Geant4 hadronic physics status and validation for large HEP detectors

J.P. Wellisch
CERN, Geneva, Switzerland

Optimal exploitation of hadronic final states played a key role in successes of all recent collider experiment in HEP, and the ability to use hadronic final states will continue to be one of the decisive issues during the analysis phase of the LHC experiments.
Monte Carlo techniques facilitate the use of hadronic final states, and have been developed for many years. We will give a brief overview of the physics underlying hadronic shower simulation, discussing the three basic types of modeling; data driven, parametrization driven, and theory driven modeling at the example of Geant4. We will confront these different types of modeling with the stringent requirements posed by the LHC experiments on hadronic shower simulation, and report on the current status of the validation effort for large HEP applications. We will address robustness, and CPU and physics performance evaluations.

1. Model Overview

The number of model currently provided with or in development in the context of GEANT4 is growing continuously. We give an enumeration of the current status, including a brief description for each model.

1.1. Modeling Total Cross-sections

The total cross-sections for inelastic scattering, capture of neutral particles, induced fission and elastic scattering have been carried over from GEANT3.21[1]. The software design in GEANT4 allows to overload this default with specialized data-sets. Custom data sets are provided for proton induced reactions[2], neutron induced reactions[3], pion reaction cross-sections[4], and ion spallation reactions[5], as well as neutron interactions at energies below 20 MeV.

1.2. Modeling Final States

In modeling final states, three basic types of models are distinguished; Models that are predominantly based on experimental or evaluated data, models that are predominantly based on parameterizations and extrapolation of experimental data under some theoretical assumptions, and models that are predominantly based on theory.

A. Data driven models:

When experimental or evaluated data are available with sufficient coverage, the data driven approach is considered to be the optimal way of modeling. Data driven modeling is used in the context of neutron transport, photon evaporation, internal conversion, radioactive decay, capture final states, absorption at rest, and isotope production. We also use data driven modeling in the calculation of the inclusive scattering cross-sections for hadron nuclear scattering. Limitations exist at high projectile energies, for particles with short life-times, and for strange baryons, as well as the K^0 system. Theory based approaches are employed to extract missing cross-sections from the measured ones, or, at high energies, to predict these cross-sections.

The main data driven models in GEANT4 deal with neutron and proton induced isotope production, and with the detailed transport of neutrons at low energies. The codes for neutron interactions are generic sampling codes, based on the ENDF/B-VI data format, and evaluated neutron data libraries such as ENDF/B-VI[15], JENDL3.3[19], and FENDL2.2[17]. Note that any combination of these can be used with the sampling codes. The approach is limited by the available data to neutron kinetic energies up to 20 MeV, with extensions up to 30 MeV or 150 MeV for some isotopes.

The data driven isotope production models that run in parasitic mode to the transport codes are based on the MENDL[20] data libraries for proton and neutron induced production. They complement the transport evaluations in the sense that reaction cross-sections and final state information from the transport codes define the interaction rate and particle fluxes, and the isotope production model is used only to predict activation.

The data driven approach is also used to simulate photon evaporation and internal conversion at moderate and low excitation energies, and for simulating radioactive decay. Both codes are based on the ENSDF[16] data of nuclear levels, and transition, conversion, and emission probabilities. In the case of photon evaporation the data are supplemented by a simple theoretical model (giant dipole resonance) at high excitation energies.

Finally, data driven modeling is used in the simulation of the absorption of particles coming to a rest, mainly for μ^-, π^-, K^-, and $\bar{p}$, in order to describe the fast, direct part of the spectrum of secondaries, and in the low energy part of the modeling of elastic scattering final states in scattering off Hydrogen.

B. Parameterized models:

Parameterizations and extrapolations of cross-sections and interactions are widely used in the full range of hadronic shower energies, and for all kinds of reactions. In GEANT4, models based on this paradigm are available for low and high particle energies respectively, and for stopping particles. They are exclusively the result of re-writes of models available from GEANT3.21, predominantly GEISHA[22]. They include induced fission, capture, and elastic scattering, as well as inelastic final state production.

