

# **Hadronic Physics II**

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## Outline

- (Short) Reminder
- NeutronHP (ParticleHP)
- Radioactive Decay
- Nucleus-nucleus (ion-ion)
- Gamma/lepton-nuclear
- Stopping Physics
- Exercises



## Reminder: Hadronic Models, Cross Sections, Framework, Physics Lists

### Hadronic interactions

- Hadrons (π±, K±, K°L, p, n, α, etc.), produced in jets and decays, travel through the detector (H, C, Ar, Si, Al, Fe, Cu, W, Pb...)
- Therefore we need to model hadronic, strong interactions hadron – nucleus -> anything
- In principle, QCD is the theory that describes all hadronic interactions in practice, perturbative calculations are applicable only in a tiny (but important !) phase-space region

the hard scattering at high transverse momentum whereas for the rest, *i.e.* most of the phase space soft scattering, re-scattering, hadronization, nucleus de-excitation only approximate models are available

 Hadronic models are valid for limited combinations of particle type – energy – target material

## **Partial Hadronic Model Inventory**



#### Hadronic Interactions from TeV to meV



Hadronic Cross Sections and (Final-State) Models

- In Geant4, there is a clear separation between cross sections related to the probability of an elastic or inelastic hadron-nucleus interaction, and therefore to the length that a hadron projectile flies in a material before interacting – and final-state models – related to the number, type and properties of the produced secondaries
- For each combination of projectile energy target
  - ≥ 1 cross sections must be specified in a physics list : the first available is used
  - 1 or 2 (final-state) models must be specified in a physics list : if two, a random number is thrown to decide which of the two models to use
    - Assumed a linear probability as a function of the energy, over an interval called **transition region**, defined arbitrarily to get smooth observables

## Hadronic Framework







Energy

### **Transition between Final-State Models**







## FTFP\_BERT

Recommended physics list for High-Energy Physics. Its main components are :

- **FTF** (Fritiof) hadronic string model, used above 3 GeV
- **BERT** (Bertini-like) intra-nuclear cascade model, used below 6 GeV
- Nucleus de-excitation : Precompound + evaporation models
- Neutron capture
- Nuclear capture of negatively charged hadrons at rest
- Hadron elastic
- Gamma- , electron- , and muon-nuclear
- Standard electromagnetic physics
- NO : neutron-HP , radioactive decay , optical photons

## A few other Physics Lists

- FTFP\_BERT\_HP : as FTFP\_BERT, but with NeutronHP for neutrons Ekin < 20 MeV</p>
  - Shielding : similar to FTFP\_BERT\_HP, but using for ions also the QMD (Quantum Molecular Dynamics) model
    - QMD used in the range [100 MeV/A, 10 GeV/A]; BIC is used below 90 MeV/A; FTFP is used above 9.99 GeV/A
- FTFP\_INCLXX : similar to FTFP\_BERT, but using INCLXX for some particles
  - Protons, neutrons, charged pions below 20 GeV; FTFP above 15 GeV
- QGSP\_BERT : similar to FTFP\_BERT, but using QGS (Quark Gluon String) model at high energies
  - [3, 6] GeV transition BERT FTFP ; [12, 25] GeV transition FTFP QGSP
- QGSP\_BIC : similar to FTFP\_BERT but using QGS and BIC (Binary Cascade) instead of FTF and BERT when possible
  - Protons, neutrons : BIC < 6 GeV , FTFP in [3, 25] GeV , QGSP > 12 GeV
     Pions & kaons : BERT < 6 GeV , FTFP in [3, 25] GeV , QGSP > 12 GeV



# NeutronHP (ParticleHP)

## An interesting complication: Neutrons

- Neutrons are abundantly produced
  - Mostly "soft" neutrons, produced by the de-excitation of nuclei, after hadron-nucleus interactions
  - It is typically the 3<sup>rd</sup> most produced particle (after electrons and gammas)
- Before a neutron "disappears" via an inelastic interactions (or decays or exits the world volume), it can have many **elastic scatterings** with nuclei, and eventually can "thermalize" in the environment
- CPU time can vary by an order of magnitude depending on the physical accuracy of the **neutron transportation** simulation
  - For typical high-energy applications, a simple treatment is enough (luckily!)
  - For other applications, a more precise, data-driven and isotope-specific treatment is needed, especially for neutrons with kinetic energies below ~ MeV

