PHYSICS CONTENT OF GEANT4

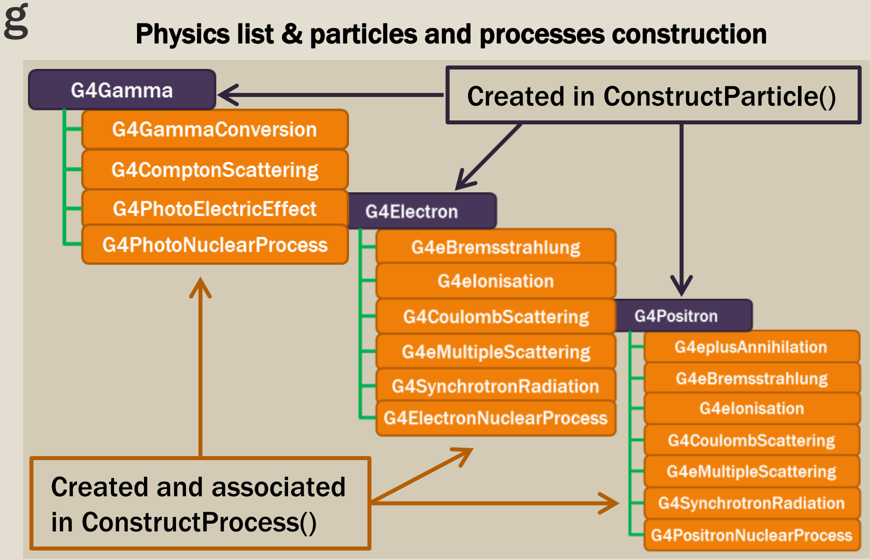
"MORE ON PHYSICS"

Geant4 PHENIICS & IN2P3 Tutorial,
22 – 26 May 2023,
Orsay

Marc Verderi
LLR, Ecole polytechnique

INTRODUCTION

- We have seen that:
  - Geant4 organizes physics modeling with the "physics list" concept.
  - Physics lists create in memory
    - particle types,
    - processes,
      - and bind these processes to the particles.
  - Tools (constructors, modular physics lists, etc.) help to build these more easily.



- We now look into more details to the physics content(s) provided in the concrete implementation of processes
  - Eg : what is there in G4ionIonisation ?

CREDITS

- For the EM physics, Vladimir Ivanchenko (CERN) and Mihaly Novak, Michel Maire and Sébastien Incerti (IN2P3).
- For Hadronic physics, Dennis Wright, Tatsumi Koi (SLAC) and Alberto Ribon (CERN) presentations, Davide Mancusi (CEA) INCL paper
- Both sources may have more filiation.

OUTLINE

I. Generalities
II. EM physics
III. Optical Physics
IV. Decay Physics
V. Hadronic Physics (tomorrow)

I. GENERALITIES

THE PHYSICS PACKAGES

- The processes are located under
  - geant4/source/processes
- Which holds the packages:
  - biasing
  - cuts
  - decay
  - electromagnetic
  - hadronic
  - management
  - optical
  - parameterisation
  - phonon
  - scoring
  - transportation

THE PHYSICS PACKAGES

- The processes are located under the directory
  - geant4/source/processes
- Which holds the packages:
  - biasing, technical, interfaces for biasing
  - cuts, technical, utilities for production thresholds
  - decay, physics, decay of particles with lifetime > 0
  - electromagnetic, physics, gamma, X-ray & charged particles
  - hadronic, physics, hadron& gamma-/lepto-nuclear
  - management, technical, general interfaces to all processes
  - optical, physics, optical photon processes
  - parameterisation, technical, interfaces for fast simulation
  - phonon, physics, phonon transport
  - scoring, technical, interfaces for scoring
  - transportation, technical, geometry boundaries and field

PHYSICS MODELING APPROACHES

- Physics packages have evolved their own designs
  - Driven by physics specificities
- They share however similar approaches:
  - Physics quantities (cross-sections, stopping powers, final states) are computed by means of:
    - Parameterizations
      - "Heuristic" formulae established on some measurements
      - Approach gradually deprecated in Geant4
    - Databases
      - Usually large data sets of direct measurements of quantities (cross-sections, final states, etc.)
      - Very much used in hadronic physics
        - low energy neutrons, radioactive decays, etc.
      - But also in electromagnetic physics, specially at low energy
        - effects of detailed atomic structure, etc.
    - Theory-driven models
      - Based partly or fully on theoretical considerations
      - More often the case at high energies
  - Approaches are mixed in processes and/or physics lists
    - trying to provide "at best" combinations.

THE PHYSICS DATASETS (GEANT4 V11.1)

Details at http://geant4.web.cern.ch/support/data_files_citations

NameVersion	Env. Var. Name	Physics coverage	#Mb
G4NDL4.7	G4NEUTRONHPDATA	Neutron data files with thermal cross-sections	1063
G4EMLOW8.2	G4LEDATA	data files for low energy electromagnetic processes	314
G4PhotonEvaporation5.7	G4LEVELGAMMADATA	data files for photon evaporation (from ENSDF)	9.6
G4RadioactiveDecay5.6	G4RADIOACTIVEDATA	data files for radioactive decay hadronic processes (from ENSDF)	1.0
G4SAIDDATA2.0	G4SAIDXSDATA	data files from evaluated elastic cross-sections in SAID data-base	0.037
G4PARTICLEXS4.0	G4PARTICLEXSDATA	data files for evaluated particle XS on natural composition of elements	11.7
G4ABLA3.1	G4ABLADATA	data files for nuclear shell effects in INCL/ABLA hadronic model	0.105
G4INCL1.0	G4INCLDATA	data files for proton and neutron density profiles in INCL	0.094
G4PII1.3	G4PIIDATA	data files for shell ionization cross-sections	4.1
RealSurface2.2	G4REALSURFACEDATA	Optional data files for measured optical surface reflectance	126.4
G4ENSDFSTATE2.3	G4ENSDFSTATEDATA	Data files for nuclides properties	0.284
G4TENDL1.4	G4PARTICLEHPDATA	Optional data files for incident particles	870

LAST GENERAL PAPER

- Take advantage of last published paper !
  - Provides a full overview of Geant4,
  - including physics options,
  - All this in one single paper

- ***Available in open access***

II. EM PHYSICS

GEANT4 EM PHYSICS PACKAGES

- **Standard**
  - γ, $e^{\pm}$ up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- **Muons**
  - up to 1 PeV
  - energy loss propagator
- **X-rays**
  - X-ray and optical photon production
- **High-energy**
  - processes at high energy (E>10 GeV)
  - physics for exotic particles
- **Polarization**
  - simulation of polarized beams
- **Low-energy**
  - Livermore library
    - γ, e^{-} from 10 eV up to 1 GeV
    - polarized processes
  - PENELOPE rewrite (2008 version)
    - γ, e^{-} , e^{+} from 100 eV up to 1 GeV
    - hadrons and ions up to 1 GeV
  - Atomic de-excitation
    - fluorescence + Auger
- **Geant4-DNA**
  - microdosimetry models for radiobiology
    - from 0.025 eV to 10 MeV
- **Adjoint**
  - Sub-library for reverse Monte Carlo simulation from the detector of interest back to source of radiation

EM DESIGN : PROCESSES & MODELS

- A physics process is described by a process class (G4VEmProcess):
  - Naming scheme : « G4ProcessName »
  - For example: G4Compton for photon Compton scattering

- A physics process can be hold several models, each model being described by a model class (G4VEmModel):
  - Naming scheme : G4ModelNameProcessNameModel or G4ModelNameModel …
    - For example: G4LivermoreComptonModel
  - Models are valid in certain energy ranges and can be assigned to G4Regions
    - Meaning the EM physics level description can be adapted to the regions

- Models implement the physics contents, ie:
  - Cross section and stopping power
  - Sample selection of atom in compound
  - Final state (kinematics, production of secondaries…)

EXAMPLE : MULTIPLE SCATTERING FOR e^{-}

- **In G4EmStandardPhysics constructor:**

```
…
G4double highEnergyLimit = 100*MeV;
…
G4eMultipleScattering* msc = new G4eMultipleScattering;
G4UrbanMscModel* msc1 = new G4UrbanMscModel();
G4WentzelVIModel* msc2 = new G4WentzelVIModel();
msc1->SetHighEnergyLimit(highEnergyLimit);
msc2->SetLowEnergyLimit(highEnergyLimit);
msc->AddEmModel(0, msc1);
msc->AddEmModel(0, msc2);
```

