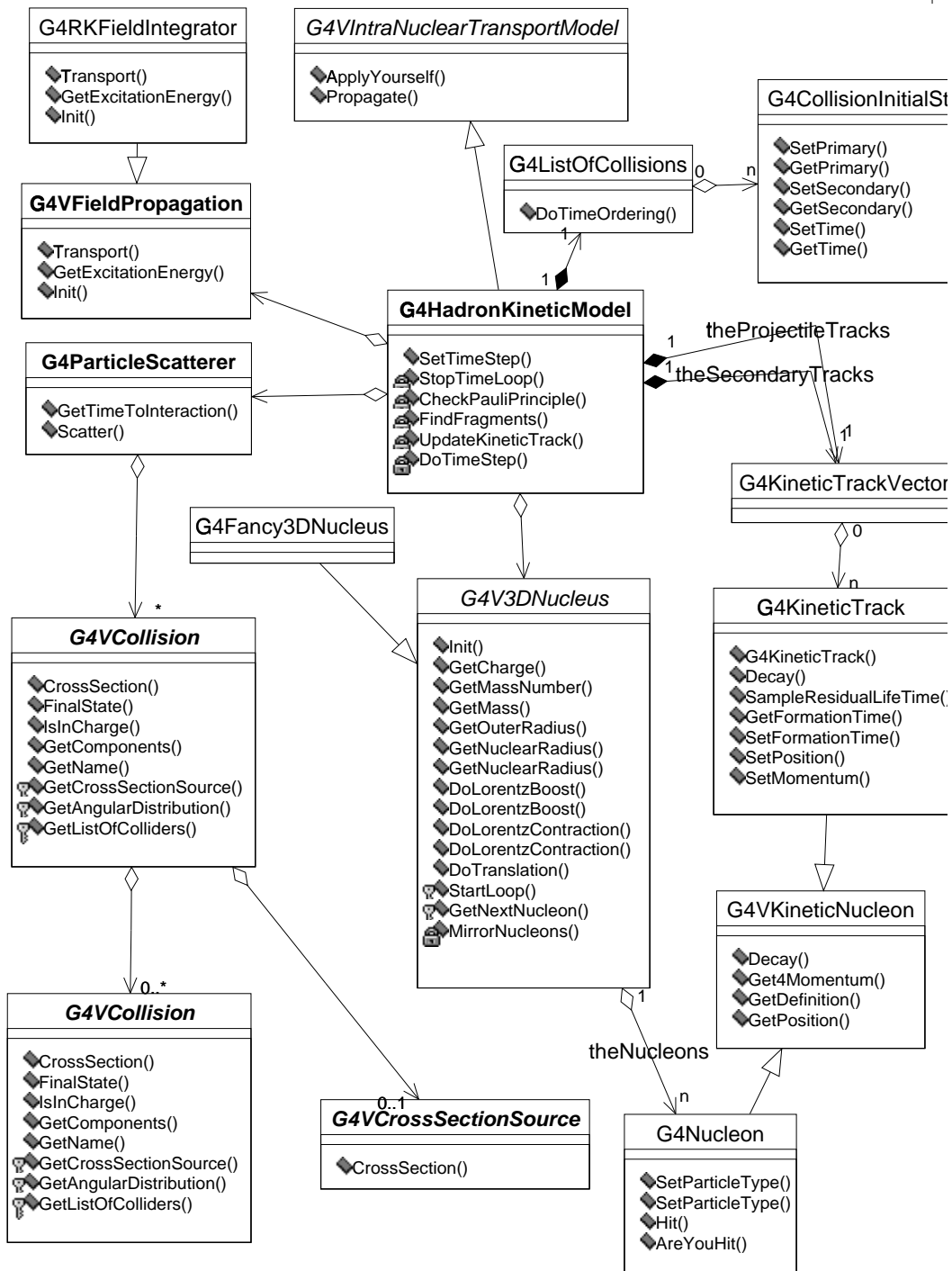


Figure 1: An overview of the Hadron Kinetic Model design: top level class diagram.

