Geant4 Hadronic Models

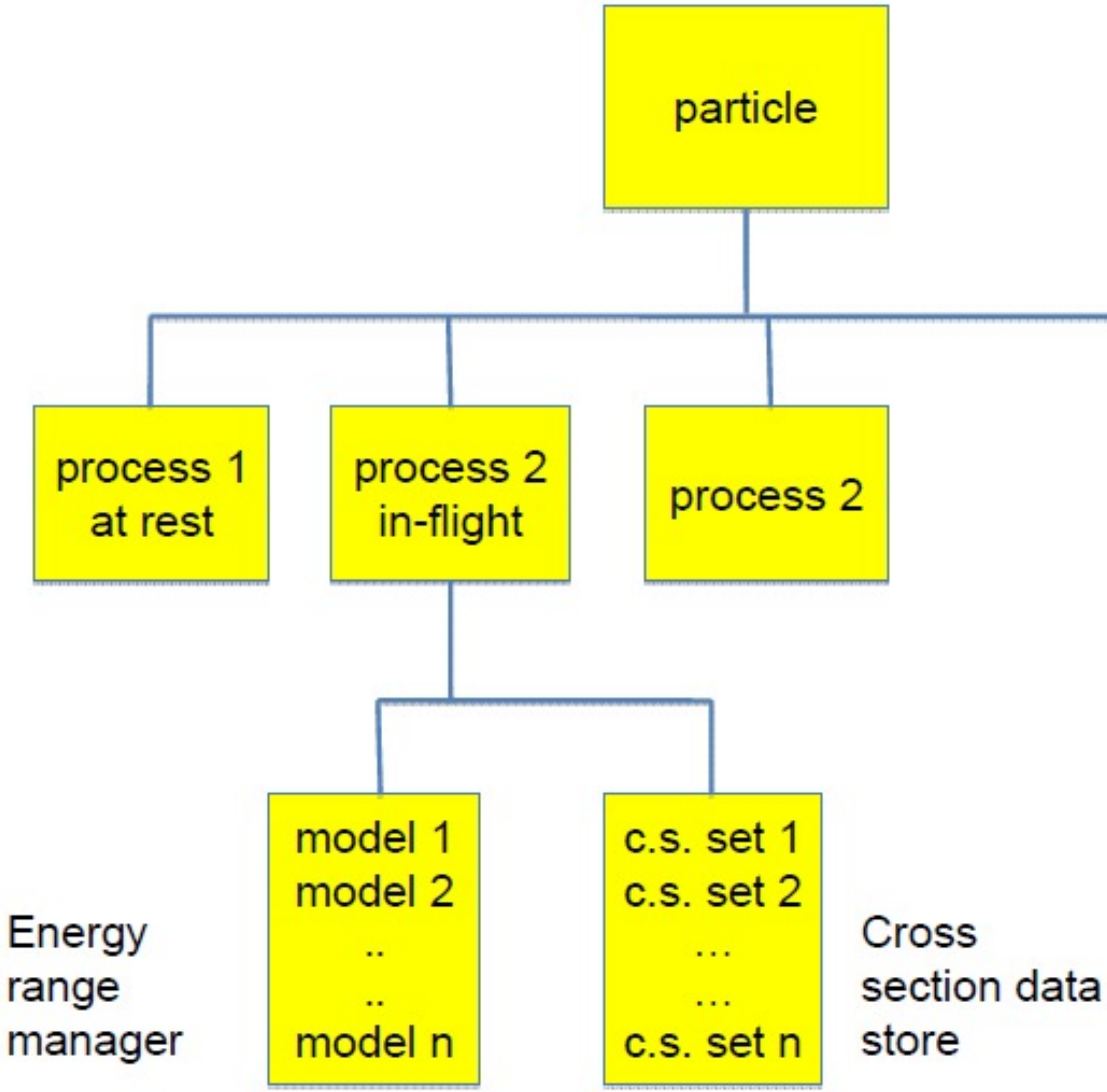
Geant4 and its Application to HEP and Astrophysics
December 5, 2022

Sunanda Banerjee

Hadronic Processes, Models and Cross Sections

- In Geant4 physics is assigned to a particle through processes
- Each process may be implemented
  - directly, as part of the process, or
  - in terms of a model class
- Geant4 often provides several models for a given process
  - user must choose
  - can, and sometimes must, have more than one per process
- A process must also have cross sections assigned
  - here too, there are options

Models and Cross Sections



Cross Sections

- Default cross-section sets are provided for each type of hadronic process
  - fission, capture, elastic, inelastic
  - can be overridden or completely replaced

- Different types of cross-section sets exist
  - some contain a few numbers to parametric the cross-section as a function of energy
  - some represent large databases
  - some are purely theoretical (equation driven)

Alternative Cross Sections

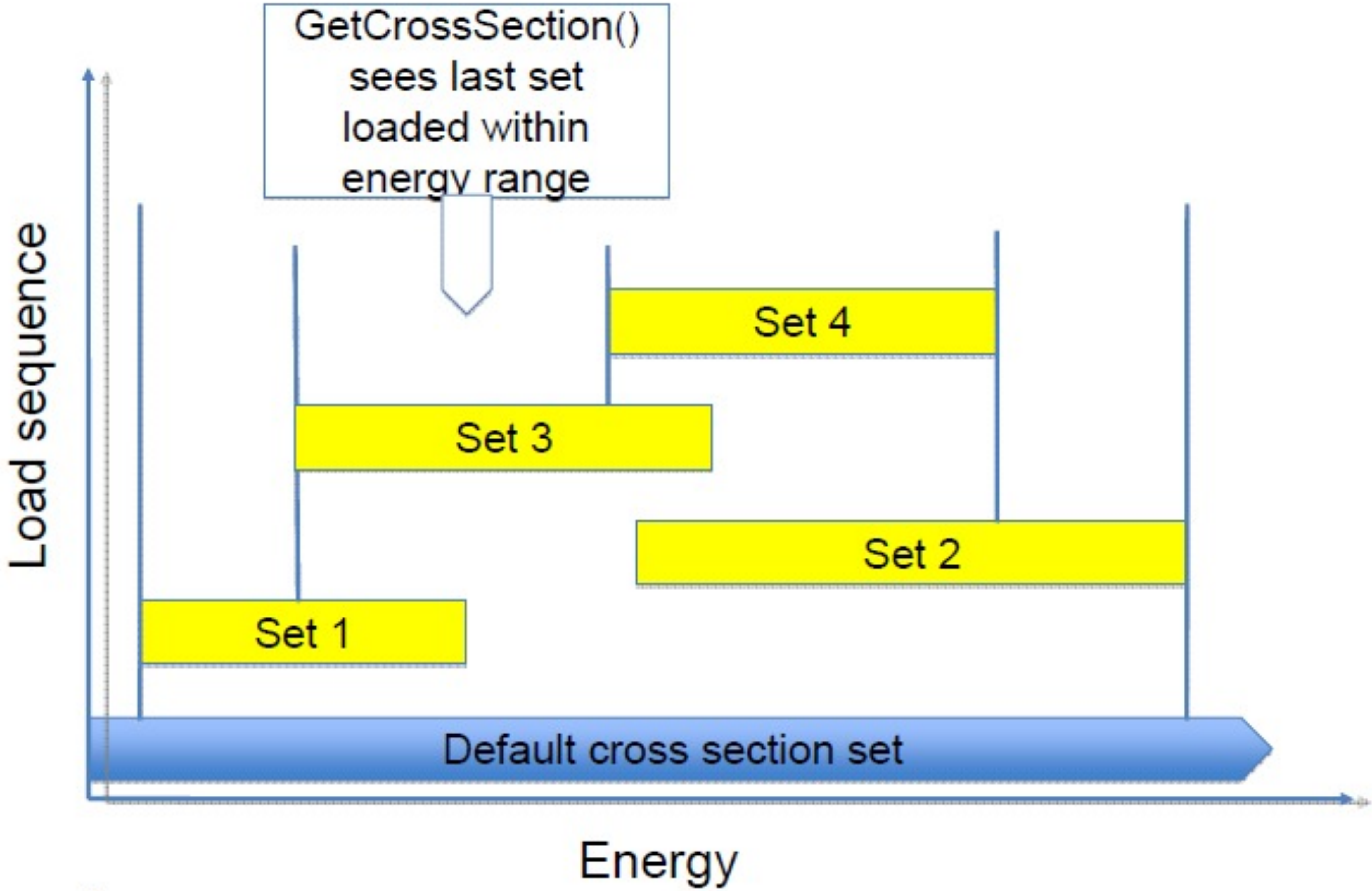
- Cross-section databases are available for low-energy neutrons
  - G4NDL available among the Geant4 distribution files
  - Livermore database (LEND) is also available
  - these are available with or without thermal cross-sections

- Cross section table is available for medium energy neutrons and protons
  - 14 MeV < E < 20 MeV

- Several alternatives exist for ion-nucleus cross-section
  - these are empirical and parametrised cross-section formulae with some theoretical insight
  - these are good for E/A < 10 GeV

- Alternative cross-sections also exist for pion cross-section

Cross Section Management



Data Driven Hadronic Models

- These are characterised by lots of data on
  - cross sections
  - angular distributions
  - multiplicities, etc.

- To get interaction length and final state, these models depend on interpolation of data
  - cross sections, Legendre coefficients, ..