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msc->AddEmModel(0, msc1);
msc->AddEmModel(0, msc2);
```

creation of the physics process (G4VProcess)

creation

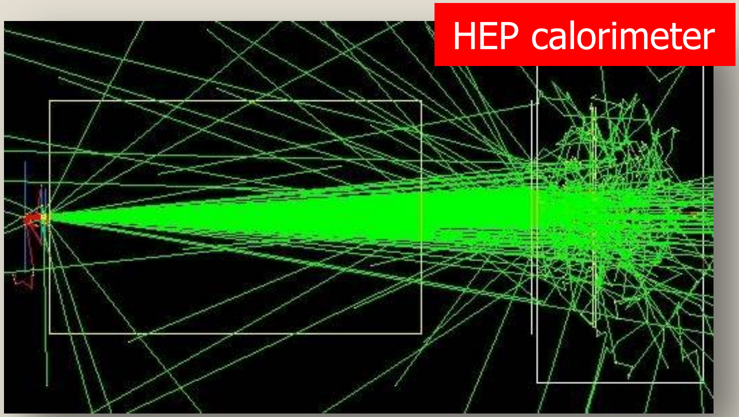
the physics models for the multiple-scattering

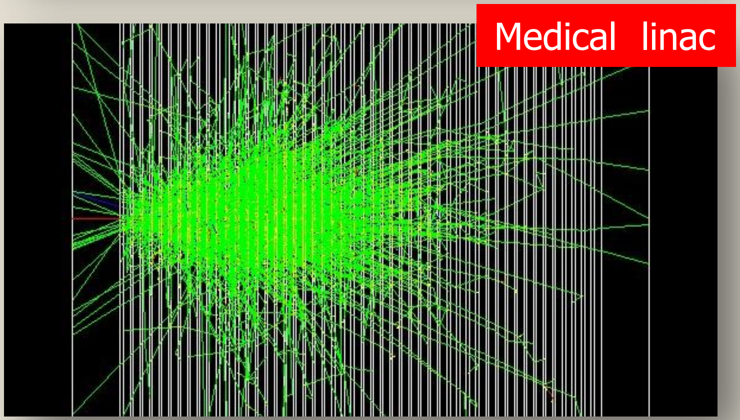
attachment to msc process

II.1 - OVERVIEW OF EM STANDARD PHYSICS

STD EM PROCESSES FOR GAMMA AND ELECTRON TRANSPORT

- **Photon processes**
  - γ conversion into e^+e^- pair
    - Bethe Heitler E < 80 GeV
    - Includes LPM effect E > 80 GeV
  - Compton scattering
    - Klein Nishina + atomic effects
  - Photoelectric effect
    - Photo-electric + atomic deexcitation
  - Rayleigh scattering
    - (except for basic EM standard)
- **Electron and positron processes**
  - Ionization
    - Moller Bhabha for cross-section
    - Berger Seltzer + atomic data for dE/dx from ioni.
  - Coulomb scattering
    - Used alone or with MSC for large angles scattering.
  - Bremsstrahlung
    - Berger Seltzer E < 1 GeV
    - Includes LPM effect E > 1 GeV
  - Positron annihilation





- Suitable for **HEP & many other Geant4 applications** with e^- and γ beams

II.2 – CONDENSED HISTORY MODELS

Ionization,

Multiple Scattering

STD EM PROCESS FOR HADRON AND ION TRANSPORT : IONIZATION

- EM processes take care of ionization by hadron & ion tracks
- If $\sigma(E,e)$ = cross-section for ion of energy E to eject e⁻ of energy e in current material with $n_{at.}$ atoms per unit volume:

Continuous loss from soft e⁻ ($e < e_{cut}$)

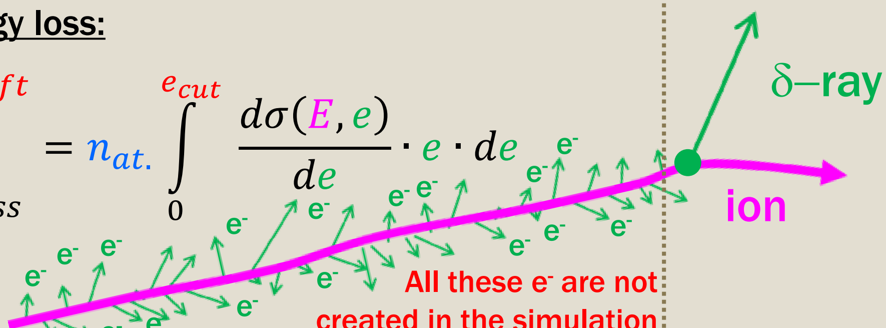
Mean energy loss:

$$\left\langle \frac{dE}{dx} \right\rangle_{loss}^{soft} = n_{at.} \int_0^{e_{cut}} \frac{d\sigma(E,e)}{de} \cdot e \cdot de$$

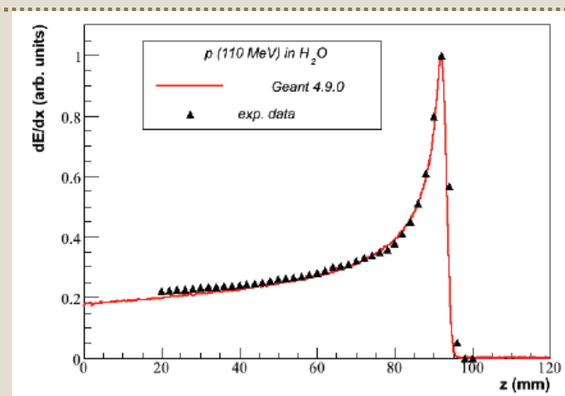
Discrete loss from hard e⁻ ($e > e_{cut}$)

Total XS for δ-ray production:

$$\sigma_{total}^{hard} = \int_{e_{cut}}^{e_{max}} \frac{d\sigma(E,e)}{de} \cdot de$$



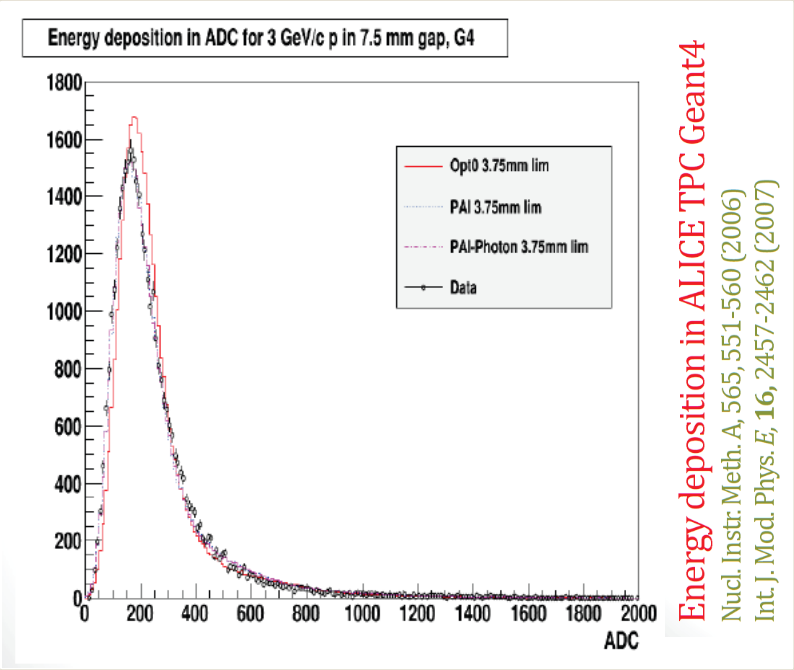
- For ions, continuous loss described:
  - By Bethe-Bloch for E > 2 MeV
    - G4BetheBlochModel
  - Bragg peak parameterization E < 2 MeV
    - Using ICRU'49
    - and NIST data
    - G4BraggIonModel



FLUCTUATION ON (MEAN) IONIZATION

- As stochastic process, **ionization has fluctuations**:
  - Simulation of discrete part (δ-ray) intrinsically takes these into account
  - Model for fluctuations **must be added to the continuous part**

- **Two models are proposed:**
  - **Urban Modelling:**
    - Based on simplified atomic model:
      - Assumed only **two levels E_1, E_2**
    - Particle-atom interactions can be:
      - An excitation of atom with energy loss $E = E_1 - E_2$
      - An ionization, with energy loss distribution $\sim 1/E^2$
    - **G4UniversalFluctuation** class
  - **PAI (photo-absorption ionization)**
    - Use photo-absorption cross-section data
    - Energy transfers sampled with production of e^- and γ
    - Very slow model, to be used in sensitive area
      - Meant for (very) thin detectors
    - **G4PAIModel** (e^-) & **G4PAIPhotModel** (e^-, γ)



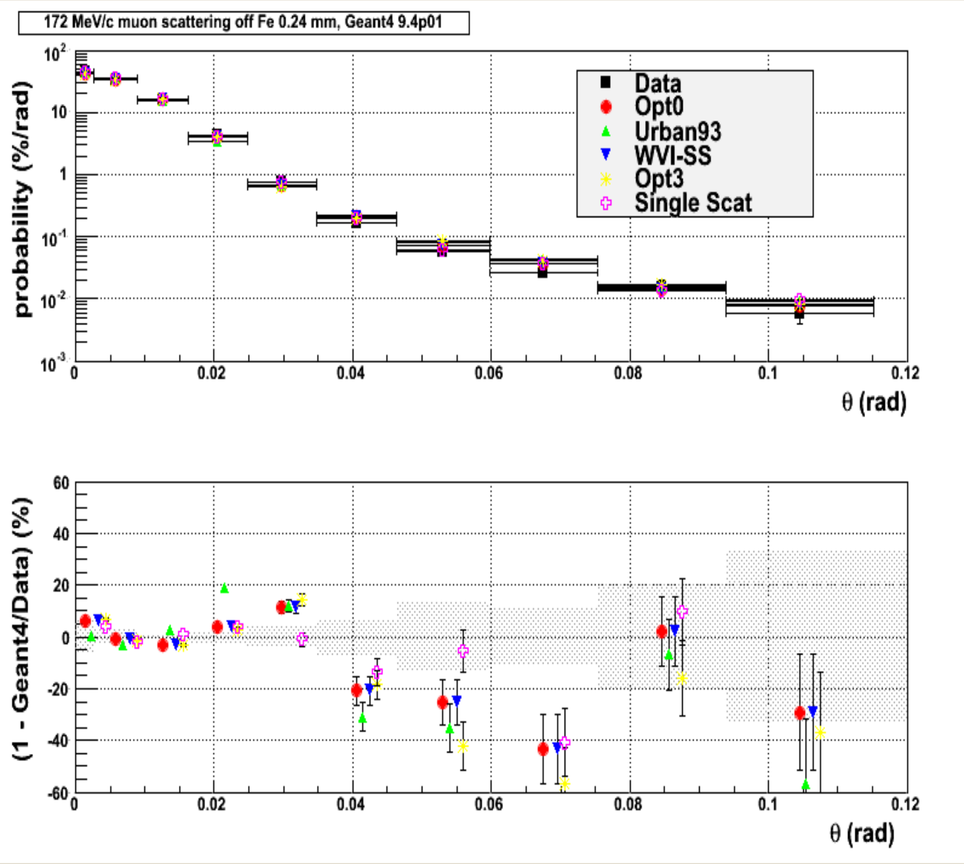
IONIZATION PROCESSES AND MODELS

Table 2
List of GEANT4 ionization processes and models with recommended energy range.

Particle	Process	Model	Energy range
$e-/e+$	G4eIonisation	G4MollerBhabhaModel	10 keV–10 TeV
$e-/e+$		G4PenelopeIonisationModel	0.1 keV–5 GeV