C. Theory based models:

Theory based modeling is the basic approach in many models that are provided by or in development for GEANT4. It includes a set of different theoretical approaches to describing hadronic interactions, depending on the addressed energy range and CPU constraints.

Parton string models for the simulation of high energy final states ($E_{CMS} > O(5\text{ GeV})$) are provided and in further development. Both diffractive string excitation, and dual parton model or quark gluon string model are used. String decay is generally modeled using well established fragmentation functions. The possibility to use quark molecular dynamic is currently in preparation.

In the energy regime below 5 GeV center of mass energy, intra-nuclear transport models are provided. For cascade type models a re-write of HETC[6] as well as INUCL[7] is in provided, as well as an implementation of a time-like cascade[8]. For quantum molecular dynamics models, an enhanced version of UrQMD[9], as well as various variants of ablation/abrasion models are being written.

Note that the cascade models are based on average geometrical descriptions of the nuclear medium, and take effects like Pauli-blocking, coherence length and formation times into account in a effective manner. Scattering is done as in the QMD, with the possibility to use identical scattering implementations. The QMD models calculate the interaction Hamiltonian from two- and three-body interactions of all particles in the system, and solve the Newtonian equations of motion with this time-dependent Hamiltonian numerically. Scattering is done using smeared resonance cross-sections, taking Pauli's principle into account by investigating local phase-space. The approach promises to give all correlations in the final state correctly, and has no principle limitations in its applicability at low energies. It is very CPU expensive.

At energies below O(100 MeV) we provide the possibility to use exciton based pre-compound models to describe the energy and angular distributions of the fast particles. In this area one model is released, and one more is in preparation.

The last phase of a nuclear interaction is nuclear evaporation. In order to model the behavior of excited, thermalised nuclei, variants of the classical Weisskopf-Ewing model are used. Specialized improvements such as Fermi's break-up model for light nuclei, and multi-fragmentation for very high excitation energies are employed. Fission, and photon evaporation can be treated as competitive channels in the evaporation model.

As an alternative for, among others, intra-nuclear transport, the chiral invariant phase-space decay model CHIPS is in development. It is a quark-level 3-dimensional event generator for fragmentation of excited hadronic systems into hadrons, and is expected to find applicability in a wide range of hadron and lepton nuclear interactions, once fully explored.

A theoretical model for coherent elastic scattering was added recently, using the Glauber model and a two Gaussian form for the nuclear density. This expression of the density allows to write the amplitudes in analytic form. Note that this assumption works only since the nucleus absorbs hadrons very strongly at small impact parameters, and the model describes nuclear boundaries well.

For lepton nuclear interactions, muon nuclear interactions are provided. Here the leptonic vertex is calculated from the standard model, and the hadronic vertex is simulated using a suitable set of models from the above described. Neutrino nuclear interactions will be added in due course.

2. Sample data driven models

As an example of a data driven model, we briefly describe the models for neutron and proton induced isotope production. These models are running in parasitic mode to the GEANT4[10] transport models, and can be used in conjunction with any set of models for final state production and total cross-sections. They have been written to allow for detailed isotope production studies, covering most of the spallation neutron and proton energy spectrum. They are based on evaluated nucleon scattering data for kinetic energies below 20 MeV, and a combination of evaluated data and extrapolations at energies up to 100 MeV. The upper limit of applicability of the model is 100 MeV nucleons kinetic energy.

The evaluated data libraries that are the basis of the GEANT4 neutron transport and activation library G4NDL0.2 are Brond-2.1[11], CENDL2.2[12], EFF-3[13], ENDF/B-VI.0[15], ENDF/B-VI.1, ENDF/B-VI.5, FENDL/E2.0[17], JEF2.2[14], JENDL-FF[19], JENDL-3.1, JENDL-3.2, and MENDL-2[20].