- Examples:
  - neutrons with E < 20 MeV
  - coherent elastic scattering (pp, np, nn)
  - radioactive decays

Theory Driven Hadronic Models

- These are dominated by theoretical arguments (QCD, Glauber theory, exciton model, …)

- Final states (number and type of particles in the final sate with their energy and angular distributions) are determined by sampling theoretically calculated distributions

- This type of models is preferred as they ate the most predictive

- Examples:
  - quark-gluon string models (projectiles with E > 20 GeV)
  - intra-nuclear cascade models (intermediate energies)
  - nuclear de-excitation and break-up

Parametrised Hadronic Models

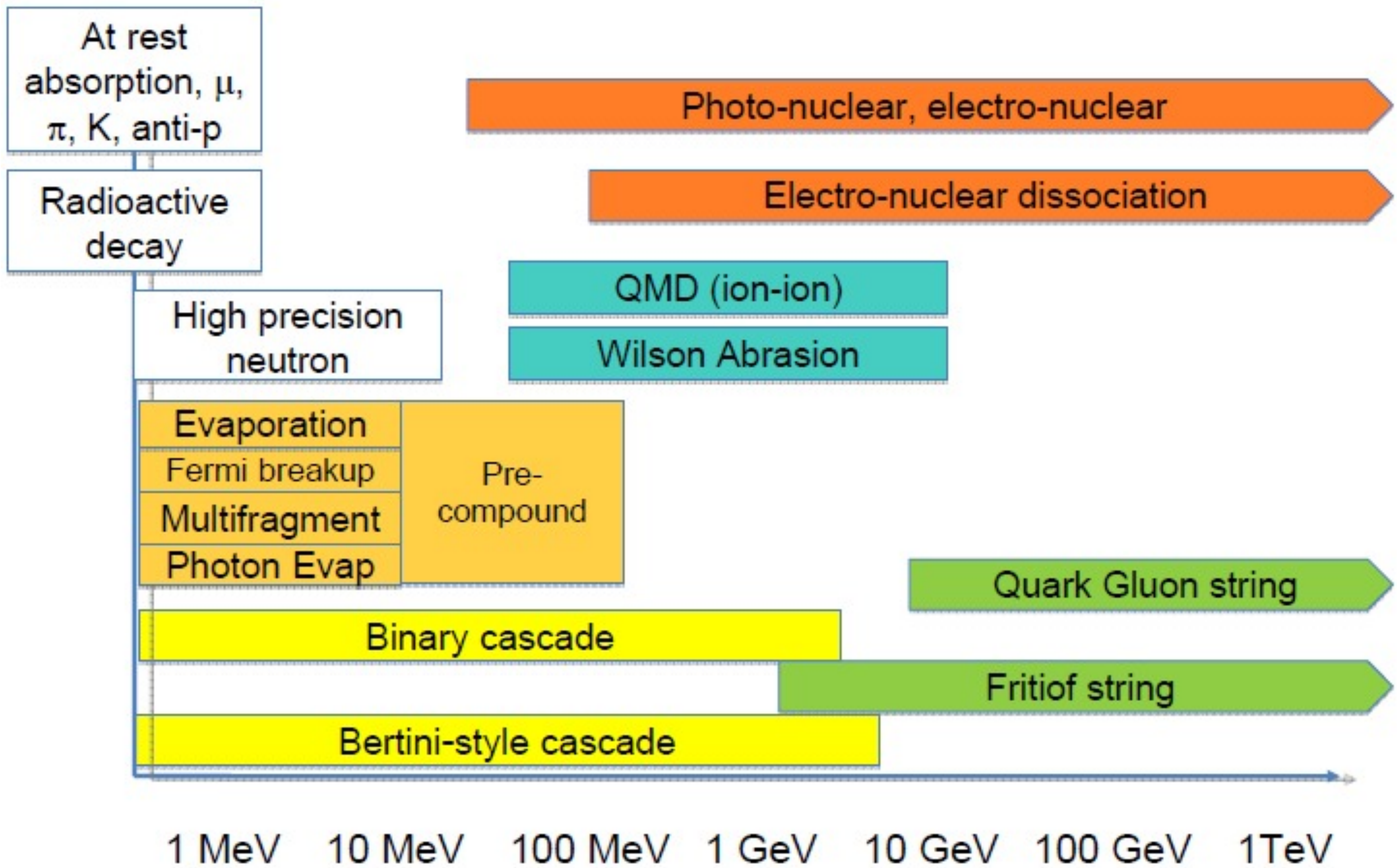
- Current versions do not contain any parametrised version. In versions preceding Geant4 10.0, two models existed. They were re-engineered versions of the Fortran Gheisha code used in Geant3

- These models depended mostly on fits to data with some theoretical guidance

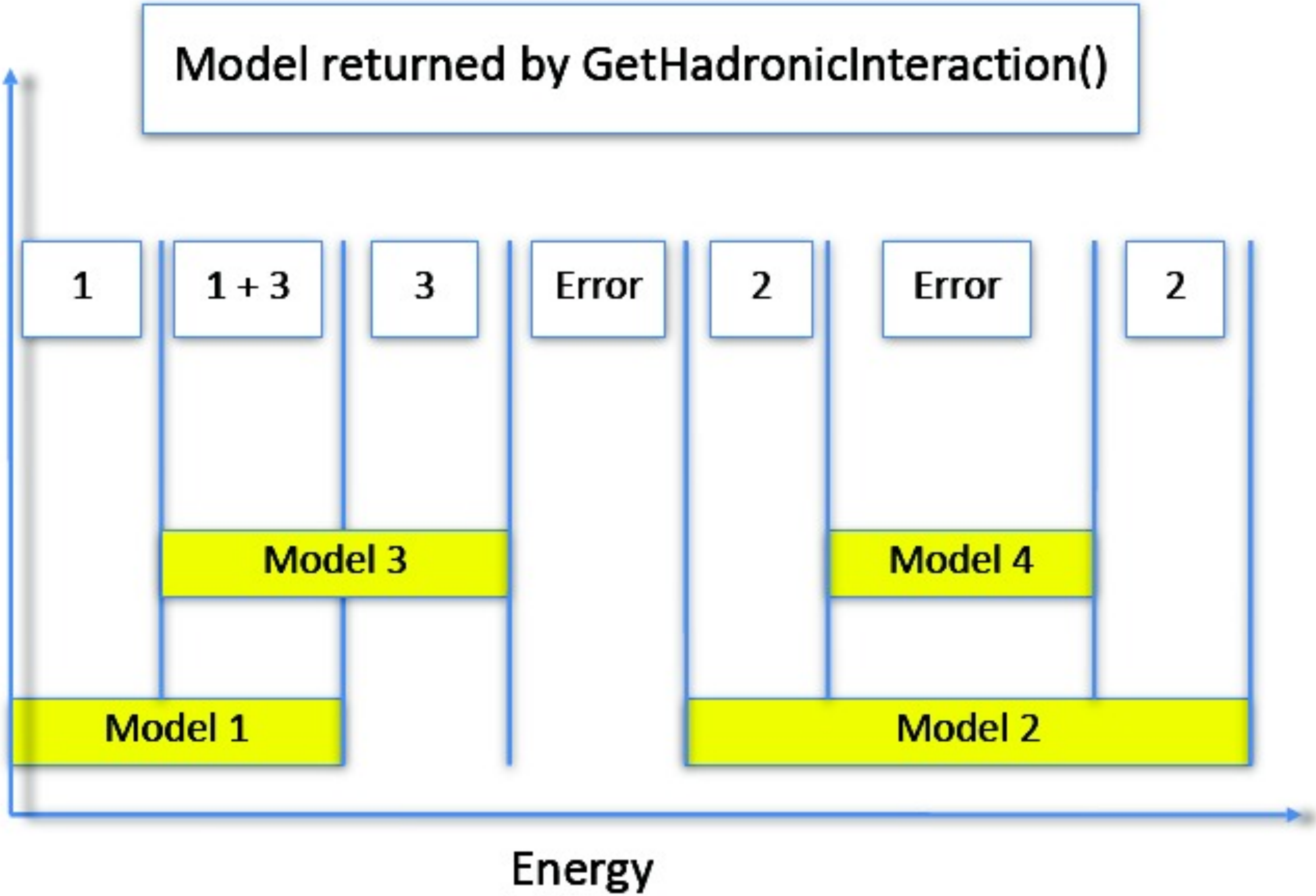
- Two such models existed:
  - Low Energy Parametrised (LEP) for E < 20 GeV
  - High Energy Parametrised (HEP) for E > 20 GeV
  - each type referred to a collection of models (one for each type of hadron)

- These codes were fast and existed for all types of particles. But they were not detailed enough and there was no-one to maintain these codes