$e-$		G4LivermoreIonisationModel	0.1 keV–1 MeV
All		G4PAIModel	0.1 keV–10 TeV
All		G4PAIPhotModel	0.1 keV–10 TeV
Muons	G4MuIonisation	G4BraggModel	0.1 keV–0.2 MeV
		G4BetheBlochModel	0.2 MeV–1 GeV
		G4MuBetheBlochModel [51]	1 GeV–10 PeV
Hadrons	G4hIonisation	G4BraggModel	1 keV–2 MeV
		G4BetheBlochModel	2 MeV–10 TeV
		G4ICRU73QOModel [52]	5 keV–10 MeV
Ions	G4ionIonisation	G4BraggIonModel	(1 keV–2 MeV)/u
		G4BetheBlochModel	(2 MeV–10 TeV)/u
		G4IonParametrisedLossModel [53]	(1 keV–1 GeV)/u

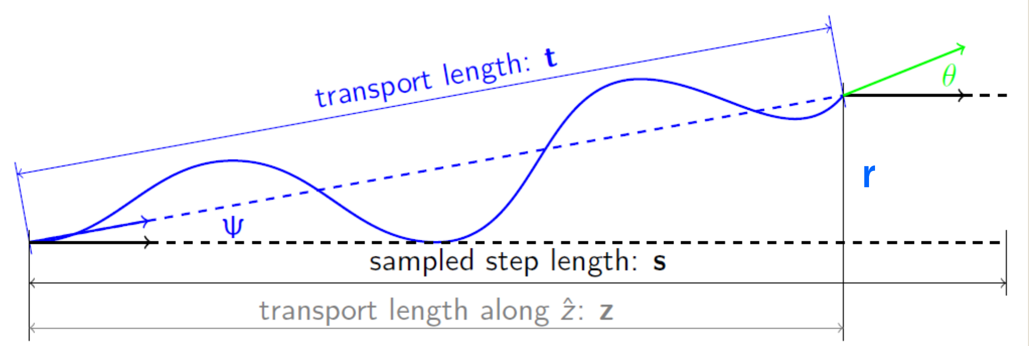
MULTIPLE COULOMB SCATTERING (MSC)

- Charged particles traversing a finite thickness of matter suffer *numerous* elastic Coulomb scattering
  - > 10^6 / mm !
- The **cumulative effect** of these small angle scatterings is a **net deflection** from the original particle direction
- **MSC implementation determines accuracy and CPU performance of simulation**



MSC ALGORITHM

- **Legend**
  - True path length : t
  - Geometrical displacement : z
  - Lateral displacement : r
  - Angular deflection : (θ,ψ)



- **The algorithm performs several steps for the simulation of MSC which are essentially the same for many « condensed » simulations**
  - The physics processes and the geometry select the step length; MSC performs the $t \leftrightarrow z$ transformation only
  - The transport along the initial direction is not MSC's business
  - Sampling of scattering angle (θ,ψ)
  - Computing of lateral displacement and relocation of particle

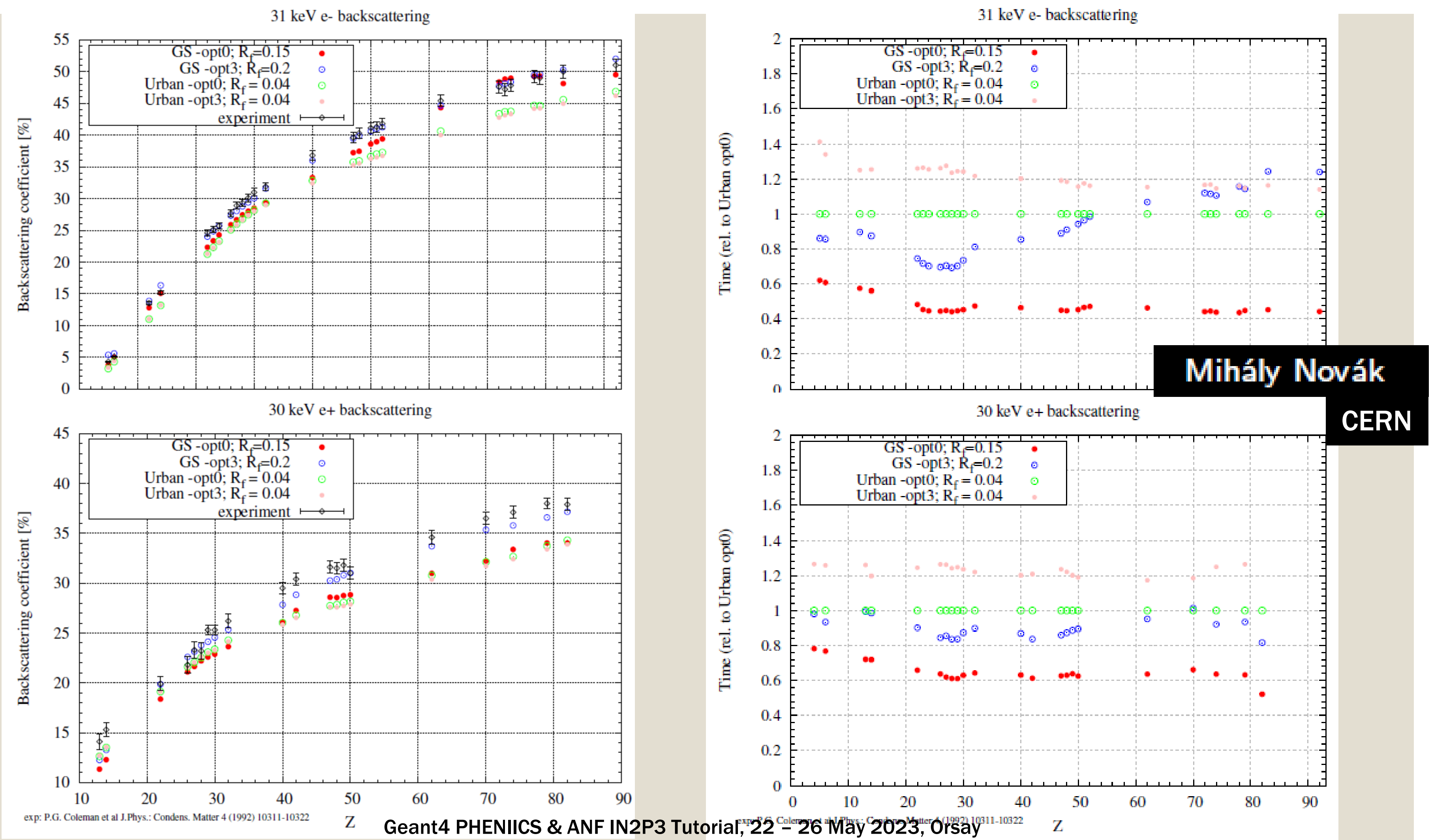
MSC AND SINGLE SCATTERING MODELS

Model	Particle type	Energy limit	Specifics and applicability
Urban (Urban 2006)	Any	-	Default model for electrons and positrons below 100 MeV, (Lewis 1950) approach, tuned to data, used for LHC production.
Screened Nuclear Recoil (Mendenhall and Weller 2005)	p, ions	< 100 MeV/A	Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space app.
Goudsmit-Saunderson (Kadri 2009)	e^+, e^-	< 1 GeV	Theory based cross sections (Goudsmit and Saunderson 1950). EPSEPA code developed by Penelope group, final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
Coulomb scattering (2008)	any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons
WentzelVI (2009)	any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons.
Ion Coulomb scattering (2010) Electron Coulomb scattering (2012)	Ions e^+, e^-	-	Model based on Wentzel formula + relativistic effects + screening effects for projectile & target. From the work of P. G. Rancoita, C. Consolandi and V. Ivantchenko.

MSC CLASSES

- Processes per particle type are available
  - G4eMultipleScattering for e+/e-
  - G4MuMultipleScattering for µ+/µ-
  - G4hMultipleScattering for hadrons and ions
- L. Urban model
  - G4UrbanMscModel :
    - The most established Geant4 scattering model
- Combined multiple and single scattering model:
  - G4WentzelVIModel + G4eCoulombScatteringModel
    - Applied for high energy e+-, muons, hadrons
- Alternative single and multiple scattering models are available to users
  - see extended examples…

AN INTERESTING REWRITE : GOUDSMIT-SAUNDERSON MODEL

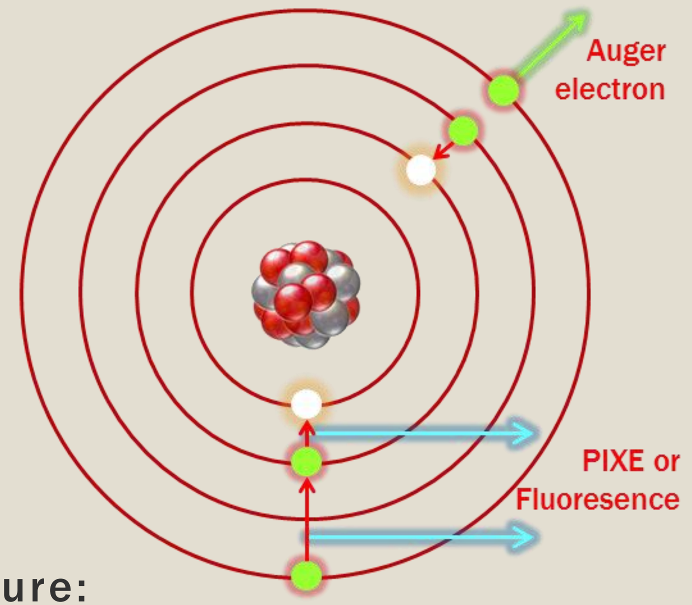


II.3 - ATOMIC DE-EXCITATION

Fluo-
rescence,
Auger &
PIXE

ATOMIC DE-EXCITATION/RELAXATION

- Atom's shell configuration can be disturbed:
  - Directly for electromagnetic interactions :