The G4NDL selection was guided in large parts by the FENDL2.0 selection. Additions to and small mod-

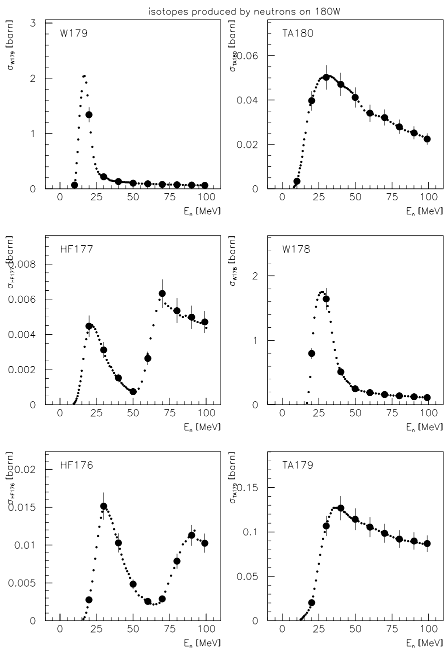

Figure 1: Isotope production cross-sections for neutron induced production of important isotopes as simulated using the isotope-production code in GEANT4. Large points are simulation results, small points are evaluated data from the MENDL2 data library.

ifications of this selection were possible due to the structure of the SHAPE GEANT4 neutron transport code and the use of the file system to maximize the flexibility of the data formats. The inclusion of the MENDL data sets is fundamental for these models.

Figure 1 shows an example of the simulated cross-section in comparison to evaluated data from the MENDL collection, using 10^6 events at each energy. A systematic error of 15% was added to the simulation results, to take the error in the extrapolation of the total cross-sections into account. For a complete description and a more comparisons, see[21].

3. Sample parametrized models

Parameterization based models have been found to be very powerful in the case of calorimeter simulation. Without giving a detailed description of these models, we want to illustrate the predictive power for the case of the GEANT4 high energy models in Fig. 2 for production of neutral pions in interactions of kaons and pions with Gold and Aluminum.

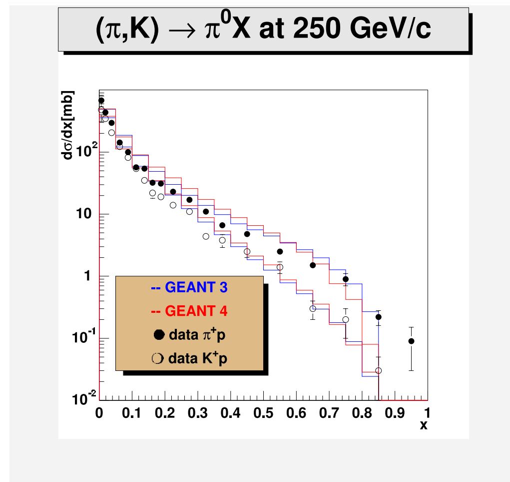

Figure 2: Comparison of production cross-sections of neutral pions in kaon and pion induced reactions with measurement.

4. Sample theory driven models

Given that the chiral invariant phase-space decay model CHIPS is a rather new development and is developed only within GEANT4, we choose this as an example for a theory based model. CHIPS is a quark-level 3-dimensional event generator for fragmentation of excited hadronic systems into hadrons. An important feature is the universal thermodynamic approach to different types of excited hadronic systems including nucleon excitations, hadron systems produced in e^+e^- interactions, high energy nuclear excitations, etc.. Exclusive event generation, which models hadron production conserving energy, momentum, and charge, generally results in a good description of particle multiplicities and spectra in multi-hadron fragmentation processes. To illustrate the predictive possibilities of this ansatz, we show a comparison between CHIPS predictions and measurement in the case of proton anti-proton annihilation in Fig. 3. For details of the model please see[23], [24], and [25].

5. Sample of a recent development

The most recent developments in Geant4 hadronics concern the cascade codes. They have first been released for public use beginning 2003. They include a novel modeling Ansatz for cascade calculations, that we called Binary Cascade, which we find to have significant predictive power. It shall serve here as an example for a recent development.