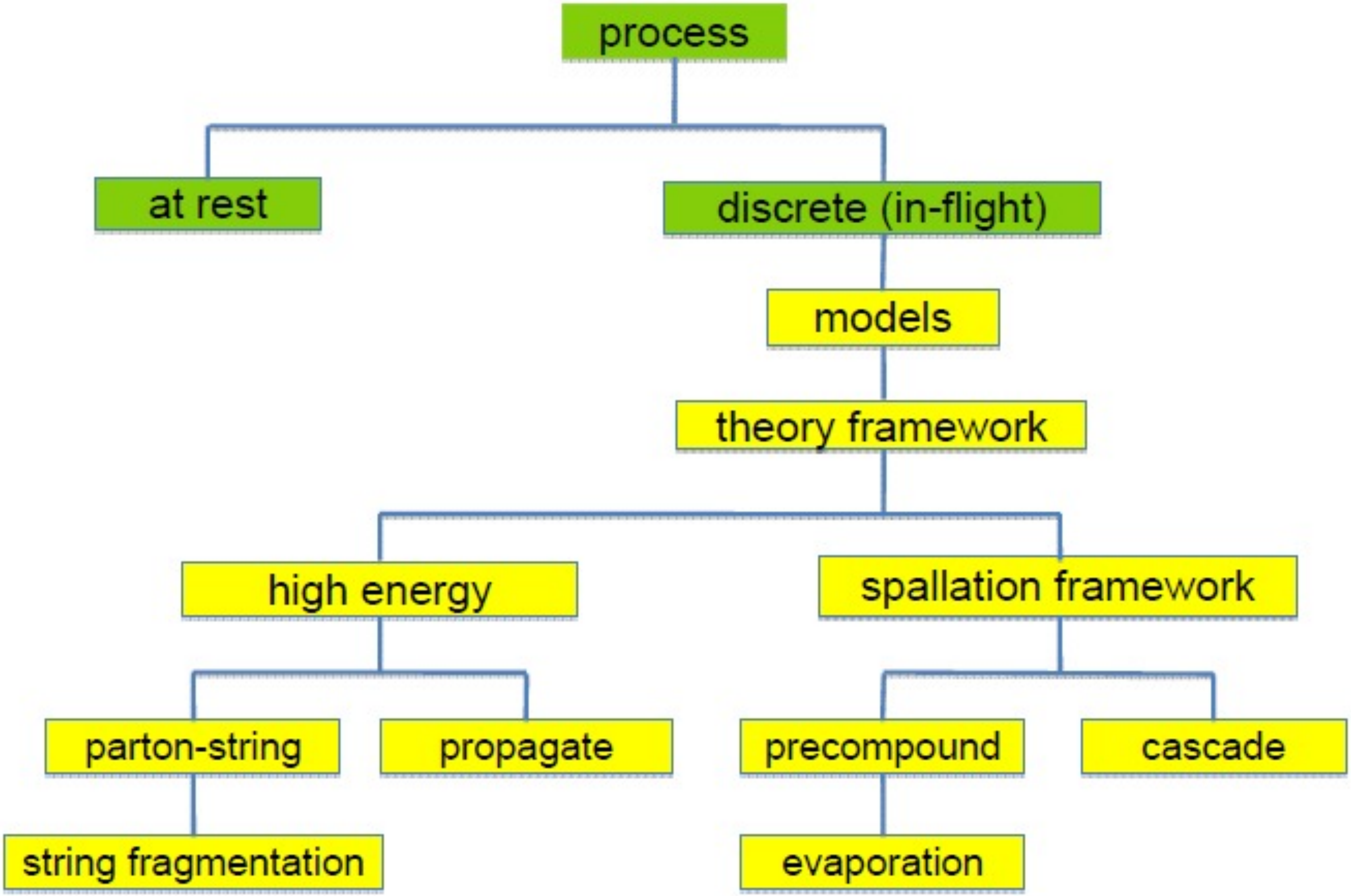
Partial Hadronic Model Inventory



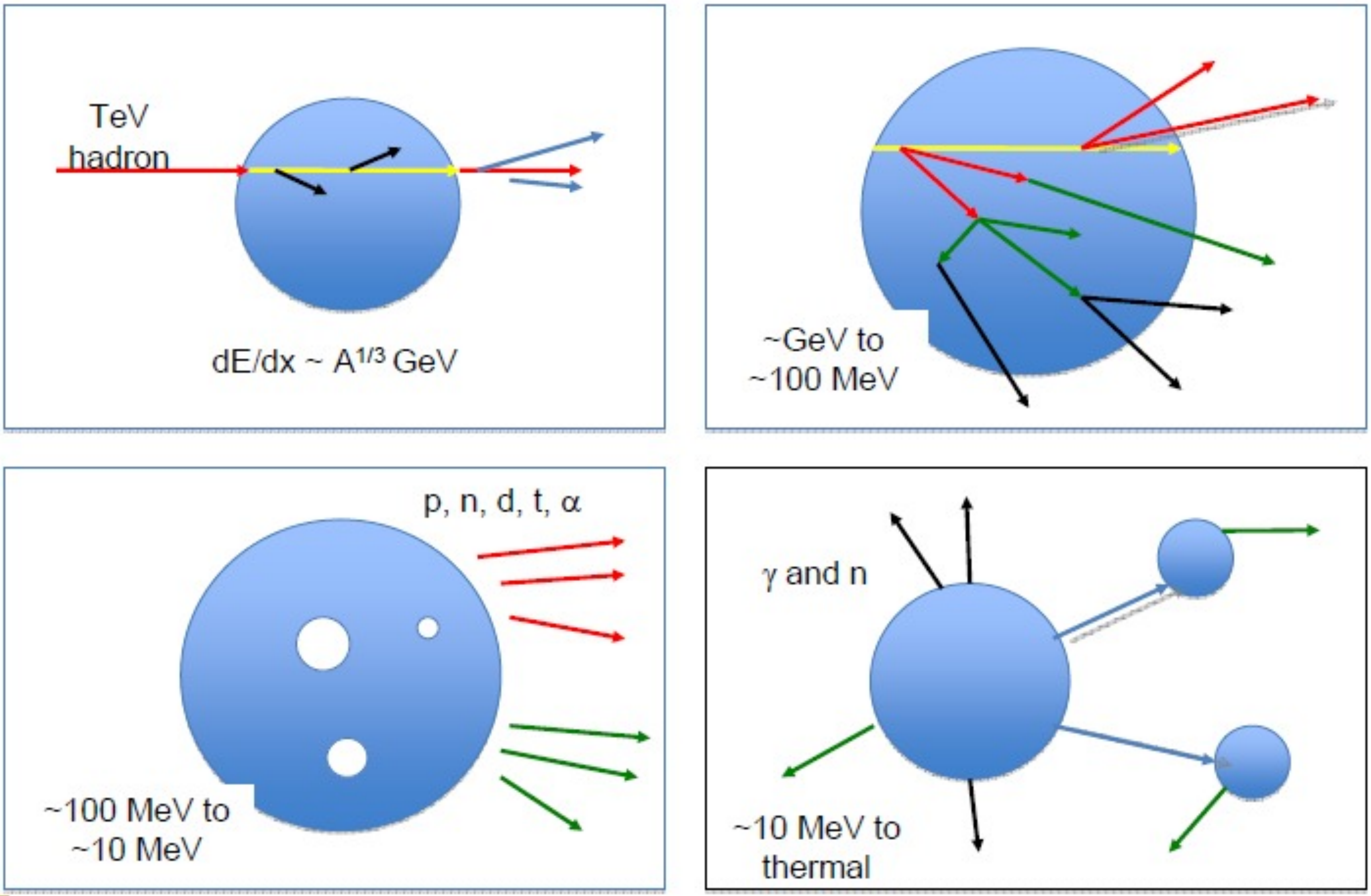
Model Management



Hadronic Model Organisation



Hadronic Interaction from TeV to meV



Hadron Elastic Scattering

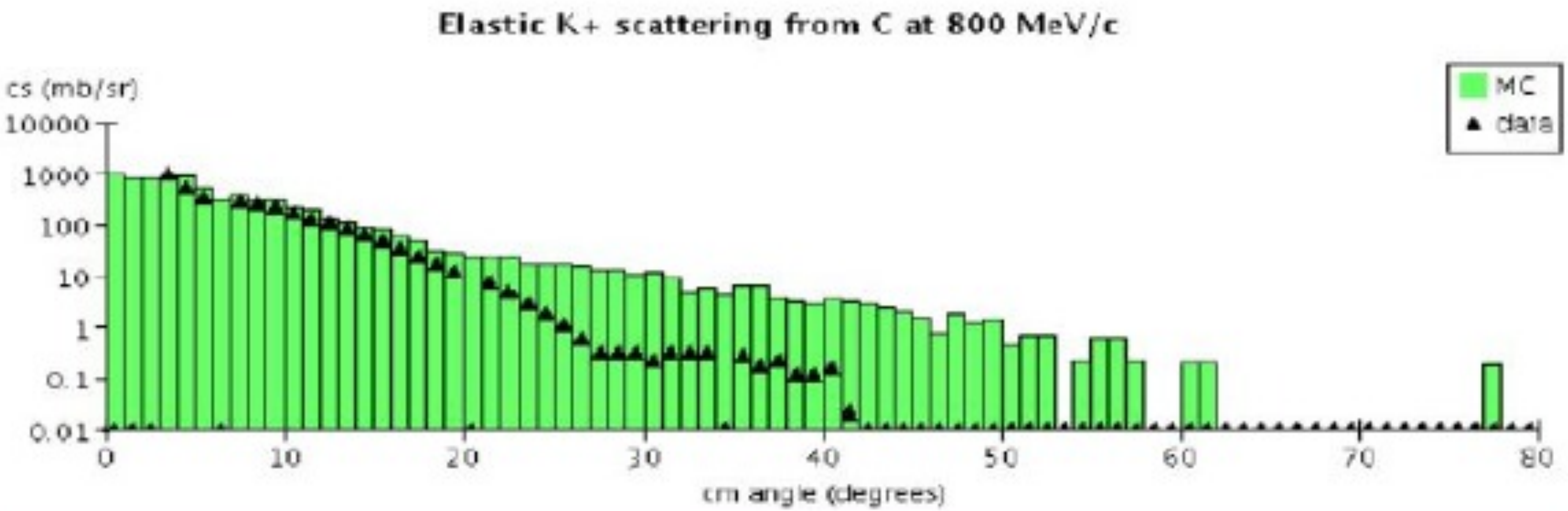
- G4WHadronElasticProcess: general elastic scattering
  - valid for all energies
  - valid for p, n, π , K, hyperons, anti-nucleons, anti-hyperons
  - based in part on old Gheisha code, but with relativistic corrections

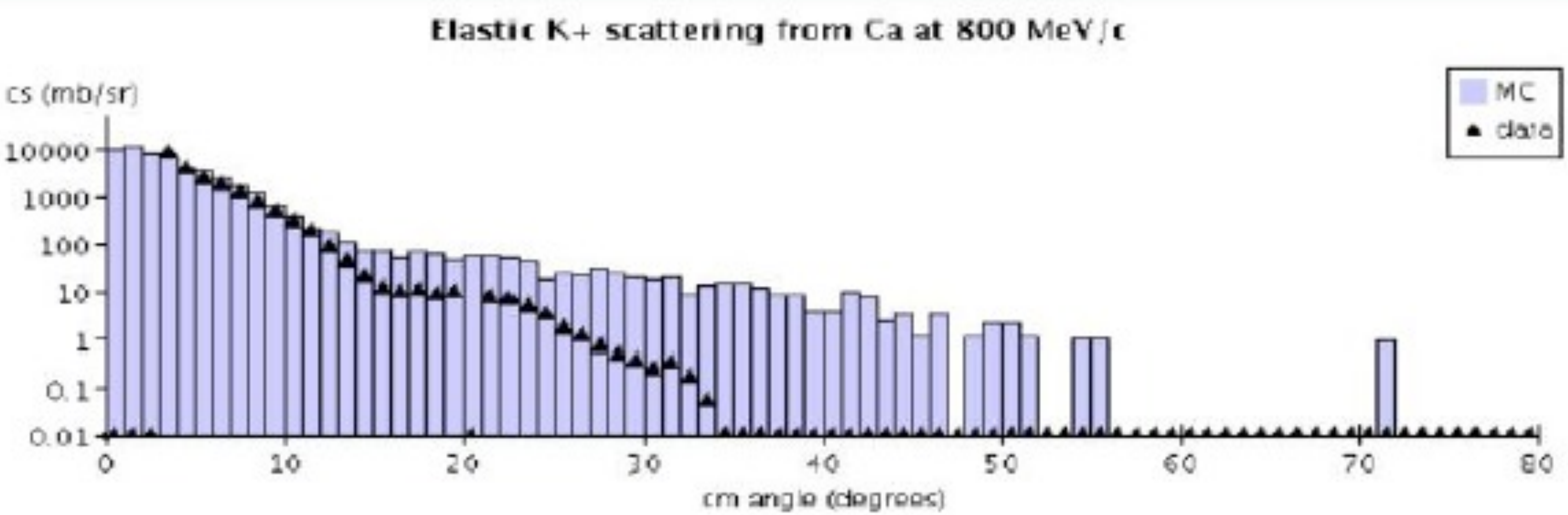
- Coherent elastic
  - G4LEpp for (p,p), (n,n) : taken from SAID phase shift analysis, good up to 1.2 GeV
  - G4LEnp for (n,p) : same as above
  - G4HadronElastic for general hadron-nucleus scattering

- Neutron elastic
  - high precision (HP) model uses data from ENDF ($E < 20$ MeV)

Elastic Scattering Validation

(G4HadronElastic)





Precompound Models

- G4PrecompoundModel is used for nucleon-nucleus interactions at low energy and as a nuclear de-excitation model within higher-energy codes

  - valid for incident p, n from 0 to 170 MeV
  - takes a nucleus from a highly excited set of particle-hole states down to equilibrium energy by emitting p, n, d, t, ^{3}He and α
  - once equilibrium is reached, four other models are called to take care of nuclear evaporation and break-up

- The parameterized models and two cascade models have their own version of nuclear de-excitation models embedded in them