    - photo-electric, Compton, ionization, …
  - Or by Z change of nucleus:
    - Radioactive decay :
      - with Z change ($\beta^{\pm}$, α, electronic capture)
    - Nuclear evaporation, etc.



- Atomic relaxation follows and atom can de-excite through:
  - Fluorescence
  - Auger
  - PIXE (Particle Induced X-Ray Emission)

- Simulation requires detailed atomic structure:
  - EADL transition probability data used (Livermore)
  - radiative: fluorescence
  - non-radiative:
    - Auger (initial & final vacancies in ≠ sub-shells)
    - Coster-Kronig (same sub-shells)

INCLUDING/ACTIVATING ATOMIC EFFECTS

- Atomic de-excitation can be activated for any EM physics options
  - See more in X-Ray Spec. 40 (2011) 135-140
- By default, reference physics include atomic deexcitation
  - As they use EM physics constructors, which include the deexcitation

- Then, atomic deexcitation can be easily (de)activated via UI commands
  - /run/initialize
  - /process/em/deexcitation regionName true false false
  - or, individually
  - /process/em/fluo true
  - /process/em/auger true
  - /process/em/pixe true

regionName: region where to activate, can be World

true false false: fluo., Auger, PIXE, resp.

/process/em/fluo, /process/em/auger, /process/em/pixe: if no region specified (as before), World is assumed

- To do the same with C++ code, use the G4EmParameters class:
  - G4EmParameters* param = G4EmParameters::Instance();
  - param->SetDeexActiveRegion(regionName,true,false,false);
  - or, individually
  - param->SetFluo(true);
  - param->SetAuger(true);
  - param->SetPixe(true);

INCLUDING/ACTIVATING ATOMIC EFFECTS

- Fluorescence is activated by default in all EM constructors
  - except in the Standard one, G4EmStandardPhysics;

- Last, no least:
  - Deexcitation module *takes into account production thresholds*
    - But deexcitation particles are generally of low energy
    - They hence might not be produced…
  - To force deexcitation particles to be produced:
    - /process/em/deexcitationIgnoreCut true
    - or, with C++:
    - param->SetDeexcitationIgnoreCut(true);

OPTIONS FOR SHELL CROSS SECTION MODELS

- Ionisation cross section models for PIXE can be changed:
  - /run/initialize
  - …
  - /process/em/pixeXSmodel Empirical
    - or ECPSSR_FormFactor or ECPSSR_Analytical
  - param->SetPIXECrossSectionModel("Empirical“);
    - or "ECPSSR_FormFactor" or "ECPSSR_Analytical"

"Energy-Loss Coulomb-Repulsion Perturbed-Stationary-State Relativistic Theory"

- Shell cross sections are available for K, L and selected M shells:
  - Empirical models:
    - from Paul "reference values" (for p and α for K-Shell) and Orlic empirical model for L shells (only for p and ions with Z>2);
  - ECPSSR_FormFactor models:
    - derive from A. Taborda *et al.* calculations of ECPSSR values directly from Form Factors and it covers K, L shells in the range 0.1-100 MeV and M shells in the range 0.1-10 MeV;
  - ECPSSR_Analytical models:
    - derive from an in-house analytical calculation of the ECPSSR theory.

- By default "Empirical" models are used and "ECPSSR_Analytical" models take over out of related energy ranges. Default setting is recommended.

- Shell cross section can also be selected for e^-, eg:
  - /process/em/pixeElecXSmodel Livermore (or Penelope)

X-Ray Spec. 40 (2011) 127-134
X-Ray Spec. 40 (2011) 135-140