Binary cascade introduces a new approach to cascade calculations, being based on a detailed 3-dimensional model of the nucleus, being based exclusively on binary scattering between reaction par-

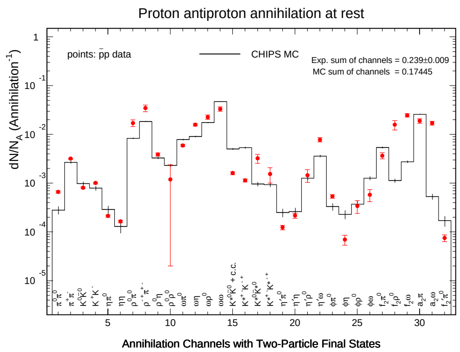

Figure 3: Comparison of the branchings in two particle final states in proton anti-proton annihilation with the predictions of CHIPS.

ticipants and nucleons within this nuclear model. In some sense this makes it a hybrid between a classical cascade code, and a quantum molecular dynamics model[27].

In binary cascading, like in QMD, each participating nucleon is described by a Gaussian wave-package.

$$\phi(x, q_i, p_i, t) = (2/(L\pi)^{3/4} exp(-2/L(x - q(t))^2 + ip_i(t)x)$$

Here x, and t are space and time coordinates, and q_i and p_i describe the particles' positions in configuration and momentum space.

The total wave-function is assumed to be the direct product of the wave-functions of the participating nucleons and hadrons, where participating means that they are either primary particles, or have been generated or freed in the process of the cascade. Note that we do not take Slaters determinant into account in the description. The wave function is not anti-symmetrized.

For such a wave-form, the equations of motion are identical in structure to the classical Hamiltonian equations, and can be solved using the well known numerical integration methods of the cascade transport approach.

In binary cascade, unlike in QMD where it can be looked at as self-generating from the system configuration, the Hamiltonian is calculated from optical potentials.

The imaginary part of the G-matrix acts like a scattering term. It is included in the model using discrete scattering and particle decay in the cascade, with free 2-body cross-sections and a geometrical interpretation of the cross-section, and effective decay width for the strong resonances.

Two examples of the model's predictive power in proton nuclear scattering are given in Fig. 5 and Fig. 4. Figure 4 shows the prediction for the total reaction cross-section in proton nuclear scattering for a set of nuclei as a function of the kinetic energy of the

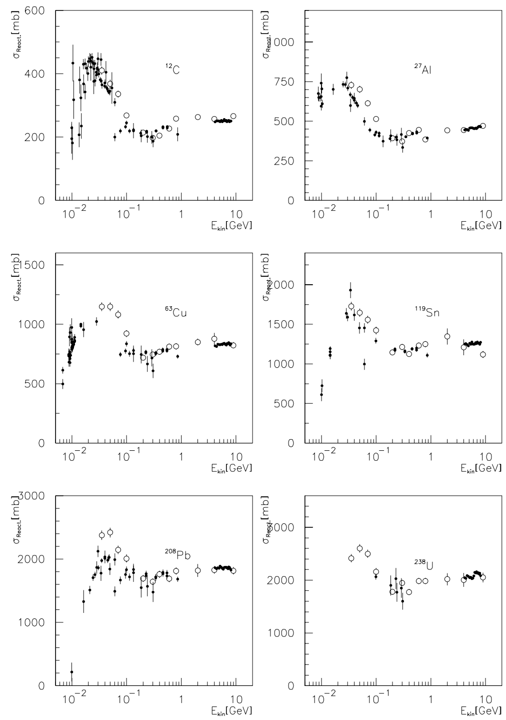

Figure 4: Prediction for the total reaction cross-section in proton nuclear scattering for a set of nuclei as a function of the kinetic energy of the proton. Open circles are cascade predictions, and points are experimental data.

proton. The data are taken from reference[28]. Figure 5 shows the neutron spectra predicted by binary cascade for proton scattering in iron at a set of initial proton energies at various scattering angles. The data stem from the EXFOR database, and include data from references [29], [30], [31], and [32].

6. Computational fundaments

In this section we give a brief impression of the usage of Object Oriented frameworks for hadronic generators in GEANT4. We have put particular focus on the level of extendibility that can and has been achieved by our Russia dolls approach to Object Oriented design, and implementation frameworks play a fundamental role in this.