Precompound Models

- Invocation of Precompound model:

```
G4ExcitationHandler* handler = new G4ExcitationHandler;
G4PrecompoundModel* preco = new G4PrecompoundModel(handler);
// Create de-excitation models and assign them to precompound model

G4NeutronInelasticProcess* nproc = new G4NeutronInelasticProcess;
  nproc->RegisterMe(preco);
  neutronManager->AddDiscreteProcess(nproc);
// Register model to process, process to particle
```

- Here the model is invoked in isolation, but usually it is used in combination with high energy or cascade models
  - a standard interface exists for this

Bertini-style Cascade Model

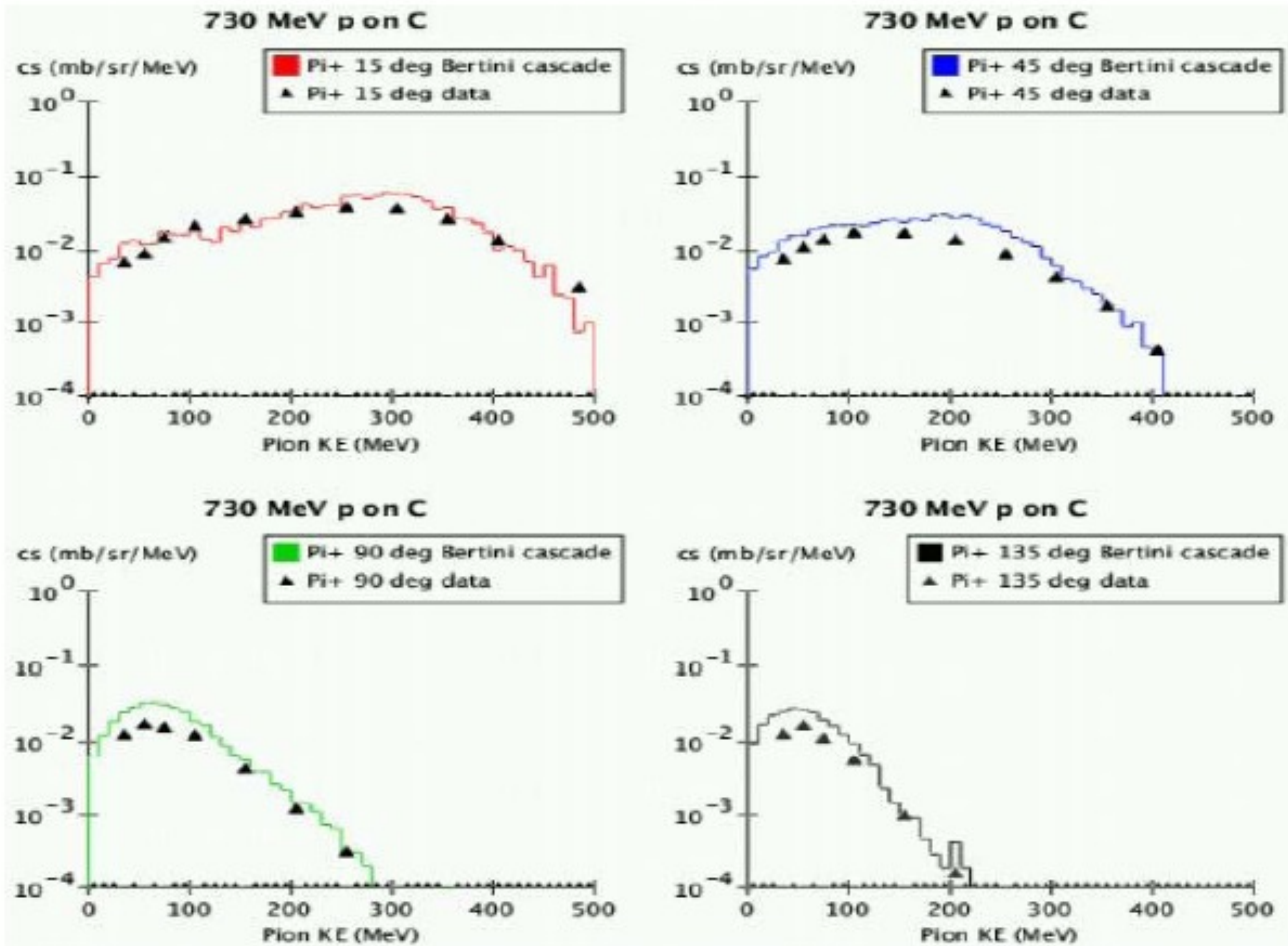
- A classical (non-quantum mechanical) cascade
  - average solution of a particle traveling through a medium (Boltzmann equation)
  - no scattering matrix calculated
  - can be traced back to some of the earliest codes (1960s)
- Core code:
  - elementary particle collisions with individual protons and neutrons: free space cross sections used to generate secondaries
  - cascade in nuclear medium
  - pre-equilibrium and equilibrium decay of residual nucleus
  - target nucleus built of three concentric shells

Using the Bertini Cascade

- In Geant4 the Bertini cascade is used for p, n, π^+, π^-, K^+, K^-, K^0_L, K^0_S, Λ, Σ^0, Σ^+, Σ^-, Ξ^0, Ξ^-, Ω^-
  - valid for incident energies of 0 – 10 GeV
  - can also be used for gammas
- Invocation sequence:

```
G4CascadeInterface* bert = new G4CascadeInterface;
G4ProtonInelasticProcess* pproc = new G4ProtonInelasticProcess;
pproc->RegisterMe(bert);
protonManager->AddDiscreteProcess(pproc);
// same sequence for all other hadrons and gamma
```

Validation of Bertini Cascade



Binary Cascade Model

- Modelling sequence similar to Bertini cascade, except
  - it's a time-dependent model
  - hadron-nucleon collisions handled by forming resonances which then decay according to their quantum numbers
  - particles follow curved trajectories in smooth nuclear potential
- Binary cascade is currently used for incident p, n and π
  - valid for incident p, n from 0 to 10 GeV
  - valid for incident π^+, π^- from 0 to 1.3 GeV
- A variant of the model, G4BinaryLightIonReaction, is valid for incident ions up to A = 12 (or higher if target has A < 12)

Using the Binary Cascade

- Invocation sequence:

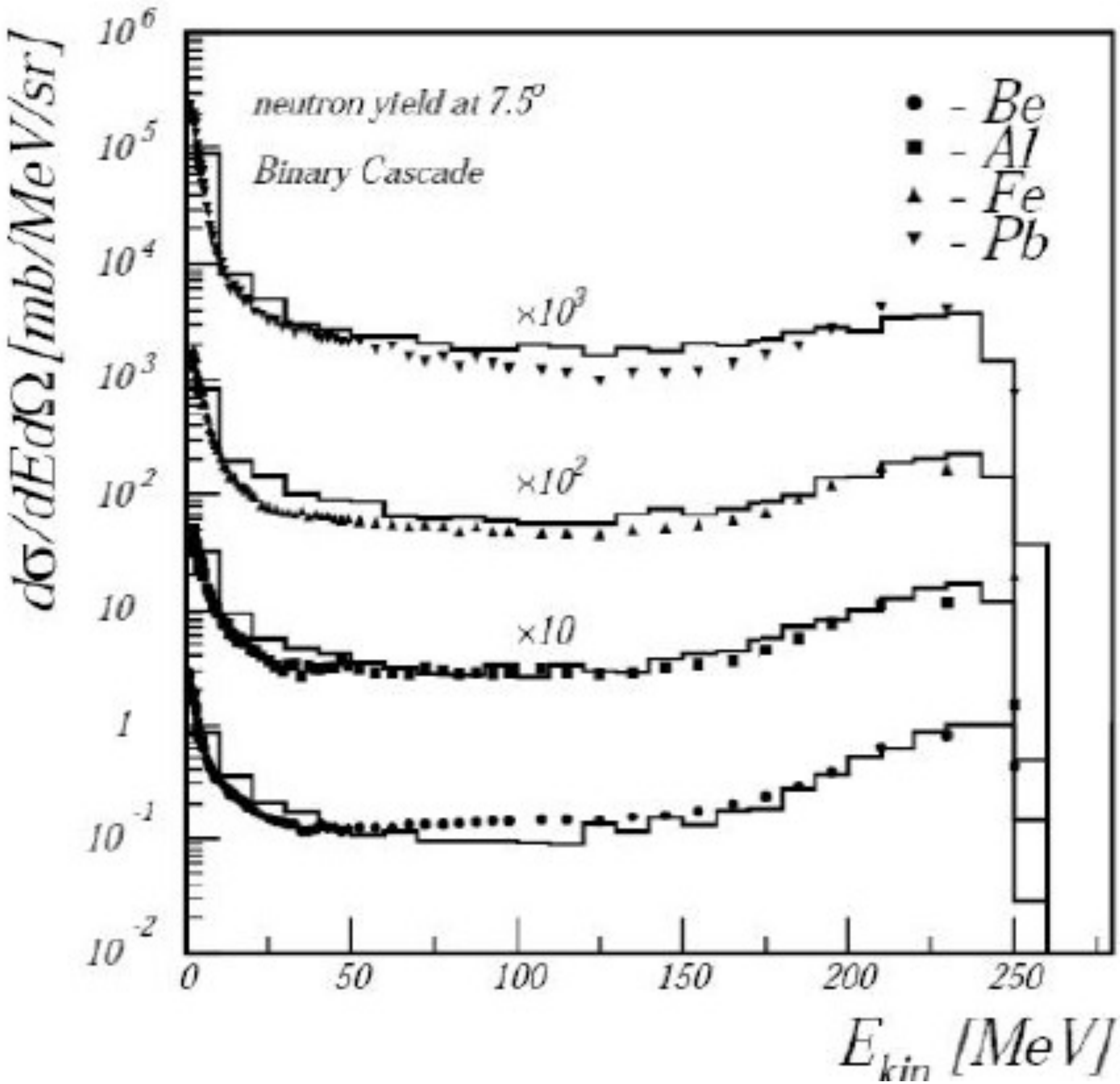
```
G4BinaryCascade* binary = new G4BinaryCascade();
    G4PionPlusInelasticProcess* piproc =
                        new G4PionPlusInelasticProcess();
    piproc->RegisterMe(binary);
    piplus_Manager->AddDiscreteProcess(piproc);
```

- Invoking BinaryLightIonReaction:

```
G4BinaryLightIonReaction* ionBinary =
                        new G4BinaryLightIonReaction();
    G4IonInelasticProcess* ionProc = new G4IonInelasticProcess();
    ionProc->RegisterMe(ionBinary);
    genericIonManager->AddDiscreteProcess(ionProc);
```