II.4 - LOW EM ENERGY

Livermore

Penelope

Ion energy loss

PURPOSE OF LOW ENERGY EM PACKAGE

- Extend coverage of Geant4 EM interactions with matter
  - for photons, electrons, positrons and ions
  - down to sub-keV scale energies

- Choices of physics models include
  - Livermore : electrons and photons [250 eV – 1 GeV]
  - Penelope : electrons, positrons and photons [100 eV – 1 GeV]
  - Microdosimetry models
    - Geant4-DNA project: [eV – ~ few 100 MeV]
    - MuElec for Silicon : [eV – 1 GeV/u]

- Possible domains of applications
  - Space science
  - Medical physics
  - Underground experiments
  - Microdosimetry for radiobiology and microelectronics
  - …

LIVERMORE MODELS
ELECTRON AND GAMMA INCIDENT (but no e^+)

- Based on publicly available **evaluated data tables** from the Livermore data library
  - EADL : Evaluated Atomic Relaxation Data Library
  - EEDL : Evaluated Electrons Interaction Data Library
  - EPDL97 : Evaluated Photons Interaction Data Library
  - Mixture of experiments and theories
  - Binding energies: Scofield
- Include elements from **Z=1 to Z=100**
  - Include atomic effects (fluorescence, Auger)
  - Atomic relaxation : Z > 5 (EADL transition data)

http://www-nds.iaea.org/epdl97

- Data tables are **interpolated** by Livermore model classes to compute
  - Total cross sections: photoelectric, Compton, Rayleigh, pair production, Bremsstrahlung
  - Shell integrated cross sections: photo-electric, ionization
  - Energy spectra: secondary e- processes
- Validity range (recommended) : **250 eV - 100 GeV**
  - Processes can be used down to 100 eV, with a reduced accuracy
  - In principle, down to ~10 eV
- Naming scheme: **G4LivermoreXXXModel** (eg. G4LivermoreComptonModel)

- Models also available as **polarized photon interactions**
- Naming scheme: **G4LivermorePolarizedXXXModel**
  - eg. G4LivermorePolarizedComptonModel

AVAILABLE LIVERMORE MODELS

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Gammas				
Compton	G4ComptonScattering	G4LivermoreComptonModel	250 eV (kill)	100 GeV
Polarized Compton	G4ComptonScattering	G4LivermorePolarizedComptonModel	250 eV (kill)	100 GeV
Rayleigh	G4RayleighScattering	G4LivermoreRayleighModel	10 eV (kill)	100 GeV
Polarized Rayleigh	G4RayleighScattering	G4LivermorePolarizedRayleighModel	250 eV (kill)	100 GeV
Conversion	G4GammaConversion	G4LivermoreGammaConversionModel	1.022 MeV	100 GeV
Polarized Conversion	G4GammaConversion	G4LivermorePolarizedGammaConversionModel	1.022 MeV	100 GeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	~ few eV	100 GeV
Polarized Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	10 eV	100 GeV
Electrons				
Ionization	G4eIonisation	G4LivermoreIonisationModel	100 eV	100 GeV
Bremsstrahlung	G4eBremsstrahlung	G4LivermoreBremsstrahlungModel	10 eV	100 GeV

PENELOPE PHYSICS
ELECTRON, POSITRON AND GAMMA INCIDENT

- Re-implementation of the low-energy models from the Monte-Carlo code PENELOPE (PENetration and Energy LOss of Positrons and Electrons) version 2008:
  - Nucl. Instrum. Meth. B 207 (2003) 107-123

- Physics models
  - Specifically developed by the group of F. Salvat *et al.*
  - Great care dedicated to the low-energy description
    - Atomic effects, fluorescence, Doppler broadening...

- Mixed approach: analytical, parameterized & database-driven
  - Applicability energy range: 100 eV – 1 GeV