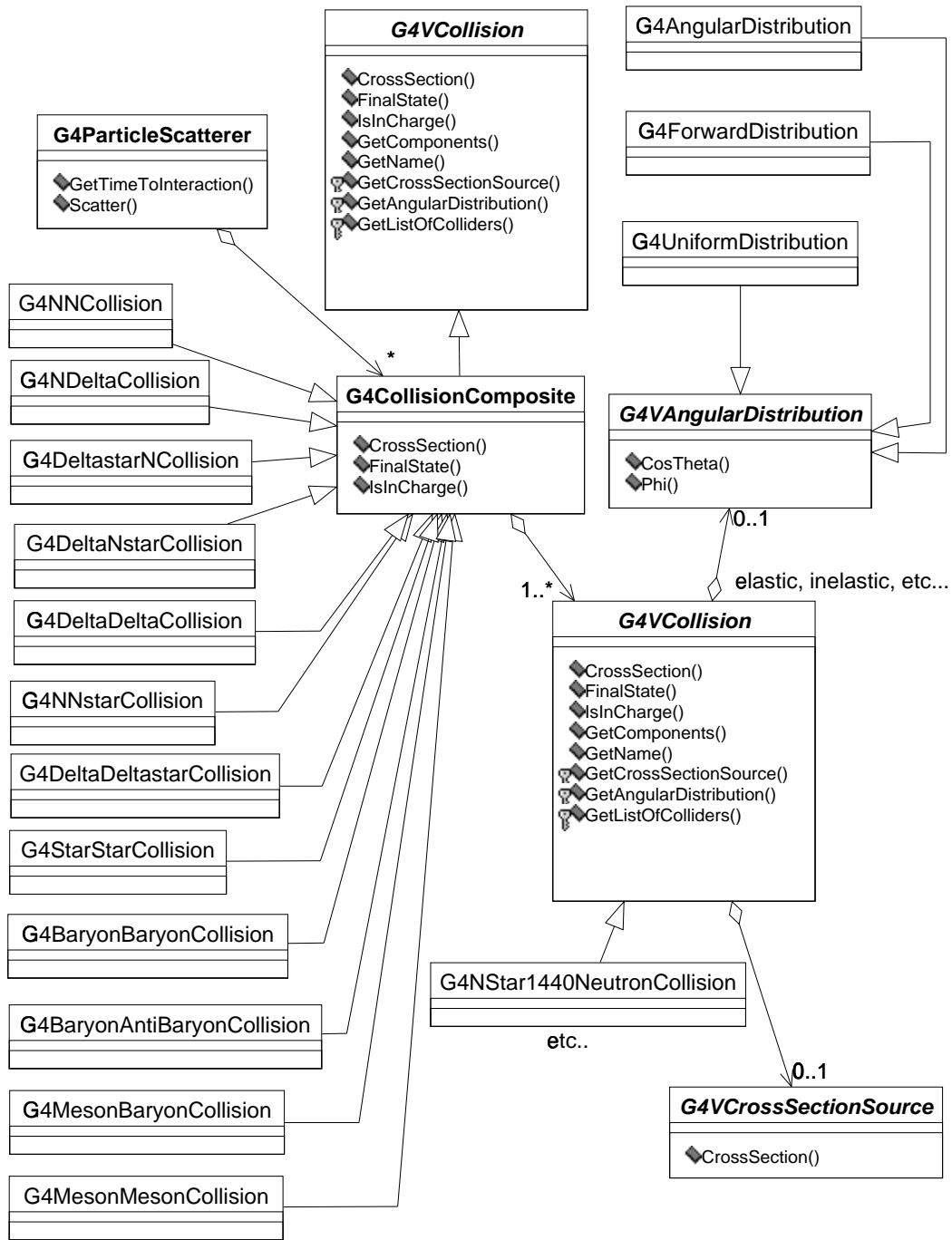


Figure 2: The Scatterer top level class diagram.