Validation of Binary Cascade

256 MeV protons



INCL++ Cascade Model

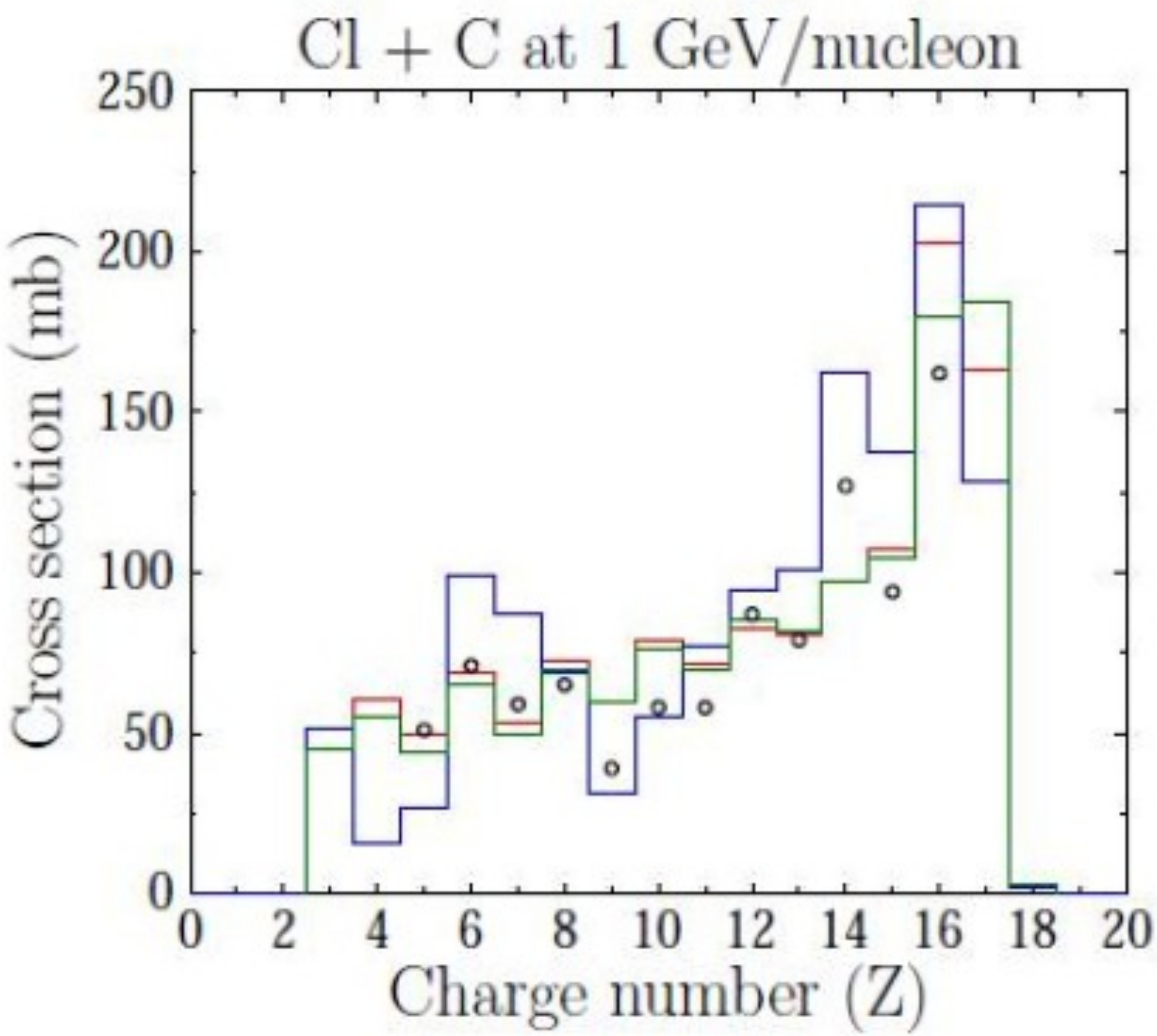
- Model elements:
  - time-dependent model
  - smooth Woods-Saxon or harmonic oscillator potential
  - particles travel in straight lines through potential
  - delta resonance formation and decay (like Binary cascade)

- Valid for incident p, n and π, d, t, ^{3}He, α from 150 MeV to 3 GeV
  - also works for projectiles up to A = 12
  - targets must be 11 < A < 239
  - ablation model (ABLA) can be used to de-excite nucleus

- Used successfully in spallation studies
  - also expected to be good in medical applications

Validation of INCL++ Cascade Model

Green: INCL4.3 Red: INCL4.2 Blue: Binary cascade



Low Energy Neutron Physics

- Below 20 MeV incident energy, Geant4 provides several models for treating neutron interactions in detail

- The high precision models (NeutronHP) are data-driven and depend on a large database of cross sections, etc.

  - the G4NDL database is available for download from the Geant4 web site
  - elastic, inelastic, capture and fission models all use this isotope-dependent data

- There are also models to handle thermal scattering from chemically bound atoms

Geant4 Neutron Data Library (G4NDL)

- Contains the data files for the high precision neutron models
  - includes both cross sections and final states
- From Geant4 9.5 onward, G4NDL is based solely on the ENDF/B-VII database
  - G4NDL data is now taken only from ENDF/B-VII, but still has G4NDL format
  - use G4NDL 4.0 or later
- Prior to Geant4 9.5, G4NDL selected data from 9 different databases, each with its own format
  - Brond-2.1, CENDL2.2, EFF-3, ENDF/B-VI, FENDL/E2.0, JEF2.2, JENDL-FF, JENDL-3 and MENDL-2
  - G4NDL also had its own (undocumented) format

G4NeutronHPElastic

- Handles elastic scattering of neutrons by sampling differential cross section data

  - interpolates between points in the cross section tables as a function of energy
  - also interpolates between Legendre polynomial coefficients to get the angular distribution as a function of energy
  - scattered neutron and recoil nucleus generated as final state

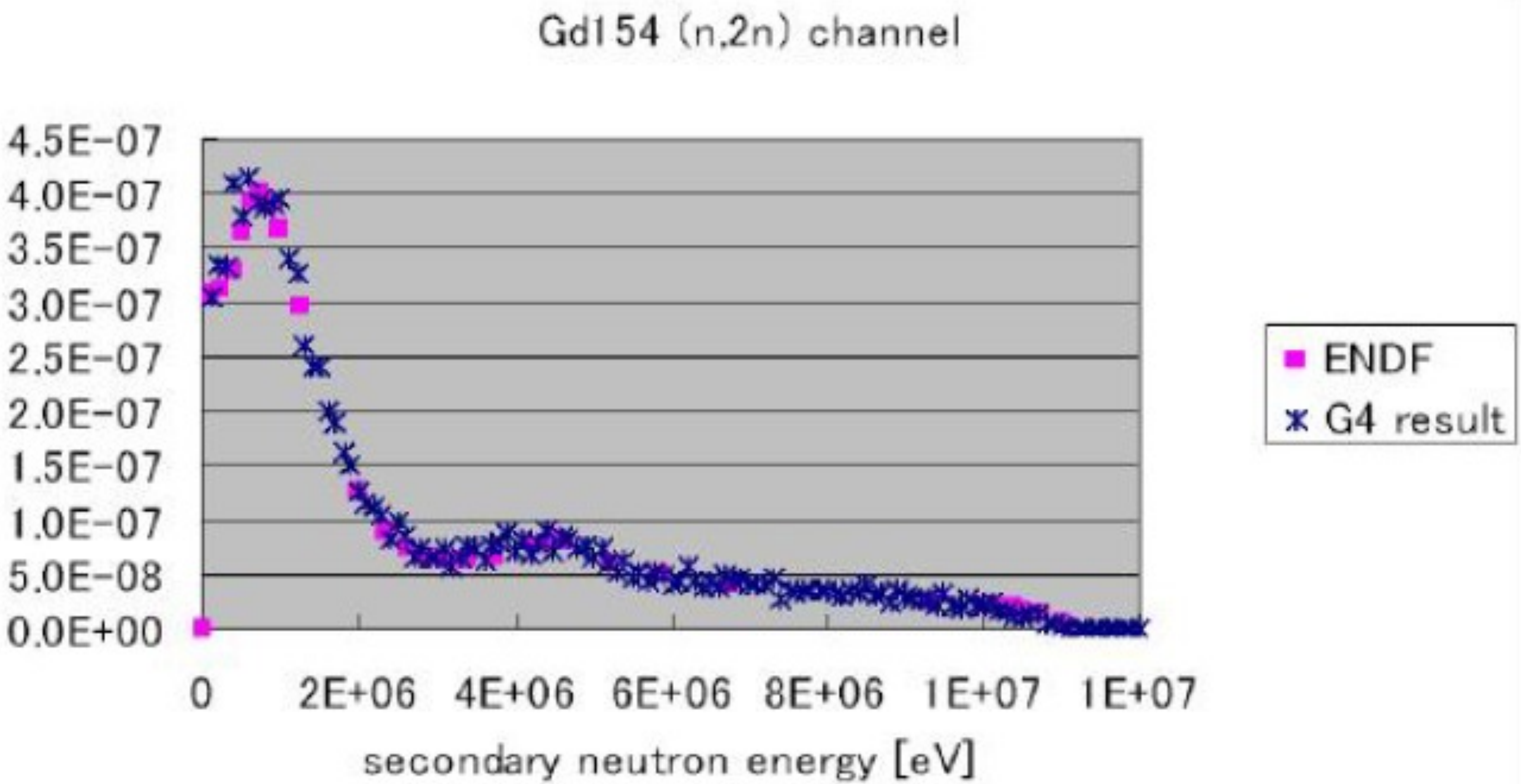
- Note that because look-up tables are based on binned data, there will always be a small energy non-conservation

  - true for inelastic, capture and fission processes as well

G4HPNeutronInelastic

- Currently supports 34 inelastic final states + n gamma (discrete and continuum)
  - n (A,Z) → (A-1, Z-1) n p
  - n (A,Z) → (A-3, Z) n n n n
  - n (A,Z) → (A-4, Z-2) d t
  - …….
- Secondary distribution probabilities
  - isotropic emission
  - discrete two-body kinematics
  - N-body phase space
  - continuum energy-angle distributions (in lab and CM)