## Neutron High Precision (HP)

- High Precision treatment of low-energy neutrons
  - Ekin < 20 MeV , down to thermal energies
  - Includes 4 types of interactions: elastic scattering, radiative capture, fission, inelastic scattering
  - Based on evaluated neutron scattering data libraries (pointed by the environmental variable G4NEUTRONHPDATA)
  - It is precise, but slow !
- Not needed for most high-energy applications; useful for:
  - Cavern background, shielding, radiation damage, radio-protection
- Not used in most physics lists
  - If you need it, use one of the \_HP physics lists: FTFP\_BERT\_HP, QGSP\_BERT\_HP, QGSP\_BIC\_(All)HP, Shielding

## Notes about NeutronHP (1/2)

- Because of several reasons (binned look-up data tables, inclusive *i.e.* incomplete, without correlations – information, *etc.*) there might be small non-conservations of energy / momentum / baryon-number
  - For all types of interactions (elastic, capture, fission and especially inelastic)
  - To avoid that, by default Geant4 uses some "tricks" (*e.g.* emitting some gammas) to conserve at least energy. This, however, can affect the average values, so for dosimetry applications — which care about energy conservation on average — the following UI command should be used to avoid any "adjustment":

#### /process/had/particle\_hp/do\_not\_adjust\_final\_state true

- Doppler broadening of the resonances, due to the thermal motion of the target nucleus, is calculated on-the-fly (from T = 0 K values)
  - CPU intense: for those applications not sensitive to neutrons below ~ 100 keV, it can be switched off by setting the following UI command

/process/had/particle\_hp/neglect\_Doppler\_broadening true

## Notes about NeutronHP (2/2)

- Geant4 Neutron Data Libraries:
  - The most recent one, G4NDL4.7.1, is based on JEFF-3.3
    - Previous ones are based on ENDF/B
    - The main motivation for using JEFF instead of ENDF/B is that it provides the closest agreemet with MCNP; moreover, it provides also trans-uranic isotopes
  - Alternative neutron data libraries for Geant4 are available from IAEA (https://www-nds.iaea.org/geant4/)
    - Based on ENDF, JEFF, JENDL, CENDL, BROND and ROSFOND neutron data libraries

## **Thermal Scattering**

- A special treatment is needed for handling neutron elastic scattering at thermal energies < 4 eV from chemically bound atoms</li>
  - At thermal neutron energies, atomic translational motion as well as vibration and rotation of the chemically bound atoms affect the neutron scattering cross section and the energy and angular distribution of secondary neutrons
  - Based on the  $S(\alpha, \beta)$  approach
    - Also known as "Thermal Scattering Law (TSL)", based on both experimental measurements and molecular dynamics calculations
  - Thermal neutron scattering files from JEFF-3.3 and ENDF/B-VIII-0 thermal data
    - There are ~30 materials : benzene, para-hydrogen, ortho-hydrogen, para-deuterium, ortho-deuterium, uranium-dioxide, ice, heavy-water, beryllium-oxide, uranium-nitride, liquid-methane, zirconium-hydride, yttrium-hydride, water, polyethylene, polymethy-methacrylate, graphite, silicium-carbide, graphite-porosity-10%, graphite-porosity-30%, beryllium-metal, iron-metal, solid-metane, aluminium-metal, sapphir, Si28, Si29, Si30, magnesium-metal, etc.
  - Can be activated with the elastic physics constructor *G4ThermalNeutrons*
    - physicsList → RegisterPhysics( new G4ThermalNeutrons(0) );

