



Hadronic Physics II

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GEANT4
A SIMULATION TOOLKIT

Outline

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

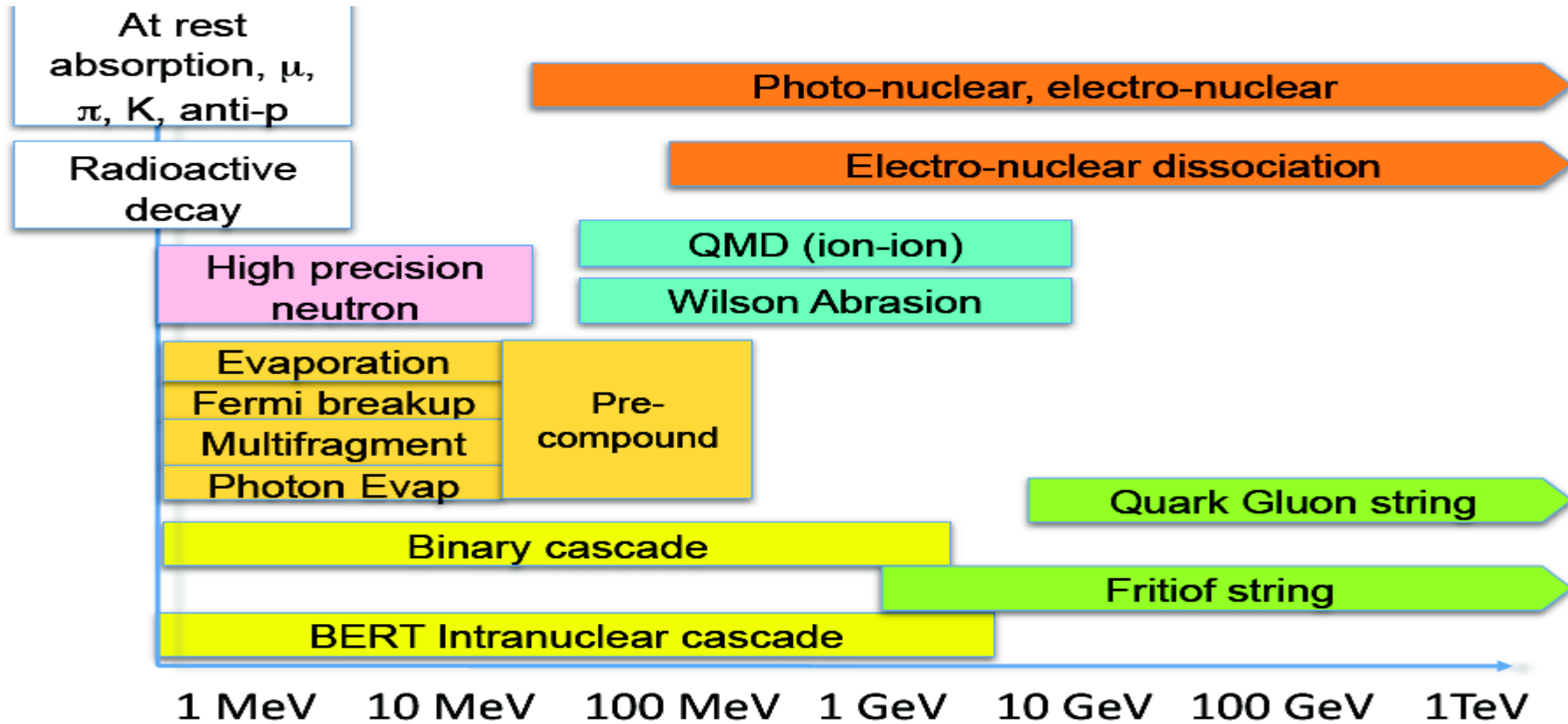


Reminder:
Hadronic Models, Cross Sections,
Framework, Physics Lists

Hadronic interactions

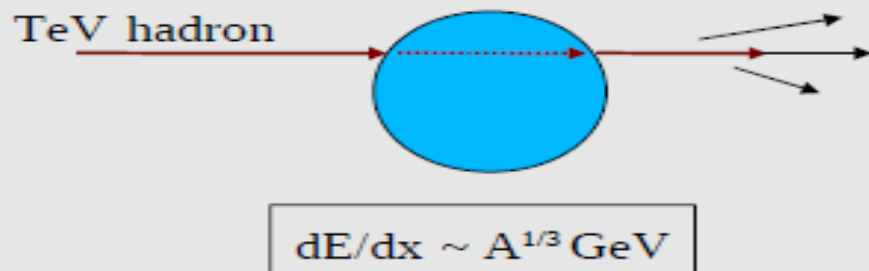
- Hadrons (π^\pm , K^\pm , K^0_L , p , n , α , *etc.*), produced in jets and decays, travel through the detector (H , C , Ar , Si , Al , Fe , Cu , W , Pb ...)
- Therefore we need to model hadronic, strong interactions
hadron – nucleus \rightarrow anything
- In principle, QCD is the theory that describes all hadronic interactions
in practice, perturbative calculations are applicable only in a tiny
(but important !) phase-space region
 - the hard scattering at high transverse momentumwhereas 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