Neutron Inelastic: ^{154}Gd (n,2n) Comparison to Data

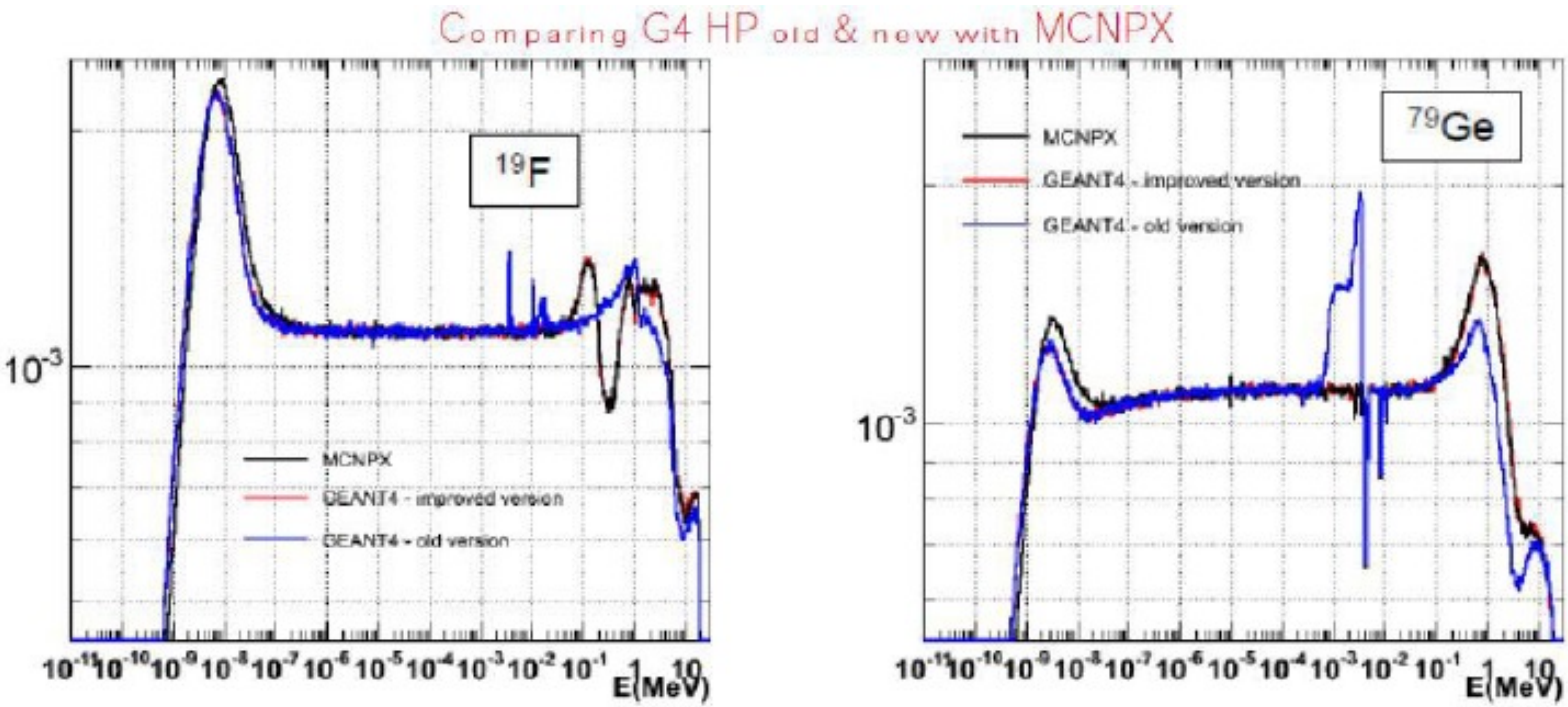


G4NeutronHPCapture

- Neutron capture on a nucleus produces photons described by either
  - the number of photons (multiplicity), or
  - photon production cross sections
- Photon spectra are either
  - discrete emission, using either cross sections or multiplicities from data libraries, or
  - continuous, with the spectrum calculated according to tabulated parameters
    - f(E->Eg) = Si pi(E) gi(E->Eg)
      where pi and gi come from the libraries

High Precision Neutrons

Comparing Geant4 with MCNPX



G4NeutronHPFission

- Currently only uranium fission data are available in Geant4
- First chance, second chance, third chance and fourth chance fission taken into account
- Resulting neutron energy distributions are implemented in different ways
  - as a function of incoming and outgoing neutron energy
  - as a Maxwell spectrum
  - as an evaporation spectrum
  - as an energy-dependent Watt spectrum
  - as Madland-Nix spectrum

Including HP Neutrons in the Physics List

- Elastic scattering

```
G4HadronElasticProcess* theNEP = new G4HadronElasticProcess;

// the cross sections
G4NeutronHPElasticData* theNEData = new G4NeutronHPElasticData;
theNEP->AddDataSet(theNEData);

// the model
G4NeutronHPElastic* theNEM = new G4NeutronHPElastic;
theNEP->RegisterMe(theNEM);
neutManager->AddDiscreteProcess(theNEP);
```

G4NeutronHPorLE Models

- The high-precision neutron models do not cover all elements or isotopes
  - often no data: latest G4NDL has 395 isotopes, but there are thousands
  - data may exist but not yet be evaluated
- A Geant4 application must have a model under all circumstances, otherwise, a fatal error occurs
- G4NeutronHPorLE models were developed to solve this problem
  - HPorLE models call the HP models if data exists
  - if no data, the Low Energy Parameterized (GHEISHA-style) model is called
  - elastic, inelastic, capture and fission provided

Thermal Neutron Scattering from Chemically Bound Atoms

- At thermal energies, atomic motion, vibration, and rotation of bound atoms affect neutron scattering cross-sections and the angular distribution of secondary neutrons

- The energy loss (or gain) of such scattered neutrons may be different from those from interactions with unbound atoms

- Original HP models include only individual Maxwellian motion of the target nucleus (free gas model)

- New behaviour handled by model and cross-section classes
  - G4HPThermalScatteringData, and
  - G4HPThermalScattering

LEND — the Livermore Neutron Models

- Provides an alternative to the HP models
  - better code design
  - faster performance
  - the Livermore database is not yet as extensive as G4NDL

- Corresponding model for each model in HP
  - elastic, inelastic, capture, fission

- Invocation in physics list:
  - use model names G4LENDElastic, G4LENDInelastic, G4LENDCapture, G4LENDFission, and cross sections G4LENDElasticCrossSection, G4LENDInelasticCrossSection, G4LENDCaptureCrossSection, G4LENDFissionCrossSection

- The Low Energy Nuclear Data files can be downloaded from the website ftp://gdo-nuclear.ucllnl.org/pub

Ion-Ion Inelastic Scattering

- Up to now, considered only hadron-nucleus interactions, but Geant4 has five different nucleus-nucleus collision models
  - G4BinaryLightIon
  - G4WilsonAbrasion/G4WilsonAblation
  - G4EMDissociationModel
  - G4QMD
  - G4Incl

- Also provided are several ion-ion cross-section data sets

- Currently, no ion-ion elastic scattering models provided

G4BinaryLightIonReaction

- This model is an extension of the G4BinaryCascade model (to be discussed later)

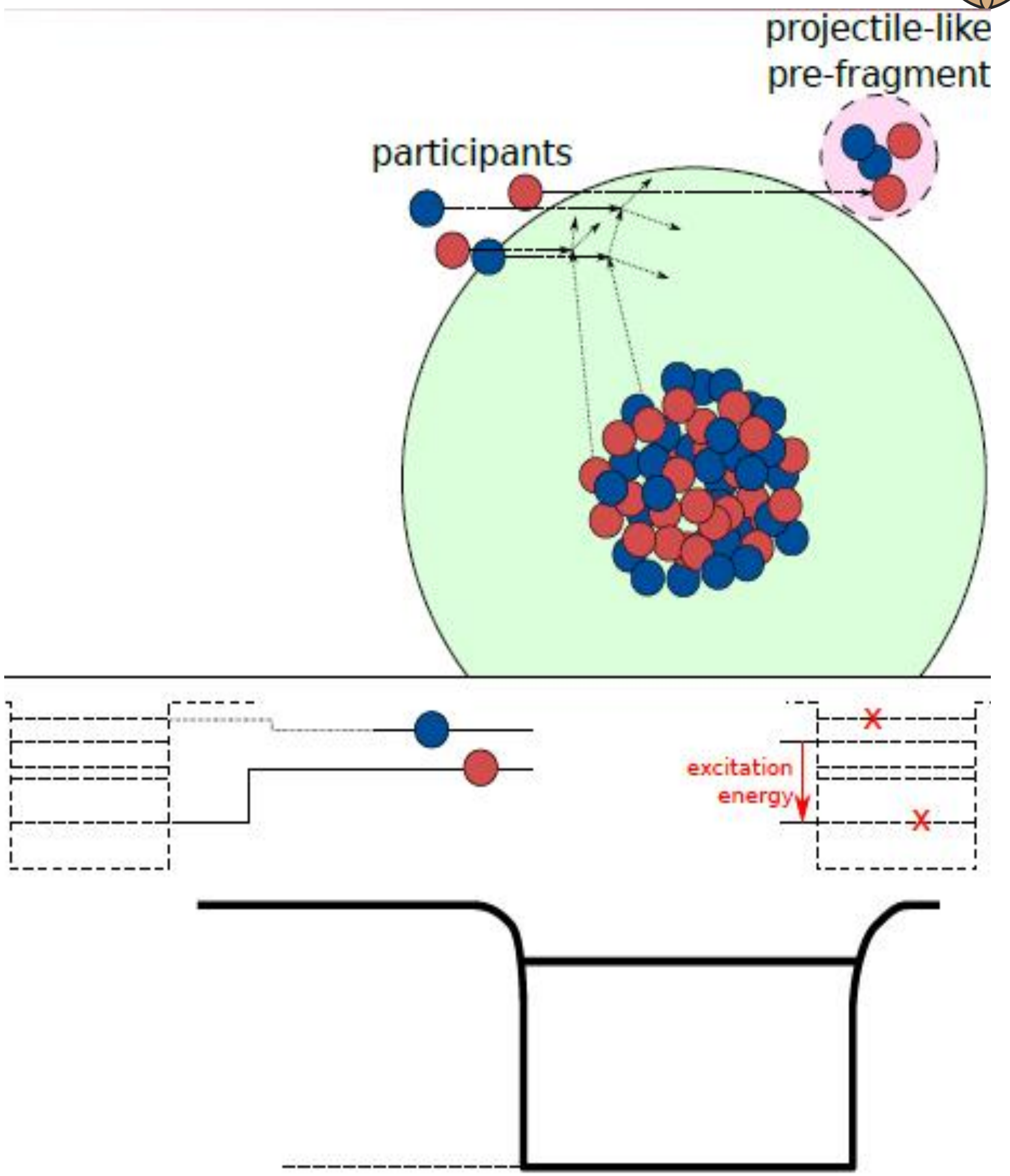
- The hadron-nuclear interaction part is identical, but the nucleus-nucleus part involves:
  - preparation of two 3D nuclei with Woods-Saxon or harmonic oscillator potentials
  - the lighter nucleus is always assumed to be the projectile
  - nucleons in the projectile are entered with their positions and momenta into the initial collision state
  - nucleons are interacted one-by-one with the target nucleus, using the original Binary cascade model