A top-level, very abstracting implementation framework provides the basic interface to the other GEANT4 categories, and fulfills the most general use-case for hadronic shower simulation, providing flexibility at the level of selecting physics processes to be included in a simulation run. It is refined for more specific use-cases by implementing a hierarchy of implementation frameworks, each level implementing the common logic of particular use-cases, and refining the granularity of delegation. Abstract classes are used as the

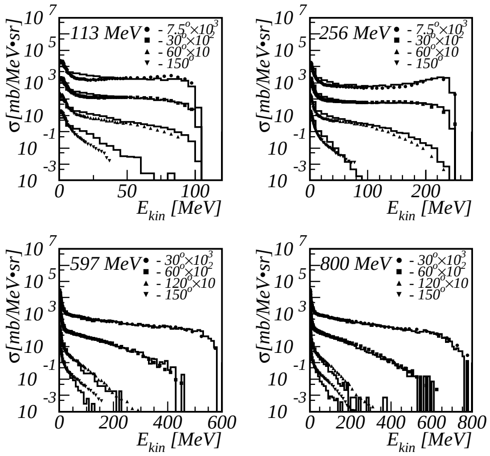

Figure 5: Neutron spectra predicted by binary cascade for proton scattering off iron at a set of initial proton energies at various scattering angles. The histogram is Monte Carlo, and the points are experimental data.

delegation mechanism[1]. All framework functional and flexibility requirements were obtained through use-case analysis. The lower level implementation frameworks address flexibility in choice of cross-sections, models for final state production, and models for isotope production (Level2), flexibility in the creation of theory driven models from components like cascades, string-parton models, pre-equilibrium decay models and evaporation phases (Level 3), flexibility of how to assemble cascade or string parton models from components like scattering terms, string excitation, field propagation, string fragmentation (Level 4), and flexibility and tailoring for fragmentation functions in string decay(Level5). For details please see reference[26].

7. Status of validation for large HEP detectors

Much work has been invested by experimental groups to use and validate GEANT4 hadronic physics for HEP detectors; in particular calorimetry, but also for tracker simulations. Very recently, these efforts were put onto a more solidly managed footing by the creation of the validation sub-project in the simulation project of the applications area of the LHC computing grid project. This effort is now being et up and lead by Fabiola Gianotti.

[1]The same can be achieved with template specializations with slightly improved CPU performance but at the cost of more complex designs and less portability.

Prior validation efforts and usages of GEANT4 hadronics in HEP we have become aware of are enumerated below:

- ATLAS tracker test-beam simulation; data with dedicated interaction trigger,
- CMS tracker test-beam, cross-section validation,
- ATLAS Tile Calorimeter test-beam simulation,
- ATLAS Forward Calorimeter test-beam simulation,
- ATLAS End-Cap Hadronic calorimeter test-beam simulation,
- LHCb hadronic calorimeter test-beam simulation,
- BTeV Crystal test-beam simulation,
- CMS barrel combined test-beam simulation,
- CsI/GLAST test-beam simulation,
- H1 forward barrel test-beam simulation,
- ATLAS combined end-cap simulation,
- ALICE radiation protection benchmark simulation, and
- CMS activation studies.

There is a strong possibility, that the above list is not exhaustive. It may not even be representative. Is meant solely to give an impression of the extent of usage of GEANT4 hadronic physics in the HEP community.

In order to give an impression of the predictive power of Geant4 hadronic physics, results of a repetition of one of the test-beam efforts using a simplified test-beam analysis are shown in Figs.6,7,8. They include data and simulation results from published, original sources, provided by the ATLAS end-cap community.