- Also include positrons
  - Not described by Livemore models

- G4PenelopeXXXModel (e.g. G4PenelopeComptonModel)

AVAILABLE PENELOPE MODELS

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Gammas				
Compton	G4ComptonScattering	G4PenelopeComptonModel	100 eV	1 GeV
Rayleigh	G4RayleighScattering	G4PenelopeRayleighModel	100 eV	1 GeV
Conversion	G4GammaConversion	G4PenelopeGammaConversionModel	1.022 MeV	1 GeV
Photo-electric	G4PhotoElectricEffect	G4PenelopePhotoElectricModel	100 eV	1 GeV
Electrons/Positrons				
Ionization	G4eIonisation	G4PenelopeIonisationModel	100 eV	1 GeV
Bremsstrahlung	G4eBremsstrahlung	G4PenelopeBremsstrahlungModel	100 eV	1 GeV
Positrons				
Annihilation	G4eplusAnnihilation	G4PenelopeAnnihilationModel	100 eV	1 GeV

ION ENERGY LOSS MODEL

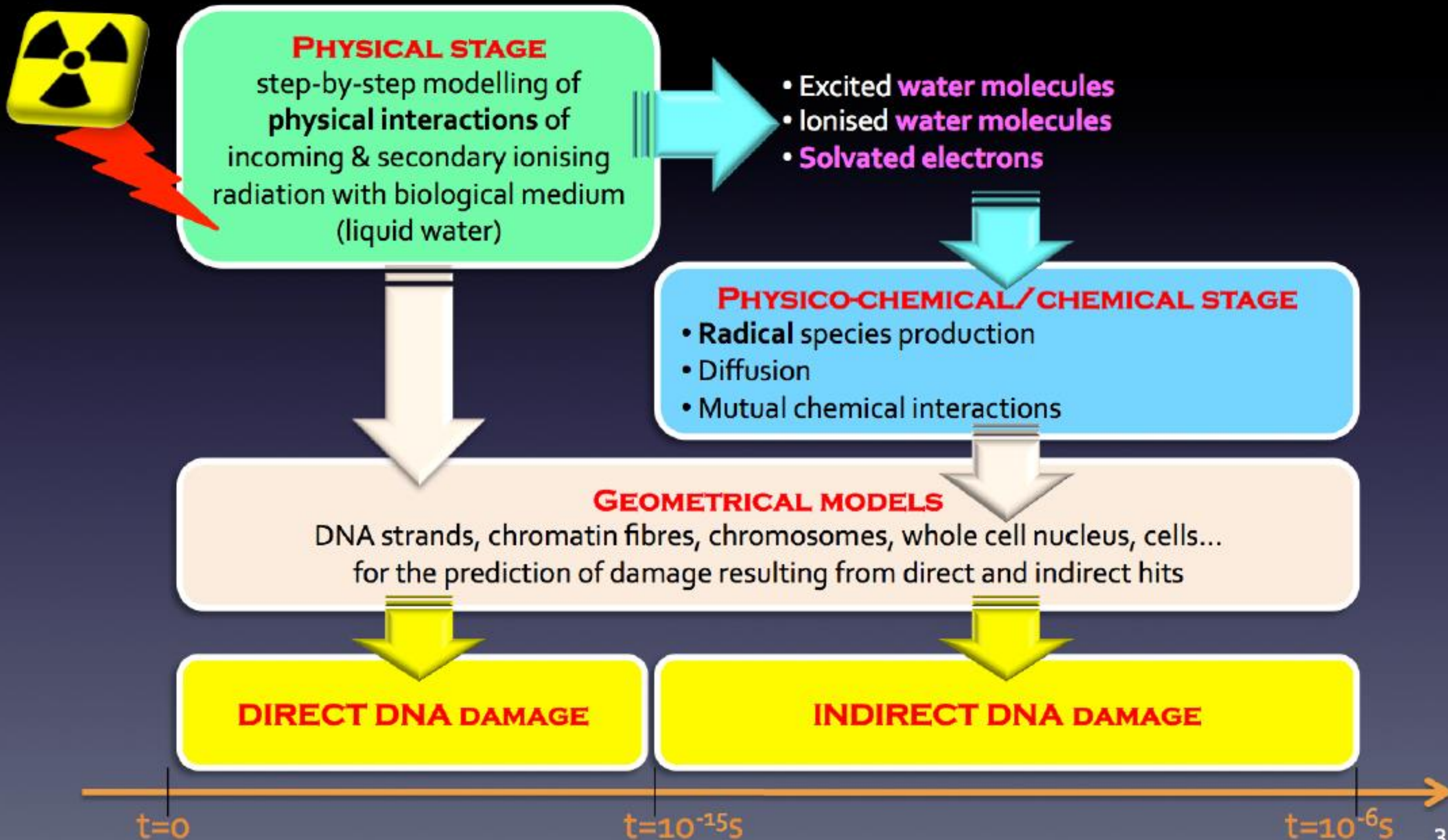
- Describes the energy loss of ions heavier than Helium due to interactions with atomic shells of target atoms
  - G4IonParametrisedLossModel class
- Primarily of interest for medical and space applications
  - See more in Nucl. Instrum. Meth. B 268 (2010) 2343-2354

- Modeling:
  - Restricted stopping powers are calculated from
    - $T < T_{Low}$: Free electron gas model
    - $T_{Low} \leq T \leq T_{High}$: parameterization (ICRU'73) approach
    - $T > T_{High}$: Bethe-Bloch formula (using eff. charge + higher ord. corr.)
    - With energy limits
      - T_{High} = 10 MeV/u (except Fe ions: T_{High} = 1 GeV/u)
      - T_{Low} = 0.025 MeV/u (lower boundary of ICRU'73 tables)
  - ICRU'73 parameterization
    - https://www.icru.org/report/stopping-of-ions-heavier-than-helium-report-73/
    - Large range of ion-materials combination:
      - Incident ions : Li to Ar, and Fe
      - 25 elemental materials, 31 compounds
    - Stopping powers based on the binary theory, effective charge approach for Fe
      - Special case: water (revised ICRU'73 tables by P. Sigmund, mean ionization potential is 78 eV)

II.5 – ULTRA-LOW EM ENERGY

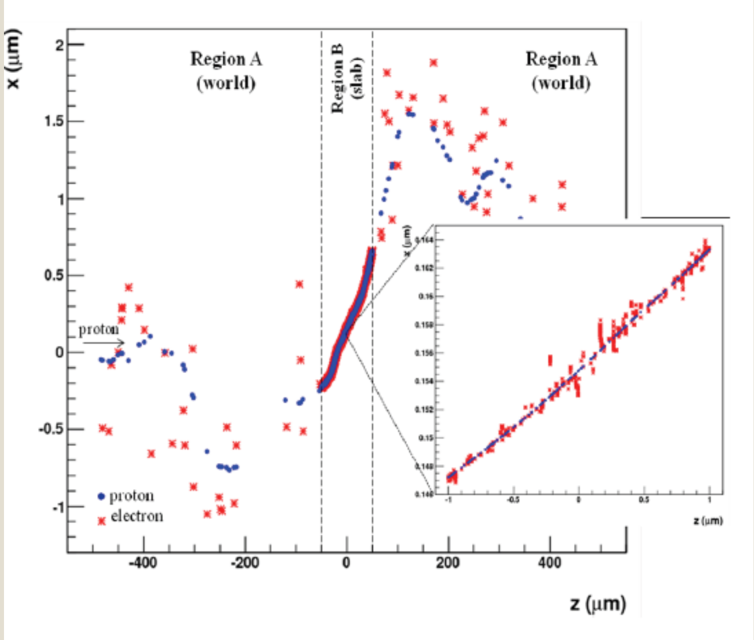
Micro-dosimetry in DNA & Silicon

How can Geant4-DNA model early DNA damage ?



GEANT4 FOR MICRODOSIMETRY IN RADIOBIOLOGY

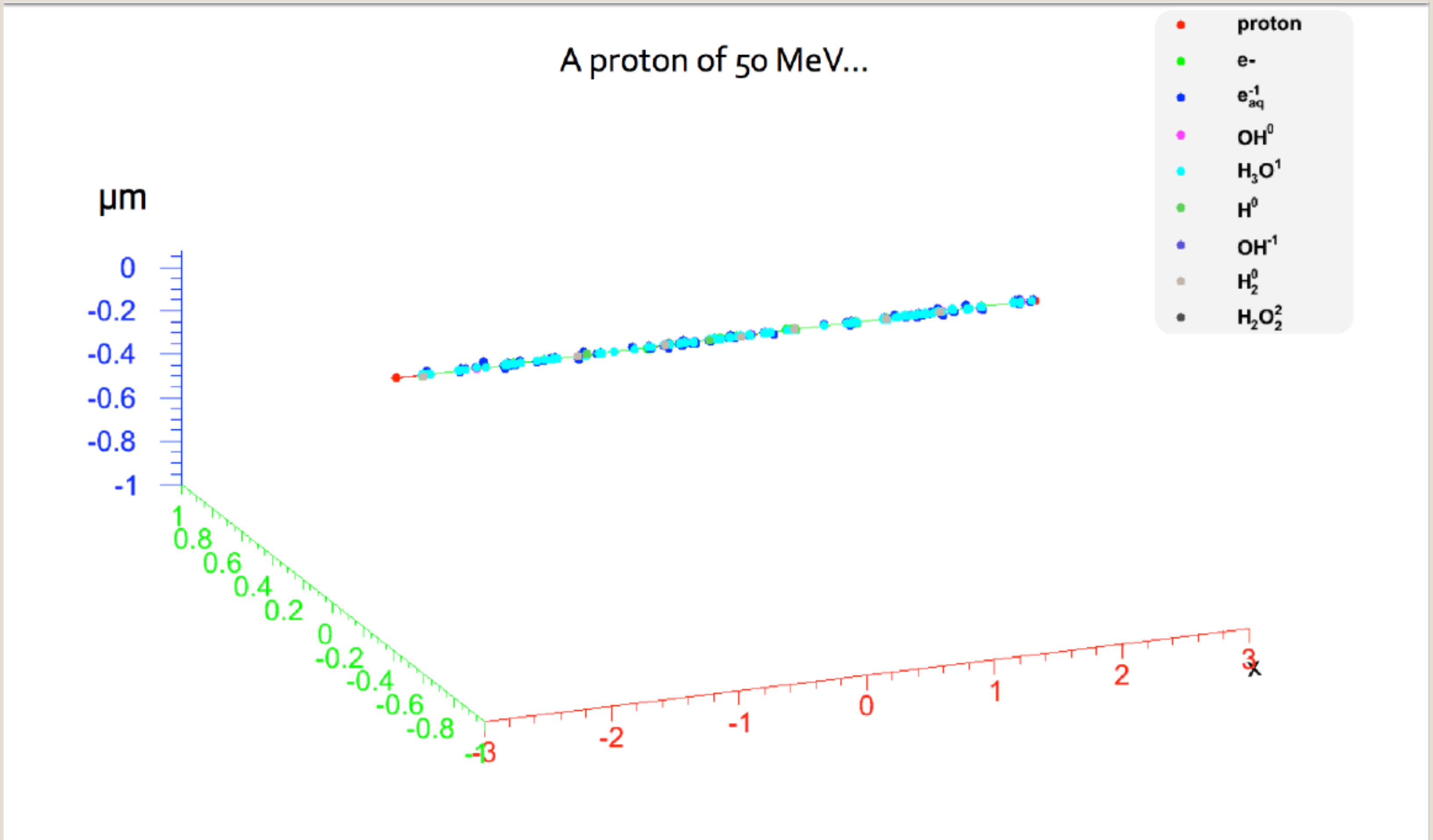
- Dedicated models for incident e^-, p, H, He, $He^{+/2+}$, C^{6+}, N^{7+}, O^{8+}, Fe^{26+}
  - They are all discrete processes
    - Ie : no "condensed history" approach applied
    - See examples/advanced/dnaphysics
  - Include elastic scattering, excitation (electronic + vibrations), ionisation and charge exchange
- For now, these models are valid for liquid water medium only
  - Extension to DNA basis and other materials on-going
- Models available in Geant4-DNA
  - may be purely analytical or use interpolated cross section data
  - are published in the literature
- Can be combined with other EM categories (Standard, Low Energy)
  - Combination done per region
    - DNA models set by G4EmConfigurator
    - See examples/advanced/microdosimetry



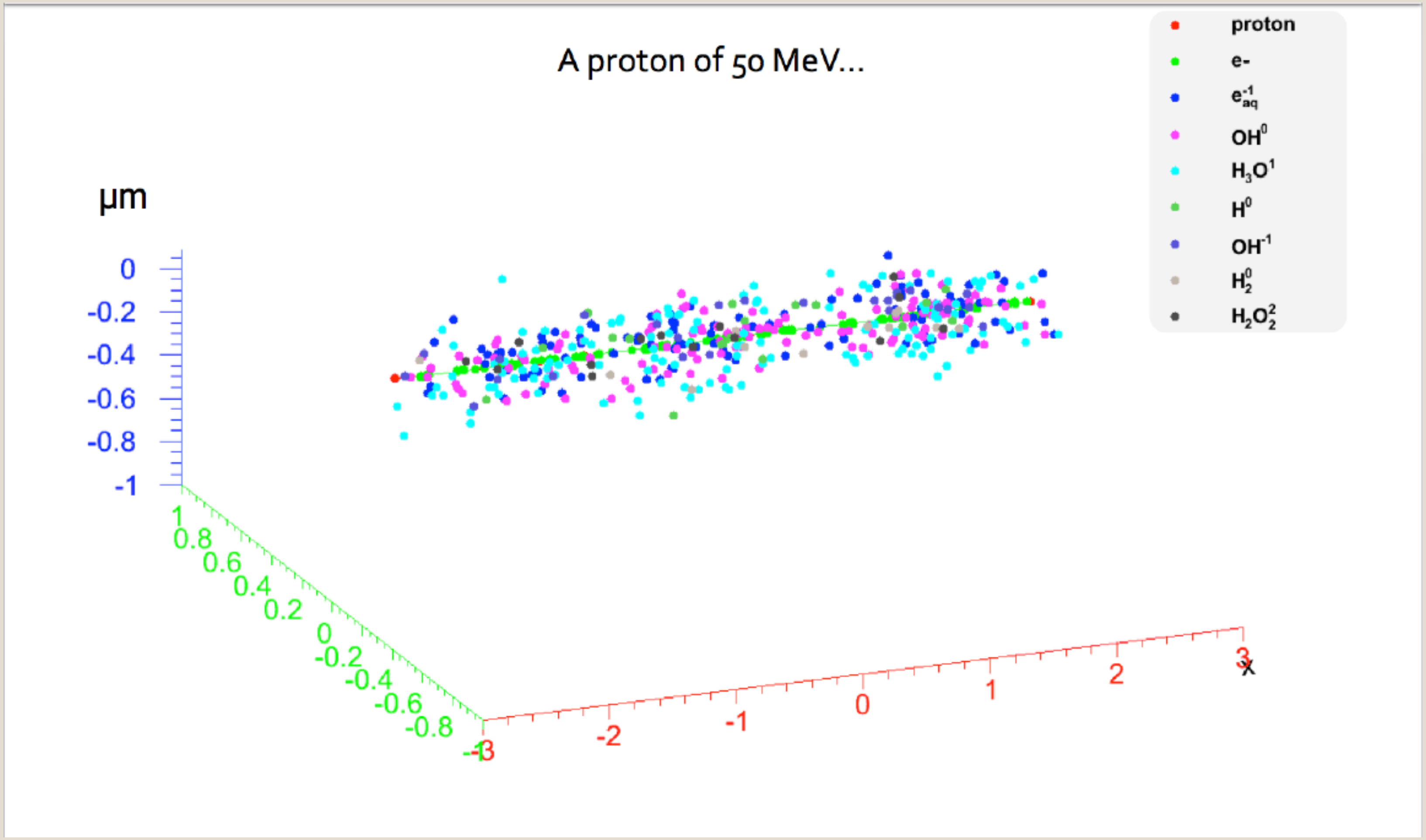
GEANT4-DNA PHYSICS PROCESSES AND MODELS

Particles	e-	p	H	He^{++}, He^{+}, He^{0}	C, N, O, Fe,…
Elastic scattering	> 9 eV – 1 MeV Screened Rutherford >7.4 eV – 1 MeV Champion	-	-	-	-
Excitation	9 eV – 1 MeV Born	10 eV – 500 keV Miller Green 500 keV – 100 MeV Born	10 eV – 500 keV Miller Green	Effective charge scaling from same models as for proton 1 keV – 400 MeV	-