or, more easily, since G4 11.2, by using one of the \_HPT physics lists

• Example: examples/extended/hadronic/Hadr04

## ParticleHP

- Extension of NeutronHP for : **p** , **d** , **t** , **3He** , **α** 
  - For high-precision inelastic interactions below **200 MeV** 
    - Of interest for medical and nuclear physics
  - Also "data"-driven, based on the **TENDL** database
    - Based mostly on **TALYS** code, with some data from **ENDF/B-VIII.0**
    - Optional database that can be downloaded from the Geant4 web site
      - G4TENDL1.4
    - Need to be pointed by the environmental variable G4PARTICLEHPDATA
  - The two codes, NeutronHP and ParticleHP, have been merged
  - Validation in progress, good comparisons so far with MCNP
  - Available only in the **QGSP\_BIC\_AIIHP** reference physics list
    - Be careful: users are reporting weird behavior of this physics list in G4 11.2 : we recommend to use 11.1 until we understand and fix the problem!

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## **Radioactive Decay**

## Nuclides in Geant4 (1/2)

- Based on data files from the Evaluated Nuclear Structure Data Files (ENSDF), Geant4 knows about ~ 6'500 nuclides with half-life > 1 ns
  - ~3'000 ground states + ~3'500 meta-stable states (isomers)
  - For Geant4 11.2, their properties (Z, A, E, τ, etc.) are in G4ENSDFSTATE2.3 (pointed by G4ENSDFSTATEDATA)
- Two ways to have radioactive nuclides either ground states or meta-stable isomers – in Geant4 :
  - **1.** Radioactive source as a primary particle (at rest or in-flight)
    - *e.g.* Na24m :

<u>/gun/particle ion</u> <u>/gun/ion 11 24 0 472. keV</u> # Z A Q E

## Nuclides in Geant4 (2/2)

- **2.** Induced radioactivity (activation) : in inelastic hadronic collisions, de-excitation nuclear models can create nuclides with half-life greater than a threshold:
  - **1 ns** by default if RDM is not used (*i.e.* for HEP applications)
    - This threshold can be changed (currently) only via C++ interface
    - Obviously, without RDM, these isomers do not decay !
  - 1 ns by default when RDM is used (either in analogue or in biasing mode)
    - This threshold can be changed via UI command

## **Radioactive Decay**

- Process to simulate radioactive decay of unstable nuclei, either in flight or at rest
- So far, implemented the following types of radioactive decays :
   α, β-, β+, γ (*i.e.* Isomeric Transitions (IT), and e- Internal Conversions (IC) )
   EC (Electron Capture), p, n, t, spontaneous-fission
  - Not yet : pp , nn ,  $\beta$ -delayed p ,  $\beta$ -delayed n ,  $\beta\beta$ -- ,  $\beta\beta$ ++ , *etc.*
- Empirical and data-driven
  - Data files from Evaluated Nuclear Structure Data Files (ENSDF)
    - As of Geant4 11.2, these are in pointed by the environmental variable
       RadioactiveDecay5.6
       G4RADIOACTIVEDATA
    - These data files contain properties such as: half-lives, nuclear level structure for parent and daughter nuclides, type of decay, decay branching ratios, energy of decay process, *etc.*

### **Radioactive Decay Chain**



EC: electron capture

IC: internal conversion

ARM: atomic relaxation model

### **Atomic Relaxation Model**



## Gamma (or Electron) Emission

- Nuclides with half-life < 1 ns are forced to decay immediately
  - This threshold can be set via UI command "/process/had/rdm/hIThreshold"
- Prompt de-excitation is done via **G4PhotonEvaporation** 
  - Uses ENSDF files with all known gamma levels for  $\sim$  3'000 isotopes (in total  $\sim$  25'500 levels with half-life > 10^-23 s )
    - As of Geant4 11.2, these are in pointed by the environmental variable
       PhotonEvaporation5.7
       G4LEVELGAMMADATA
  - Internal conversion (*i.e.* nuclear de-excitation via emission of atomic electrons) is enabled as a competing process to gamma de-excitation
- Option to disable atomic relaxation after decay
  - When Radioactive Decay is activated, Fluorescence and Auger emissions are switched on by default (overriding any EM default settings). User can use UI command to change this.