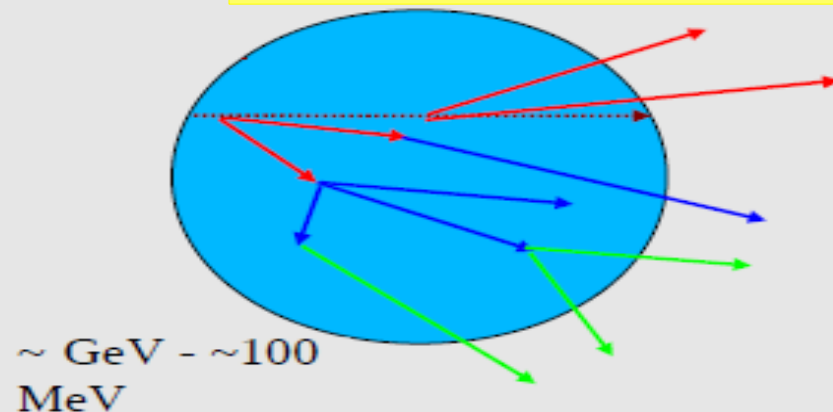


Hadronic Interactions from TeV to meV

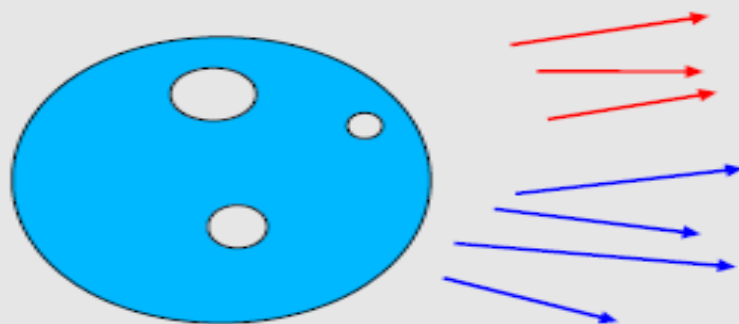
String model



Intra-nuclear cascade model

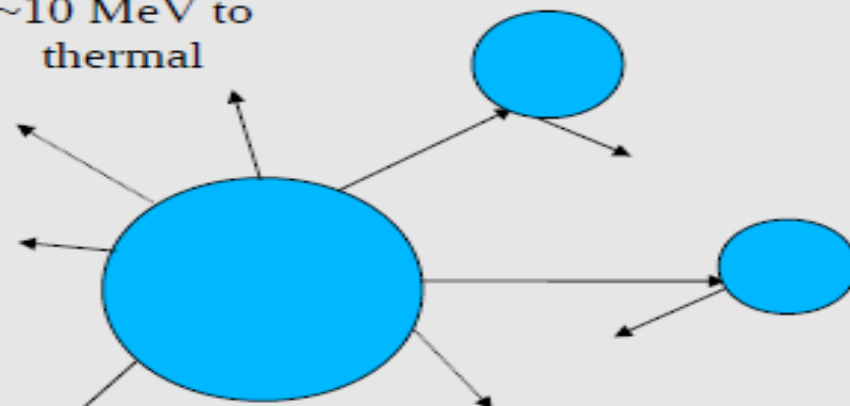


$\sim 100 \text{ MeV} - \sim 10 \text{ MeV}$