G4EMDissociation Model

- Electromagnetic dissociation is the liberation of nucleons or nuclear fragments as a result of strong EM fields
  - as when two high-Z nuclei approach
  - exchange of virtual photons instead of nuclear force
- Useful for relativistic nucleus-nucleus collisions where the Z of the nucleus is large
- Model and cross sections are an implementation of the NUCFRG2 model (NASA TP 3533)
- Can be used up to 100 TeV

INCL Nucleus-Nucleus

- INCL hadron-nucleus model used to interact projectile nucleons with target
- True potential is not used for projectile nucleus, but binding energy is taken into account
- True potential is used for the target
- Projectile nucleons can pass through to form fragments or interact with the nucleus

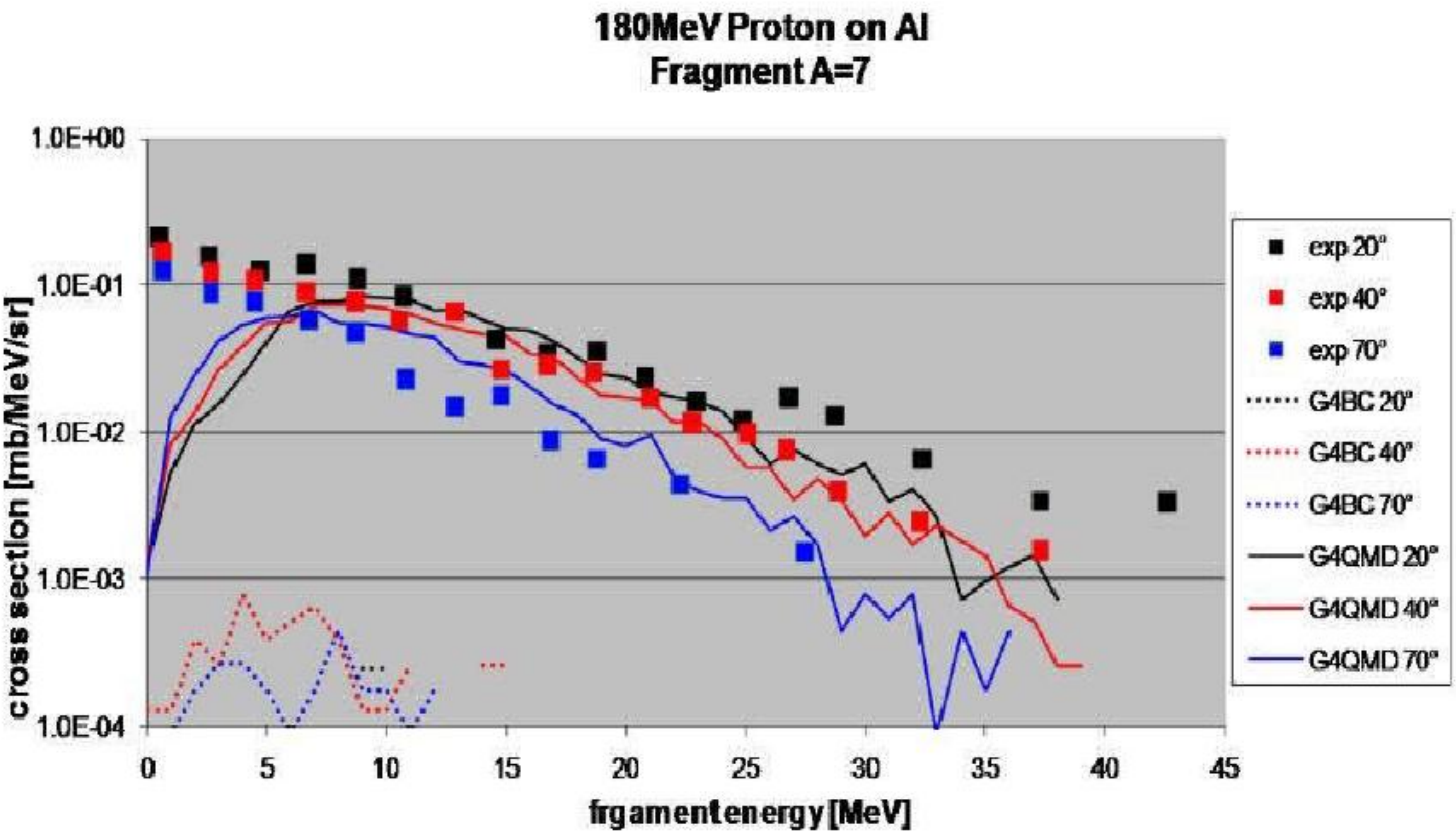


G4QMD Model

- BinaryLightIonReaction has some limitations:
  - neglects participant-participant scattering
  - uses simple time-independent nuclear potential
  - imposes small A limitation for target or projectile
  - the binary cascade base model can only go to 5-10 GeV

- A solution to this is QMD (Quantum Molecular Dynamics) model
  - an extension of the classical molecular dynamics model
  - treats each nucleon as a gaussian wave packet
  - propagation is done with scattering which takes Pauli's principle into account
  - can be used for high energy, high Z collisions

G4QMD Validation



Including QMD in the Physics List

```
• G4HadronInelasticProcess* ionInel =
          new G4HadronInelasticProcess(“ionInelastic”,
  G4GenericIon::G4GenericIon());
    // the cross sections
    G4TripathiCrossSection* tripCS = new G4TripathiCrossSection;
    G4IonsShenCrossSection* shenCS = new
  G4IonsShenCrossSection;
    ionInel->AddDataSet(shenCS);
    ionInel->AddDataSet(tripCS);
    // assign model to process
    G4QMDReaction* theQMD = new G4QMDReaction;
    ionInel->RegisterMe(theQMD);
    G4ProcessManager* pman = G4GenericIon::G4GenericIon()->
                                        GetProcessManager();
    pman->AddDiscreteProcess(ionInel);
```

Radioactive Decay

- The process to simulate radioactive decays of nuclei
  - in flight
  - at rest

- α, β^+, β^- decay, and electron capture (EC) are implemented

- Empirical and data-driven
  - data files are taken from Evaluated Nuclear Structure Data Files (ENSDF)
  - half lives, nuclear level structure for parent and daughter nuclides, decay branching ratios, the energy of the decay process

- If the daughter of nuclear decay is an isomer, prompt de-excitation is done by using G4PhotonEvaporation

- Analog (non-biased) sampling is the default

- Biased sampling is also implemented

Using Radioactive Decays

- Can be accessed with messengers (biasing options etc,)
- To activate radioactive decays through the physics list, insert

```
G4RadioactiveDecay* theDecay = new G4RadioactiveDecay;
G4ProcessManager* pmanager = G4ParticleTable::GetParticleTable()->
FindParticle(“GenericIon”)->GetProcessManager();

pmanager->AddProcess(theDecay);
pmanager->SetProcessOrdering(theDecay, idxPostStep);
pmanager->SetProcessOrdering(theDecay, idxAtRest);
```

Gamma- and Lepto-nuclear Processes

- These models are neither exclusively electromagnetic nor hadronic
  - gamma-nuclear
  - electro-nuclear
  - muon-nuclear

- Geant4 processes available:
  - G4PhotoNuclearProcess (implemented by two models)
  - G4ElectronNuclearProcess (implemented by one model)
  - G4PositronNuclearProcess (implemented by one model)
  - G4MuonNuclearProcess (implemented by two models)

- Gammas interact directly with the nucleus
  - at low energies, they are absorbed and excite the nucleus as a whole
  - at high energies, they act like hadrons (pion, rho, etc.) and form resonances with protons and neutrons

- Electrons and muons cannot interact hadronically, except through virtual photons
  - electron or muon passes by a nucleus and exchanges virtual photon
  - The virtual photon then interacts directly with the nucleus (or nucleons within the nucleus)

Neutrino Scattering

- Not directly implemented inside Geant4
  - there exist interfaces to GENIE
  - neutral current and charged current scattering could be added
- The nuclear part of the interaction is essentially done
  - can be handled by Bertini, FTF
- The weak part of interaction will take some work
  - implementation of existing formulae for sampling ν, Q^2

QCD String Models

- Fritiof (FTF) valid for
  - p, n, π, K, Λ, Σ, Ω from 3 GeV to ~TeV
  - anti-proton, anti-neutron, anti-hyperons at all energies
  - anti-d, anti-t, anti-^{3}He, anti-α with momenta between 150 MeV/nucleon and 2 GeV/nucleon

- Quark-Gluon String (QGS) valid for
  - p, n, π, K from 15 GeV to ~TeV

- Both models handle:
  - building a 3-D model of the nucleus from individual nucleons
  - splitting nucleons into quarks and di-quarks
  - formation and excitation of QCD strings
  - string fragmentation and hadronization

How the QCD String Model Works

- Lorentz contraction turns the nucleus into a pancake

- All nucleons within 1 fm of the path of the incident hadron are possible targets