#### Sampling Radioactive Decay : Analogue mode (default)

#### Several options available via UI commands :

- Enable/disable radioactive decay in various geometry volumes "/process/had/rdm/selectVolume", "/process/had/rdm/deselectVolume"
- Limits the nuclei in which radioactive decay can be applied (useful to limit the decay chain, *i.e.* to avoid decays of daughters) "/process/had/rdm/nucleusLimits"
- Supply a user-defined radioactive decay datafile for a given isotope (useful, for instance, to amplify rare decay branches)
   "/process/had/rdm/setRadioactiveDecayFile"
- Supply a user-defined evaporation datafile for a given isotope "/process/had/rdm/setPhotoEvaporationFile"
- Switch on/off atomic relaxation

"/process/had/rdm/applyARM" (default: true )

#### Sampling Radioactive Decay : **Biased** mode (alternative)

#### Several options available via UI commands :

- Set all decay branch probabilities equal "/process/had/rdm/BRbias" default: true
- "Splitting" : perform nuclear decay N times for each event "/process/had/rdm/splitNuclei" default: 1
- Activation : integrate decay chain over time windows (in seconds) "/process/had/rdm/sourceTimeProfile", "/process/had/rdm/decayBiasProfile" using Bateman equations "/process/had/rdm/analogueMC false" (default: true )
- Collimation of decay products "/process/had/rdm/decayDirection", "/process/had/rdm/decayHalfAngle"

## Using Radioactive Decay (1/2)

- Activate Radioactive Decay by one of the following 3 ways:
  - 1. Choose one of the reference physics lists that have already Radioactive Decay activated, *e.g.* any \_HP physics list or Shielding
  - **2.** Add the physics constructor *G4RadioactiveDecayPhysics* to a reference physics list (which does not have it already), *e.g.*

G4VModularPhysicsList\* physicsList = new FTFP\_BERT; physicsList->RegisterPhysics( new G4RadioactiveDecayPhysics ); runManager->SetUserInitialization( physicsList );

**3.** Do something like this in your own physics list :

G4RadioactiveDecay\* rDecay = new G4RadioactiveDecay; G4PhysicsListHelper\* plh = G4PhysicsListHelper::GetPhysicsListHelper(); rDecay -> SetICM( true ); // Internal conversion : obsolete, always true! rDecay -> SetARM( true ); // Atomic relaxation plh -> RegisterProcess( rDecay, G4GenericIon::GenericIon() );

## Using Radioactive Decay (2/2)

- Many options can be set via UI commands
- Set environmental variables to point to the data libraries:
  - G4ENSDFSTATEDATA -> G4ENSDFSTATE2.3
  - G4LEVELGAMMADATA -> PhotonEvaporation5.7
  - G4RADIOACTIVEDATA -> RadioactiveDecay5.6

in most cases, this is done automatically without the need for the user to do anything !

## Examples of using RDM

#### examples/extended/radioactivedecay

- rdecay01/
  - Shows basic features of the radioactive decay of nuclei : energy spectrum of emitted particles, time of decay, activity
  - Analogue mode only, with user-defined RadioactiveDecay and PhotonEvaporation files
- rdecay02/
  - Induced radioactivity by nuclear reactions
  - Shows advanced features *e.g.* selected decay channels, time window, *etc.* in both analogue and biasing mode
- Activation/
  - Induced radioactivity by nuclear reactions
  - Shows the evolution of each meta-stable isomer as a function of time, taking into account the time of exposure of the beam; analogue mode only



## Nucleus-Nucleus (Ion-Ion) Interactions

#### Nucleus-nucleus (ion-ion) : cross sections and final-state models

- Cross sections (elastic and inelastic)
  - Glauber-Gribov based approach
- Inelastic final-state models
  - **FTFP** model above **3** GeV/nucleon
  - BIC (Binary Cascade) model below 6 GeV/nucleon
  - INCL (Liege intra-nuclear cascade) model below **3** GeV/nucleon for **A < 18**
  - QMD (Quantum Molecular Dynamic) model between ~100 MeV/nucleon
     and ~10 GeV/nucleon
    - Since G4 11.2, there is also a light-ion QMD variant, *G4LightIonQMDPhysics*, optimised for medical applications (*i.e.* light target nuclei and projectile kinetic energy in the range 30-500 MeV/nucleon)
  - **ParticleHP** below **200** MeV/nucleon only for light ions (p, d, t, He3,  $\alpha$ )
- Elastic final-state model
  - **G4NuclNuclDiffuseElastic** for all energies