Pre-equilibrium (Precompound) model

$\sim 10 \text{ MeV}$ to thermal

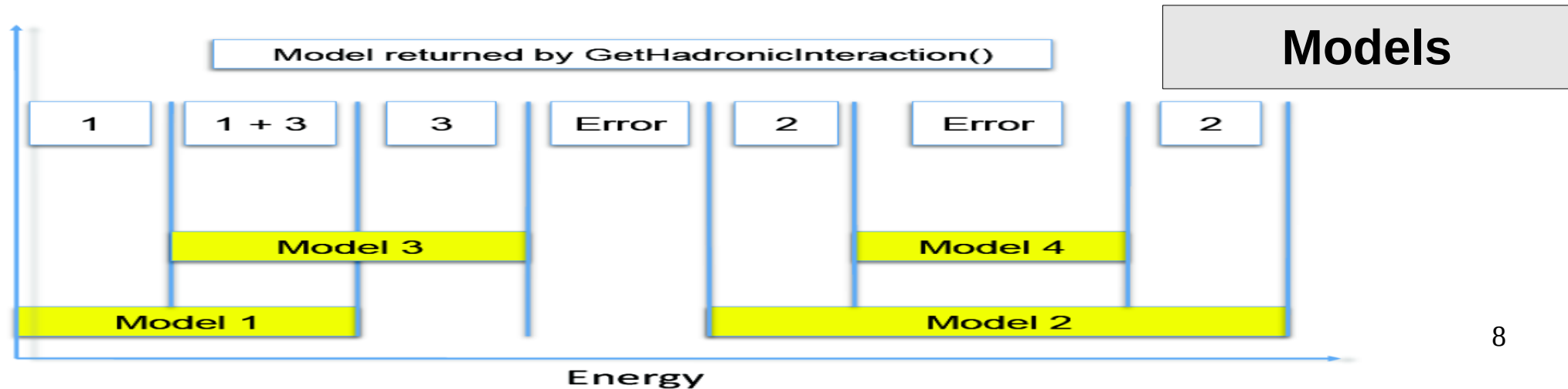


Equilibrium (Evaporation) model

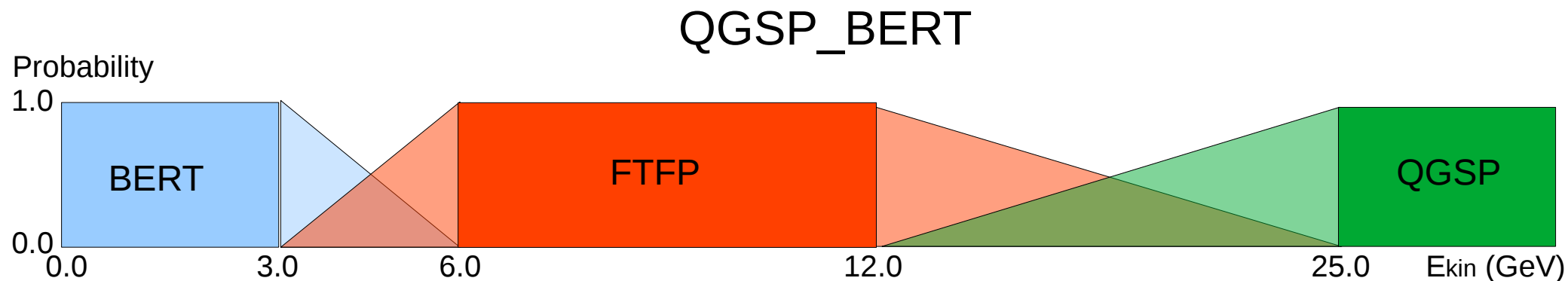
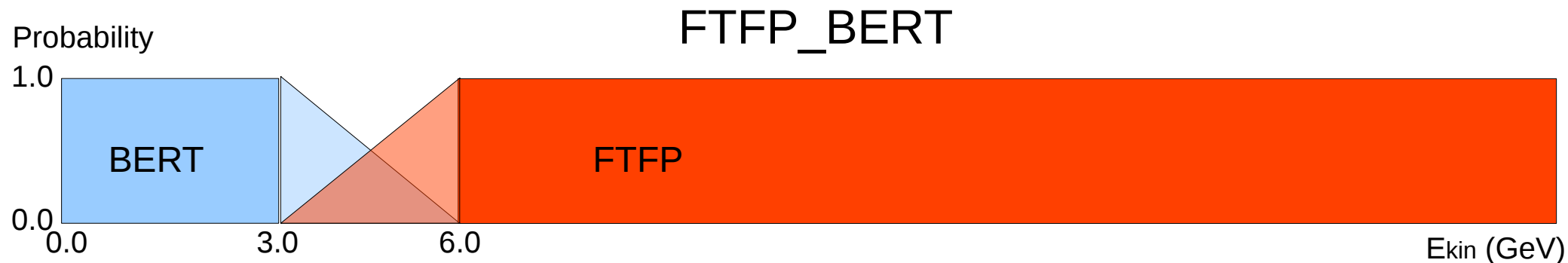
Hadronic Cross Sections and (Final-State) Models