Charge Change	-	100 eV – 100 MeV Dingfelder	100 eV – 100 MeV Dingfelder		-
Ionisation	11 eV – 1 MeV Born	100 eV – 500 keV Rudd 500 keV – 100 MeV Born	100 eV – 100 MeV Rudd		Effective charge scaling 0.5 MeV/u – 10^6 MeV/u
Vibrational excitation	2 – 100 eV Michaud et al.	-			
Attachment	4 – 13 eV Melton				

1 PICOSECOND AFTER IRRADIATION…

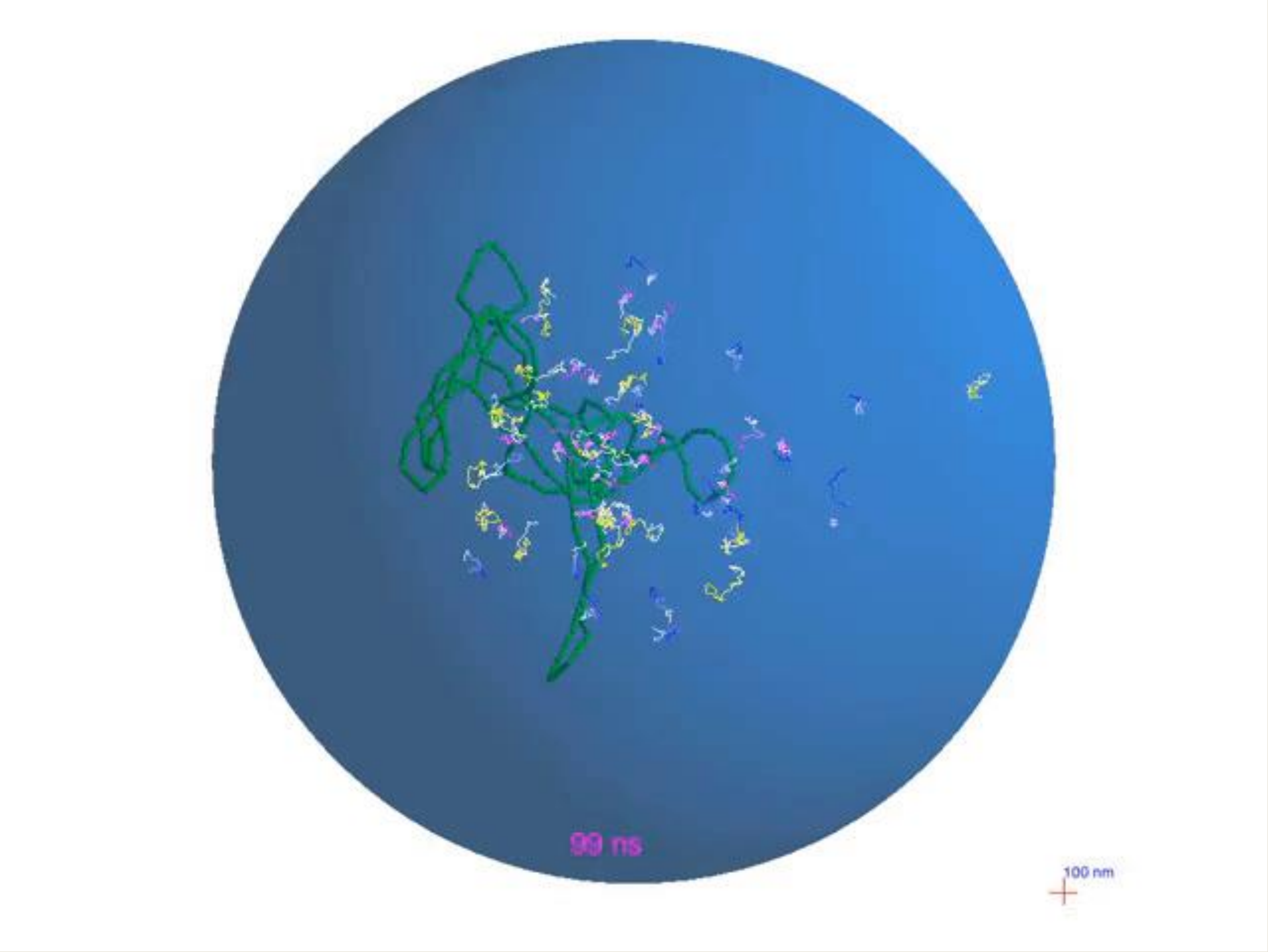


1 MICROSECOND AFTER IRRADIATION…



IRRADIATION OF A PBR322 PLASMID, INCLUDING RADIOLYSIS

- MOVIE COURTESY OF V. STEPAN (NPI-ASCR/CENBG/CNRS/IN2P3/ESA) -



DEDICATED WEB SITE

- http://geant4-dna.org/ :

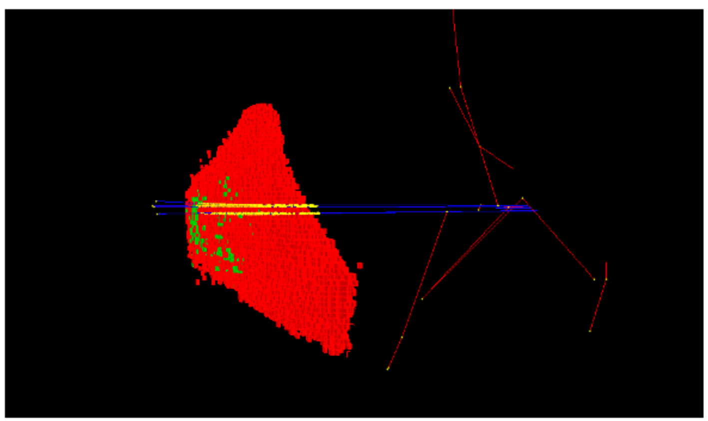
The Geant4-DNA project

Extending the Geant4 Monte Carlo simulation toolkit for radiobiology

Geant4-DNA | Software | Physics | Chemistry | Examples & tutorials | Publications | Collaboration | Funding

Welcome to the Internet page of the **Geant4-DNA project**.

The Geant4 general purpose particle-matter Monte Carlo simulation toolkit is being extended with processes for the **modeling of early biological damage induced by ionising radiation at the DNA scale**. Such developments are on-going in the framework of the Geant4-DNA project, originally initiated by the European Space Agency/ESTEC.



Microbeam irradiation of a keratinocyte with alpha particles
(see the « microbeam » Geant4 advanced example)
- courtesy of L. Garnier (CNRS/IN2P3) -

Recent posts

March 8th, 2016: our virtual machine has been updated to Geant4 10.2+P01

Dec. 4th, 2015: Geant4 10.2 has been released

Dec. 1st, 2015: a new review paper on Geant4-DNA is available, see Publications.

MicroElec : PROCESSES AND MODELS FOR MICROELECTRONICS

- Purpose
  - Extend Geant4 for the simulation of particle-matter interactions in highly integrated microelectronic components
  - for electrons, protons, heavy ions in Silicon
- Approach:
  - Same step-by-step approach as Geant4-DNA
    - Ie no “condensed history”
  - Applicable to the « G4_Si » NIST material

Nucl. Instrum. Meth B 288 (2012) 66 – 73
Nucl. Instrum. Meth B 287 (2012) 124 – 129
IEEE Trans. Nucl. Sci. 59 (2012) 2697 – 2703
Nucl. Instrum. Meth B 325 (2014) 97 - 100

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Electrons				
Elastic scattering	G4MicroElecElastic	G4MicroElecElasticModel	5 eV (kill < 16.7 eV)	100 MeV
Ionization	G4MicroElecInelastic	G4MicroElecInelasticModel	16.7 eV	100 MeV
Protons and heavy ions				
Ionization	G4MicroElecInelastic	G4MicroElecInelasticModel	50 keV/u	1 GeV/u

II.6 – UTILS

USER INTERFACES AND HELPER CLASSES

- Physics configuration and control:
  - G4EmParameters (G4EmProcessOptions obsoleting)
    - C++ interface to EM options alternative to UI commands
  - G4EmConfigurator
    - add models per energy range and geometry region

- Physics calculations:
  - Useful classes to compute physics quantities !
  - G4EmCalculator
    - easy access to cross sections and stopping powers
  - G4EmSaturation
    - Birks effect (recombination / “quenching” effects)
  - G4ElectronIonPair
    - sampling of ionisation clusters in gaseous or silicon detectors

EXAMPLE OF PHYSICS CALCULATION

- Possible to retrieve Physics quantities using a G4EmCalculator object
- Physics List should be initialized

- Example for retrieving the total cross section of a process with name procName, for particle and material matName