# Nucleus-Nucleus (ion-ion) : physics constructors and physics lists

- Physics constructors
  - **G4IonPhysics** : used in most reference physics lists; uses FTFP & BIC
  - **G4IonINCLXXPhysics** : not used in any reference physics list; uses FTFP, INCL, BIC
  - **G4IonQMDPhysics** : used only in Shielding physics list; uses FTFP, QMD, BIC
    - Since G4 11.2, there is also the variant *G4LightIonQMDPhysics*
  - **G4IonPhysicsPHP** : used only in QGS\_BIC\_AllHP physics list; uses FTFP, BIC, PHP
  - *G4IonElasticPhysics* : used in QGSP\_BIC\*, Shielding, QBBC
- Physics Lists
  - Nearly all reference physics lists use G4IonPhysics (i.e. FTFP & BIC); most physics lists do not have ion elastic
    - Exception: **QGSP\_BIC\***, **Shielding**, **QBBC** use *G4IonElasticPhysics*
  - Shielding is the only reference physics list that uses G4IonQMDPhysics (i.e. FTFP, QMD, BIC)
    - Since G4 11.2, there is an option to use *G4LightIonQMDPhysics* instead
  - **QGSP\_BIC\_AIIHP** is the only reference physics list that uses *G4IonPhysicsPHP* (*i.e.* FTFP, BIC, PHP)



## Gamma/Lepton-Nuclear Interactions

## **Gamma-nuclear** interactions

- The same approach for all reference physics lists
  - On-going development to provide an alternative approach
- Cross sections
  - For all energies, parameterisation of experimental data by M. Kossov
  - Below 140 MeV covering the Giant Dipole Region (GDR) an extended collection of photonuclear data by IAEA is used
  - Optionally (not by default), LEND gamma cross section data below 20 MeV
- Final-state models
  - Above 3 GeV, QGSP (Quark Gluon String + Precompound/de-excitation) model
  - Between 199 MeV and 6 GeV, BERT (Bertini-like intra-nuclear cascade) model
  - Below 200 MeV, Precompound/de-excitation model
  - Optionally (not by default), LEND final-state model below 20 MeV can be used
    - If data available for a given isotope, else use BERT model

## (Charged-)Lepton-nuclear interactions

- The same approach for all reference physics lists
  - Missing tau-nuclear; on-going development to provide an alternative approach as well as this missing process (tau-nuclear)
- Cross sections
  - For electron/positron-nuclear collisions at all energies, parameterisation of experimental data by M. Kossov
  - For muon-nuclear at all energies, Kokoulin's theoretical computation
- Final-state models
  - Based on the equivalent photon approximation: first a virtual gamma is produced; then it is converted to a real gamma, which interacts with a target nucleus
  - Below 10 GeV, BERT (Bertini-like intra-nuclear cascade) model
  - Above 10 GeV, FTFP (Fritiof + Precompound/de-excitation) model
    - The real gamma is treated as a neutral pion (with the same total energy)

## Neutrino-nuclear interactions

- Most neutrino experiments are currently using an external package, GENIE, interfaced to Geant4, for neutrino-nuclear interactions
- By default, there are no neutrino-nuclear processes in Geant4
- However, electron-, muon- and tau-neutrino and anti-neutrino charged and neutral current interactions can be activated via UI commands
  - For any reference physics list
  - Implemented relatively recently, physics validation on-going
  - Neutrino oscillations in vacuum are included (since G4 11.2)
    - Not yet neutrino oscillations in matter