- 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



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 : **P**recompound + 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 $E_{kin} < 20$ MeV
 - **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 3rd 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
 - **$E_{kin} < 20 \text{ MeV}$** , 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, 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 agreement 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 $< 4 \text{ eV}$ from chemically bound atoms
 - 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-methane, aluminium-metal, sapphir, Si28, Si29, Si30, magnesium-metal, etc.
 - Can be activated with the elastic physics constructor ***G4ThermalNeutrons***
 - *physicsList* \rightarrow *RegisterPhysics(new G4ThermalNeutrons(0));*
 - 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_AllHP** reference physics list



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 11.1 , 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 :
/gun/particle ion
/gun/ion 11 24 0 472. keV # Z A Q E

Nuclides in Geant4 (2/2)

2. Induced radioactivity (activation) :

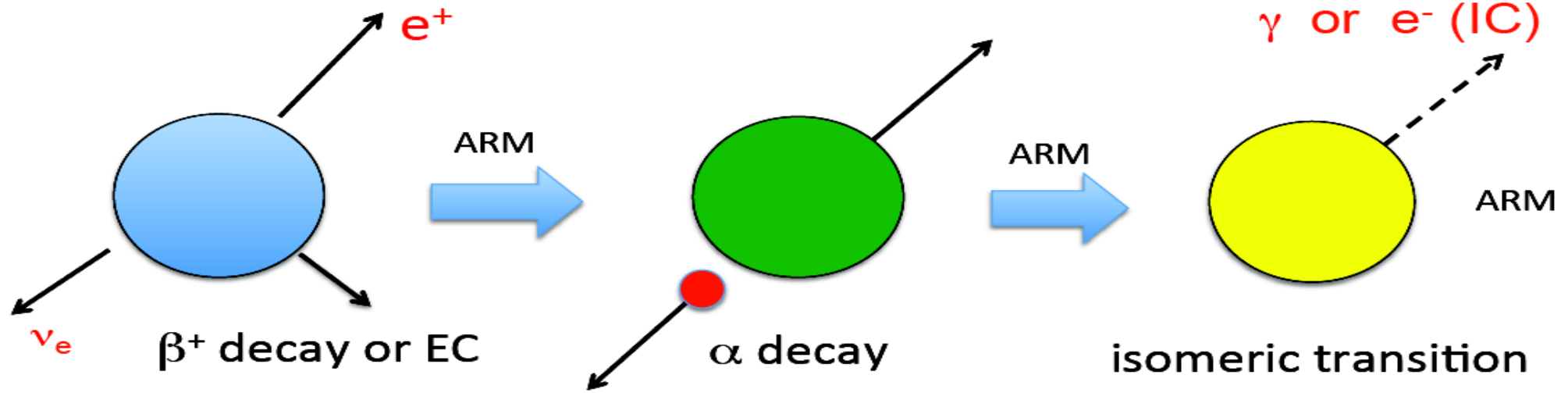
in inelastic hadronic collisions, de-excitation nuclear models can create nuclides with half-life greater than a threshold:

- **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 , β -delayed p , β -delayed n , $\beta\beta^{--}$, $\beta\beta^{++}$, *etc.*
- Empirical and data-driven
 - Data files from Evaluated Nuclear Structure Data Files (**ENSDF**)
 - As of Geant4 11.1 , these are in **RadioactiveDecay5.6** pointed by the environmental variable **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