8. Conclusions

Taking the view of the LHC experiments, it has become evident that all modeling techniques - data driven, parameterization driven, and theory driven - are need to satisfy all LHC needs in an optimal manner. Data driven modeling is known to provide the best, if not only, approach to low energy neutron transport for radiation studies in large detectors. Parametrization driven modeling has proven to allow for tuning of the hadronic shower Monte Carlo for particle energies accessible to test-beam studies, is the most CPU performent possibility for calorimeter simulation, and is also widely used in this field. Theory

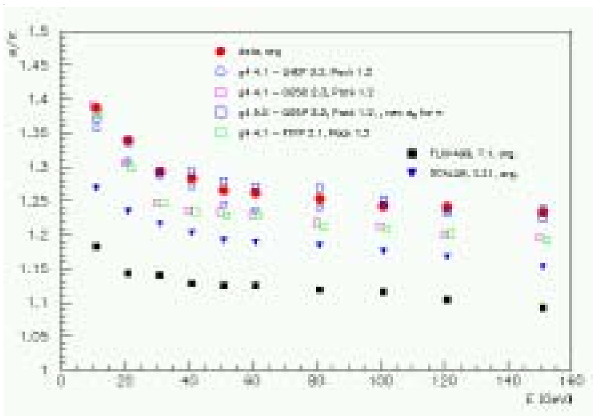

Figure 6: Prediction of the e/pi ratio for the ATLAS end-cap calorimetry. Open circles are results of the simplified analysis, full points are results of the full analysis.

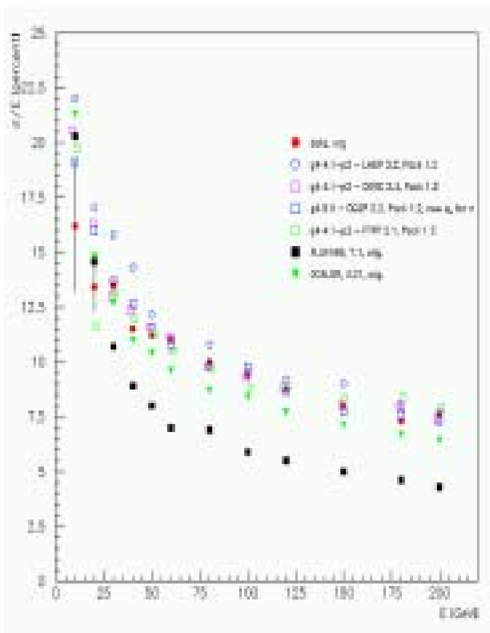

Figure 7: Prediction of the energy resolution for the ATLAS end-cap calorimetry. Open circles are results of the simplified analysis, full points are results of the full analysis.

driven modeling is the approach that promises safe extrapolation of results toward energies beyond the test-beam region, and allows for maximal extendibility and customizability of the underlying physics.

The use of state of the art software technology is the key that allows for distributed development of the physics base of a hadronic shower simulation tool-kit in the Geant4 context. It allows the work of many experts in the field to be combined in a coherent manner, and offers the user the possibility to unify their

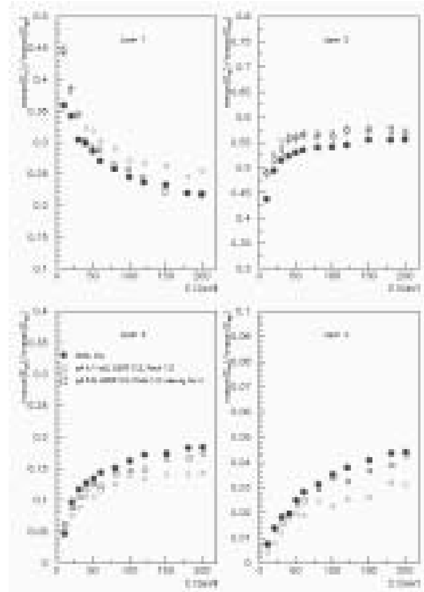

Figure 8: Prediction of the e/pi ratio for the ATLAS end-cap calorimetry. Open circles are results of the simplified analysis, full points are results of the full analysis.

knowledge in a single executable program in a manner that he deems optimal for his particular problem. This is a completely new situation. In a very short time it has lead to an unexpectedly wide range of modeling possibilities in Geant4, and an unprecedented ease of flexibility of usage of models and cross-sections.

At the time of writing, Geant4 hadronic physics has become a very widely used program, with a predictive power in terms of physics that is as good or better than GEANT3 at its best.

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