# **Stopping Physics**

## Reminder of "Capture At Rest"

- In Nature, particles are never completely "at rest" *i.e.* with zero kinetic energy in the Lab. frame – however, given the typical simplified treatment in simulations of low-energy (≤ 1 keV) particles, charged particles can come completely at rest in Geant4 !
- In Geant4, µ- and negatively charged hadrons have a nuclear capture at rest process (independent from their inelastic process, used for "in-flight" interactions)
  - $\mu-$ ,  $\pi-$ , K-, anti-p,  $\Sigma-$ , anti- $\Sigma+$ ,  $\Xi-$ , anti- $\Xi+$ ,  $\Omega-$ , anti-d, anti-t, anti-He3, anti- $\alpha$
  - For at-rest processes, the **lifetime** (instead of the cross section as for an in-flight process) is related to the probability that such a process occurs
  - The capture at rest process competes against the **decay** process

## Stopping Physics (1/2)

- The same stopping physics is present in nearly all reference physics lists
  - Only FTF\_BIC & QGS\_BIC use a slightly different model for antiproton and antineutron annihilation (Fritiof/Binary instead of Fritiof/Precompound)
  - In INCL-based physics lists (*e.g.* FTFP\_INCLXX, QGSP\_INCLXX, *etc.*), the intra-nuclear cascade model INCL is used for antiproton annihilation at rest (as well as in-flight)
    - Large interest in antiproton physics at low energies (CERN and astro-particle experiments)
- Simple treatment of the EM cascade
  - Emission of **X-rays** and **Auger electrons** due to the capture of the (negatively charged) particle from an external shell down to the inner K-shell
  - Approximated treatment from old measurements for µ- capture, applied identically to all other particles types
    - For some applications, it is important to correlate the hadronic products of the nuclear capture with the EM emissions
    - On-going development to have a more accurate description of "muonic atoms"
    - Attempts to have dedicated EM cascade for antiproton annihilation

## Stopping Physics (2/2)

- For the hadronic part of the nuclear capture, these are the final-state hadronic models that are (currently) used:
  - **BERT** (Bertini-like) intranuclear cascade model for:

 $\mu-$  ,  $\pi-$  , K- ,  $\Sigma-$  ,  $\Xi-$  ,  $\Omega-$ 

- FTF (Fritiof) string model, coupled to either Precompound/de-excitation (in most of physics lists) or Binary Cascade (only in FTF\_BIC & QGS\_BIC) for: *anti-*p, *anti-*Σ+, *anti-*Ξ+, *anti-*d, *anti-*t, *anti-*He3, *anti-*α
  - For annihilation at rest, a string model is at the limit of its applicability, therefore for more accurate simulations (as required in particular for the rich antiproton physics research at CERN and in astro-particle experiments) an intra-nuclear cascade approach, such as INCL, is recommended
  - Since G4 11.2, INCL-based physics lists (*e.g.* FTFP\_INCLXX, QGSP\_INCLXX, *etc.*) use the intra-nuclear cascade model INCL for antiproton annihilation at rest (as well as in-flight)



## Exercises

### Exercise 1 : NeutronHP

- Consider the example:
  - geant4/examples/basic/B4/B4a
- Enlarge the calorimeter (from a typical EM to a typical HAD)
  - In the method B4DetectorConstruction::DefineVolumes increase both nofLayers and calorSizeXY by a factor of 10
- Observe how the execution time changes
  - Consider a *pi* beam of **10 GeV** energy
  - With **FTFP\_BERT** physics list
  - With **FTFP\_BERT\_HP** physics list
  - With **FTFP\_BERT\_HPT** physics list
  - With FTFP\_BERT\_HPT physics list and replacing the active material *liquidArgon* with *e.g. G4\_WATER*

## Exercise 2 : Radioactive Decay

- Consider the example:
  - geant4/examples/extended/radioactivedecay/rdecay01/
- Study the decay of As74
  - Which has a rather complicated decay scheme in  $\beta$  ,  $\beta$ + and EC
  - in both analogue and biased modes
    - You can limit the decay chain, *i.e.* to avoid to decay its daughters, as follows /process/had/rdm/nucleusLimits 74 74 33 33