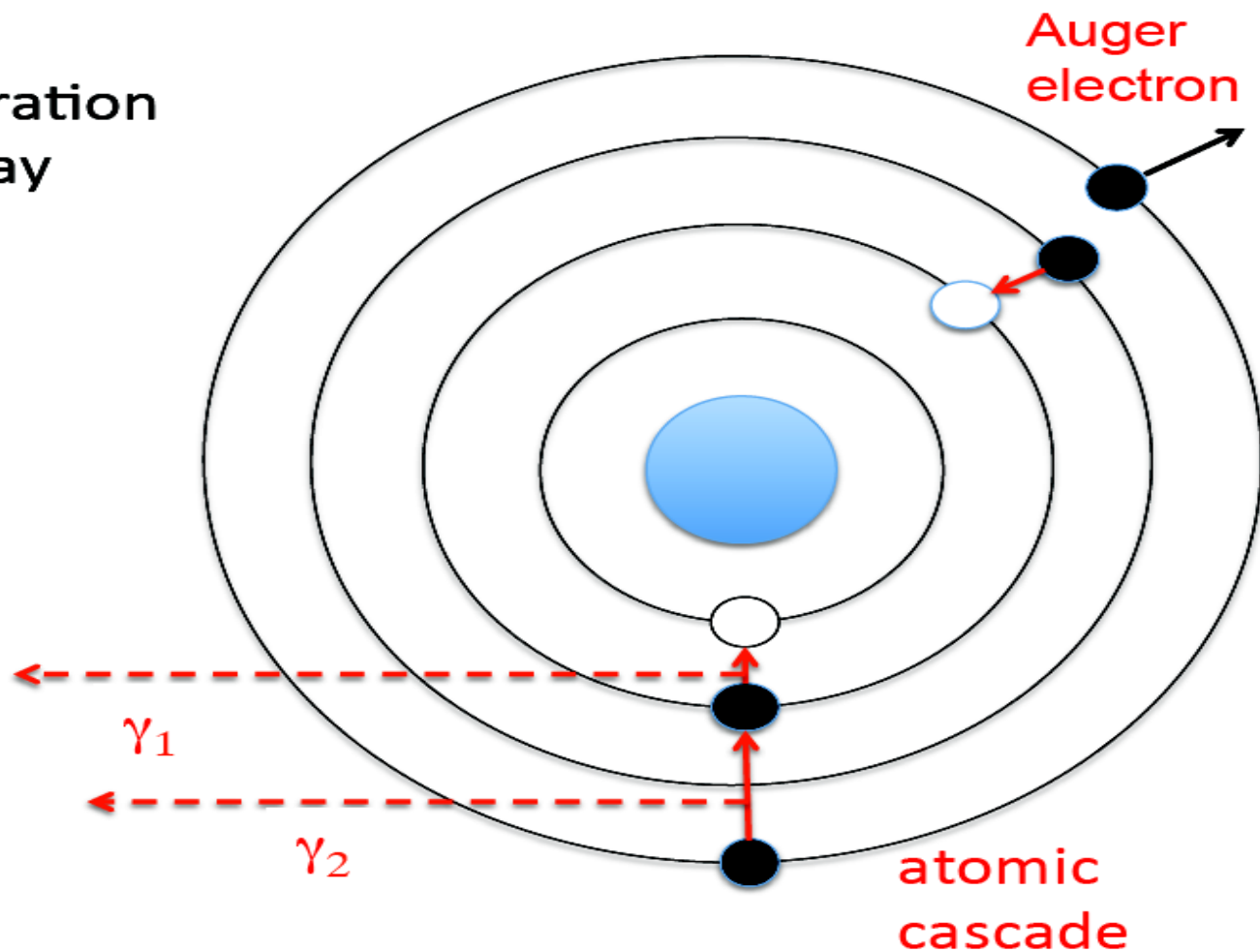
Atomic Relaxation Model

electron shell configuration
may change after decay

inner holes filled by
atomic cascade

either photons or
Auger electrons are
emitted

fluorescence option
also available



Gamma (or Electron) Emission

- Nuclides with half-life $< 1 \text{ ns}$ are forced to decay immediately
 - This threshold can be set via UI command `/process/had/rdm/hlThreshold`
- 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 $> 10^{-23} \text{ s}$)
 - As of Geant4 11.1 , these are in **PhotonEvaporation5.7** pointed by the environmental variable **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 (up to **~1** TeV/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
 - **ParticleHP** below **200** MeV/nucleon only for light ions (p, d, t, He3, α)
- Elastic final-state model
 - **G4NuclNuclDiffuseElastic** for all energies

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

- **Physics constructors**

- ***G4IonPhysics*** : used in most reference P.L. ; uses **FTFP** & **BIC**
- ***G4IonINCLXXPhysics*** : not used in any reference P.L. ; uses **FTFP**, **INCL**, **BIC**
- ***G4IonQMDPhysics*** : used only in **Shielding** P.L. ; uses **FTFP**, **QMD**, **BIC**
- ***G4IonPhysicsPHP*** : used only in **QGS_BIC_AllHP** P.L. ; 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**)
- **QGSP_BIC_AllHP** 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 not yet included, but under development



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)
 - μ^- , π^- , K^- , *anti-p* , Σ^- , *anti- Σ^+* , Ξ^- , *anti- Ξ^+* , Ω^- , *anti-d* , *anti-t* , *anti-He3* , *anti- α*
 - 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 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)
 - On-going development for extending `INCL` intra-nuclear cascade model to 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:
 μ^- , π^- , K^- , Σ^- , Ξ^- , Ω^-
 - **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, could be promising



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_HP + thermal scattering** physics list
 - With **FTFP_BERT_HP + thermal scattering** 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 β^- , β^+ 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*