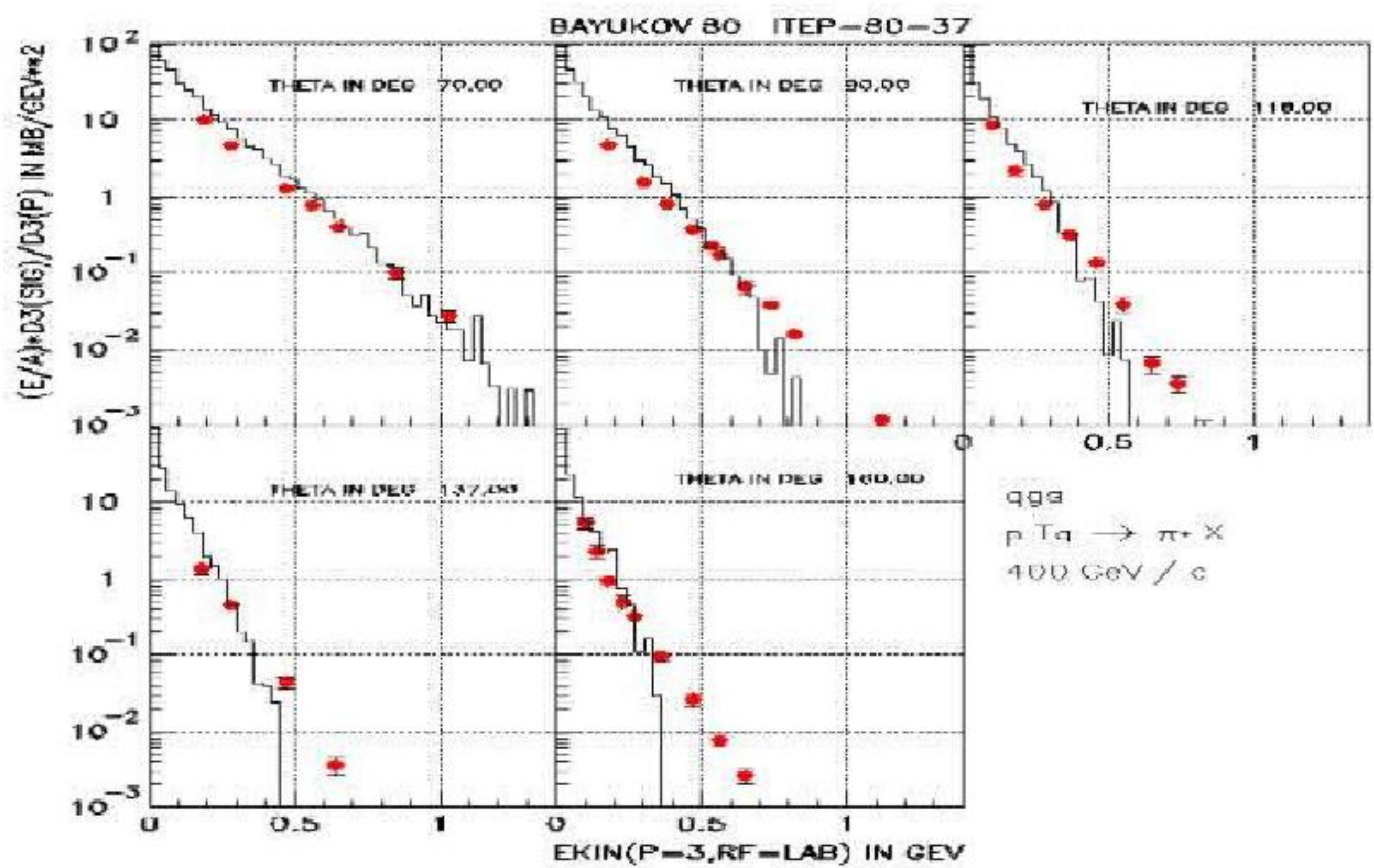
- Excited nucleons along the path collide with neighbours
  - n + n → nΔ, NN, ΔΔ, NΔ, ..
  - essentially a quark-level cascade in the vicinity of path → Reggeon cascade

- All hadrons are treated as QCD strings
  - the projectile is a quark-antiquark pair or quark-diquark pair
  - target nucleons are quark-diquark pairs

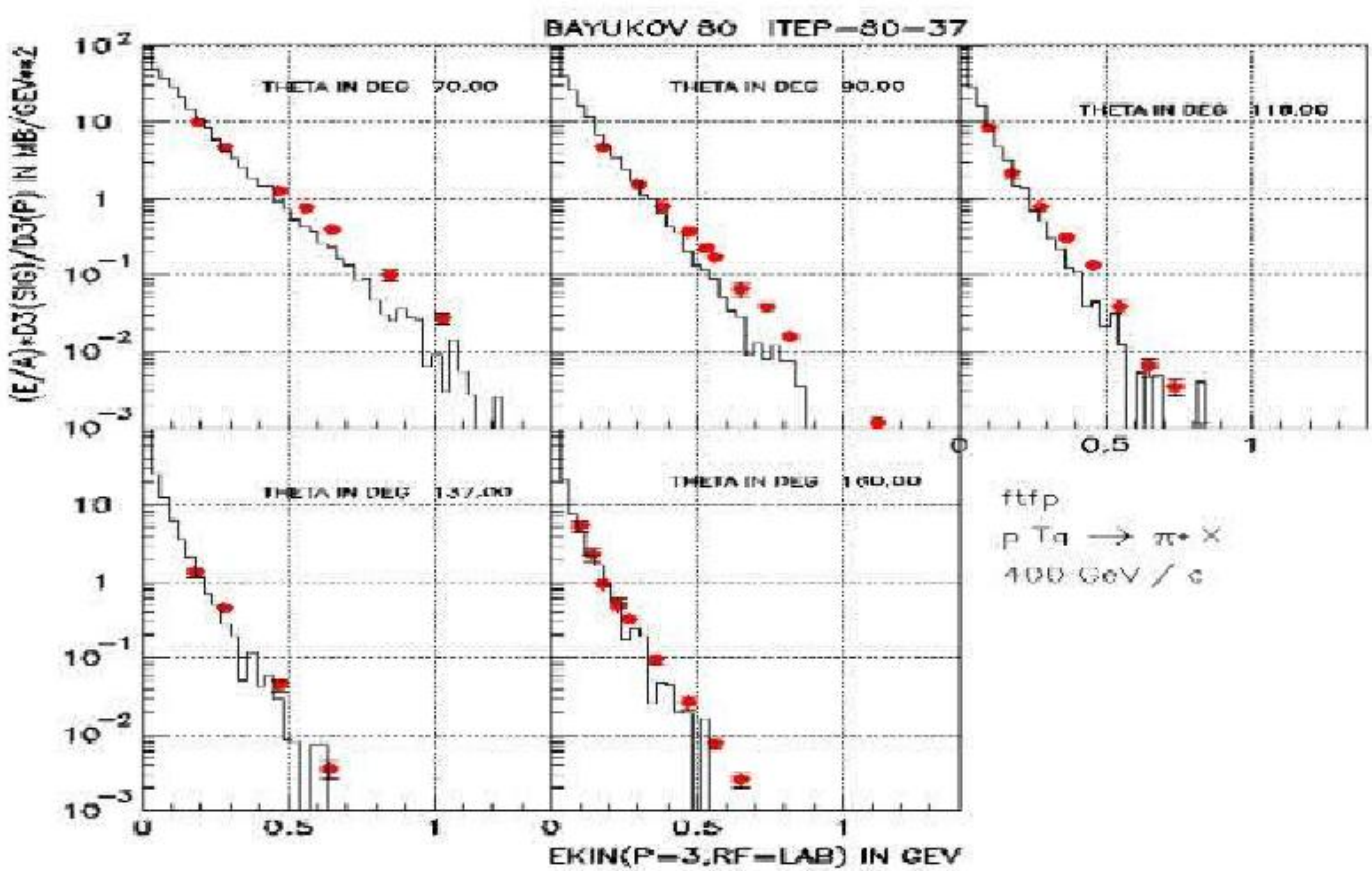
How the QCD String Model Works

- Hadron excitation is represented by a stretched string
  - the string is a set of QCD colour lines connecting the quarks
- When a string is stretched beyond a certain point it breaks
  - replaced by two shorter strings with newly created quarks, anti-quarks on each side of the break
- High-energy strings then decay into hadrons according to fragmentation functions
  - fragmentation functions are theoretical distributions fitted to experiment
- The resulting hadrons can then interact with the nucleus in a traditional cascade

QGS Validation



FTF Validation



Adding FTF Model to the Physics List (1)

- G4TheoFSGenerator* heModel = new G4TheoFSGenerator("FTFP");

```
// model class that contains the sub-models

// Build the high energy string part of the interaction
G4FTFModel* ftf = new G4FTFModel;        // string interaction code
G4ExcitedStringDecay* esdk =              // string decay code
          new G4ExcitedStringDecay(new G4LundFragmentation);

ftf->SetFragmentationModel(esdk);
// assign decay code to model

heModel->SetHighEnergyGenerator(ftf);
// assign string sub-model to high energy model
```

Adding FTF Model to the Physics List (2)

```
// Now set the de-excitation models to handle the nuclear after the
    // high energy interaction
    G4GeneratorPrecompoundInterface* intfce =
                                 new G4GeneratorPrecompoundInterface;
    G4PrecompoundModel* preco =
           new G4PreCompoundModel(new G4ExcitationHandler);
   // precompound model handles medium energy de-excitation
   // G4ExcitationHandler does low energy de-excitation

   intfce->SetDeExcitation(preco);    // assign de-excitation models

   heModel->SetTransport(intfce);   // assign to high energy model
```

Capture Processes and Models

- G4PionMinusAbsorptionAtRest
  - process with direct implementation (no model class)
- G4PionMinusAbsorptionBertini **
  - at rest process implemented with Bertini cascade model
- G4KaonMinusAbsorption
  - at rest process with direct implementation
- G4AntiProtonAnnihilationAtRest
  - process with direct implementation
- G4FTFCaptureAtRest **
  - process implemented for anti-protons by FTF model

** recommended

- G4MuonMinusCaptureAtRest
  - process with direct implementation (no model class)
- G4AntiNeutronAnnihilationAtRest
  - process with direct implementation
- G4HadronCaptureProcess
  - in-flight capture for neutrons
  - model implementations:
    - ❖G4NeutronHPCapture (below 20 MeV)

Fission Processes and Models

- G4HadronFissionProcess can use two models
  - G4NeutronHPFission (specifically for neutrons below 20 MeV)

- A third model handles spontaneous fission as an inelastic process (rather than fission)
  - G4FissLib: Livermore Spontaneous Fission

Summary (I)

- Geant4 hadronic physics allows the user to choose how a physics process should be implemented
  - Cross-sections
  - models
- Many processes, models and cross-sections to choose from
  - The hadronic framework makes it easier for users to add more
- General hadron elastic scattering handled by G4WHadronElasticProcess
- Precompound models are available for low-energy nucleon projectiles and nuclear de-excitation
- Three intra-nuclear cascade models available to cover medium energies (up to 10 GeV)
  - Bertini-style, Binary cascade, INCL++
- There are specialized high-precision neutron models
  - HP models which use G4NDL, now based entirely on ENDF/B-VII
  - alternative LEND (Livermore) models are faster but currently less extensive – use the ENDF.B-VII library

Summary (II)

- Several models for ion-ion collisions
  - Wilson models fast, but not so detailed
  - Binary light ion cascade is more detailed but slower
  - INCL++ ion cascade
  - QMD model is very detailed but not so fast

- Radioactive decay
  - handles decay of isotopes at rest and in flight
  - ENSDF database files required

- Gamma-nuclear and lepto-nuclear processes are available for nuclear reactions initiated by non-hadrons

- Two QCD string models are available for implementing high-energy interactions:
  - Fritiof (FTF): more versatile, covers many particle types, larger energy range
  - Quark-Gluon String (QGS)

- Several stopping processes and models are available for μ, π, K, anti-p, anti-n

- Capture and fission (mostly for neutrons)

Additional Slides

G4WilsonAbrasion and G4WilsonAblation

- A simplified macroscopic model of nucleus-nucleus collisions
  - based largely on geometric arguments
  - faster than Binary cascade or QMD models, but less detailed
- These two models are used together
  - G4WilsonAbrasion handles the initial collision in which a chunk of the target nucleus is gouged out by the projectile nucleus
  - G4WilsonAblation handles the de-excitation of the resulting fragments
- Based on the NUCFRG2 model (NASA TP 3533)
- Can be used up to 10 GeV/n

Wilson Abrasion/Ablation