```
#include "G4EmCalculator.hh"
…
G4EmCalculator emCalculator;

G4Material* material =
     G4NistManager::Instance()->FindOrBuildMaterial(matName);
G4double density = material->GetDensity();
G4double massSigma =
     emCalculator.ComputeCrossSectionPerVolume(energy,
                                               particle,
                                               procName,
                                               material )/density;
G4cout << G4BestUnit(massSigma, "Surface/Mass") << G4endl;
```

- See RunAction.cc in $G4INSTALL/examples/extended/electromagnetic/TestEm0, for example.

II.6 – EM PHYSICS CONSTRUCTORS

GEANT4 STANDARD EM PHYSICS CONSTRUCTORS FOR HEP APPLICATIONS

- Constructors with variation of MSC stepping algorithms and/or parameters for speed vs. accuracy tradeoff

Constructor	Components	Comments
G4EmStandardPhysics	Default: nothing or _EM0 (QGSP_BERT, FTFP_BERT,…)	for ATLAS and other HEP simulation applications
G4EmStandardPhysics_option1	Fast: due to simpler MSC step limitation, cuts used by photon processes (FTFP_BERT_EMV)	similar to one used by CMS; good for crystals but not good for sampling calorimeters (i.e. with more detailed geometry)
G4EmStandardPhysics_option2	Experimental: similar to option1 with updated photoelectric model but no displacement in MSC (FTFP_BERT_EMX)	similar to one used by LHCb

COMBINED GEANT4 EM PHYSICS CONSTRUCTORS

- Constructors with focus on physics accuracy
- More accurate models for $e^{\pm}$ MSC (Goudsmit-Saunderson(GS)) and/or more accurate stepping algorithms (compared to HEP)
- Stronger continuous step limitation due to ionisation

Constructor	Components	Comments
G4EmStandardPhysics_option3	Urban MSC model for all particles	proton/ion therapy
G4EmStandardPhysics_option4	Most accurate combination of models (particle type and energy); GS MSC model with Mott correction and error-free stepping for $e^{\pm}$)	the ultimate goal is to have the most accurate EM physics description
G4EmLivermorePhysics	Livermore models for e^- , γ below 1 GeV and standard above; same GS MSC for $e^{\pm}$ as in option4)	accurate Livermore based low energy e^- and γ transport
G4EmPenelopePhysics	PENELOPE models for $e^{\pm}$, γ below 1 GeV and standard above; same GS MSC for $e^{\pm}$ as in option4)	accurate PENELOPE based low energy e^-, e^+ and γ transport
G4EmDNA	DNA models in selected regions	For dedicated applications

EXPERIMENTAL GEANT4 EM PHYSICS CONSTRUCTORS

- Primarily meant for developers and model validations

Constructor	Components	Comments
G4EmStandardPhysicsGS	standard EM physics and the GS MSC model for $e^{\pm}$ with HEP settings	may be considered as an alternative to EM0 i.e. for HEP
G4EmStandardPhysicsWVI	WentzelWVI + Single Scattering mixed simulation model for Coulomb scattering	high and intermediate energy applications
G4EmStandardPhysicsSS	single scattering (SS) model description of the Coulomb scattering	validation and verification of the MSC and mixed simulation models
G4EmLowEPPhysics	Monarsh University Compton scattering model, 5D gamma conversion model, WVI-LE model	testing some low energy models
G4EmLivermorePolarized	polarized gamma models	a (polarized) extension of the Livermore physics models

LEARN MORE USING EXAMPLES !
$G4INSTALL/EXAMPLES/EXTENDED/ELECTROMAGNETIC

Check basic quantities

Total cross sections, mean free paths …	TestEm0, Em13, Em14
Stopping power, particle range …	Em0, Em1, Em5, Em11, Em12
Final state : energy spectra, angular distributions	Em14
Energy loss fluctuations	Em18

Multiple Coulomb scattering

as an isolated mechanism	Em15
as a result of particle transport	Em5

More global verifications

Single layer: transmission, absorption, reflexion , atomic deexcitation, msc	Em5
Bragg curve, tallies	Em7
Depth dose distribution	Em11, Em12
Shower shapes, Moliere radius	Em2
Sampling calorimeters, energy flow	Em3
Crystal calorimeters	Em9

Other specialized programs

High energy muon physics	Em17
Other rare, high energy processes	Em6
Synchrotron radiation	Em16
Transition radiation	Em8
Photo-absorption-ionization model	Em10

Refer to section on extended examples in App. User Guide.

You are warmly invited to study these examples !

SUMMARY : WHEN/WHY USING “LOW ENERGY” EM MODELS

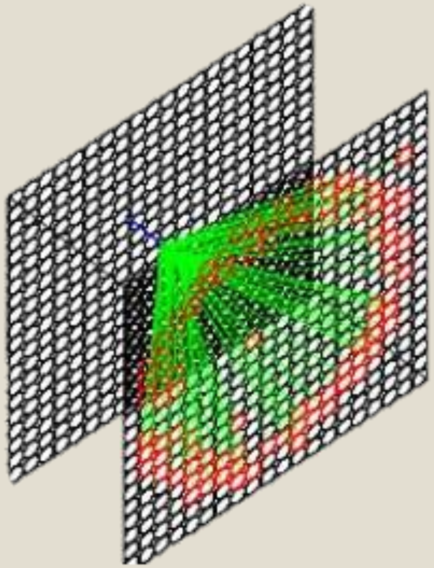
- Use Low-Energy models (Livermore or Penelope), as an alternative to Standard models, when you:
  - Need precise treatment of EM showers and interactions at low-energy:
    - keV scale or below
  - Are interested in atomic effects:
    - fluorescence x-rays, Doppler broadening, etc.
  - Can afford more CPU-intensive simulation
  - Or want to cross-check another simulation:
    - eg with a difference physic list
    - For systematic studies

- Do not use when you are interested in EM physic > MeV
  - Same results as Standard EM
  - But with strong CPU penalty

III. OPTICAL PHYSICS

OPTICAL PHOTON
ASSUMPTIONS & LIMITATIONS

- Geant4 offers some production and transport capabilities for optical photons.
  - G4OpticalPhoton is the class representing them
  - "opticalphoton" is their particle name



- As for other Geant4 particles, they are treated as "point-like" objects:
  - Allows simulating "point like" interactions ✓
    - Scattering, absorption, reflection…
  - But excludes any "wave-like" behaviors ✘
    - No phase treatment ⇒ no interferences simulated !
      - Don't expect Geant4 to simulate Young's slits experiment !
- Optical photons are treated separately from EM processes:
  - Wavelengths are much larger than atomic spacing
  - G4OpticalPhoton ≠ G4Gamma; and there is no smooth transition defined.
- Energy/momentum not generally conserved in G4 optics

OPTICAL PHOTON PROCESSES

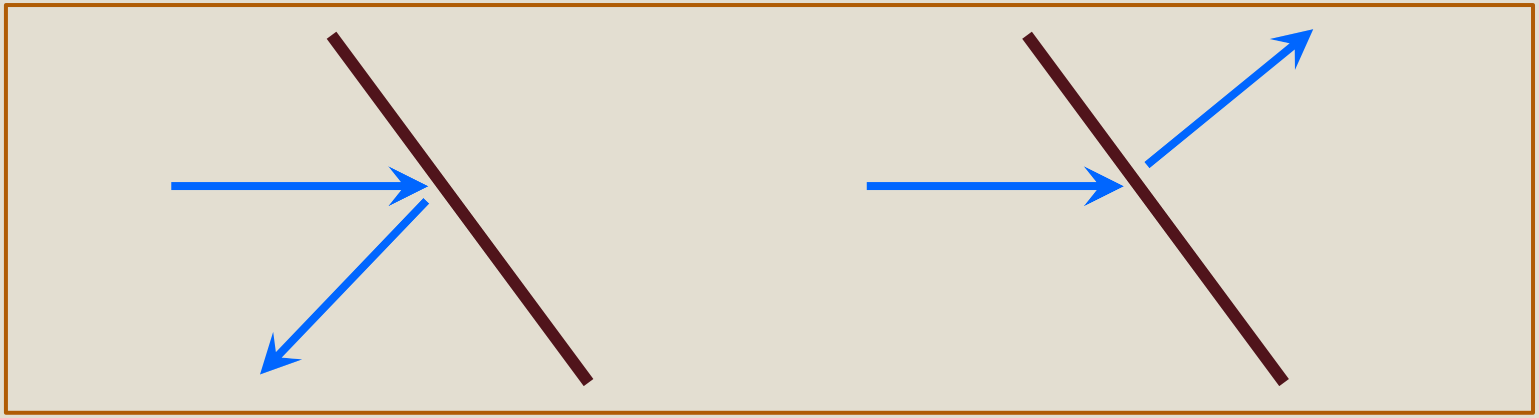
- **Production processes:**
  - G4Cerenkov
  - G4Scintillation
  - Large production of photons :
    - Use of « **fSuspend** » flag any N photons produced to track them first
- **Transport processes:**
  - G4OpBoundaryProcess
  - G4OpWLS (wavelength shifting)
  - G4OpAbsorption
  - G4OpRayleigh
- **Activating optical physics:**
  - The physics constructor G4OpticalPhysics can be used to create/activate optical physics.
  - For example, in your main(…):

```
G4VModularPhysicsList* myModularPhysicsList = new FTFP_BERT;
myModularPhysicsList->RegisterPhysics(new G4OpticalPhysics);
```

- **Optical properties definition:**
  - Optical properties attached to G4Material (by user code)
    - reflectivity, transmission efficiency, dielectric constants, surface properties, including binned wavelength/energy dependences
  - Photon spectrum attached to G4Material (by user code)
    - scintillation yield, time structure (fast, slow components)

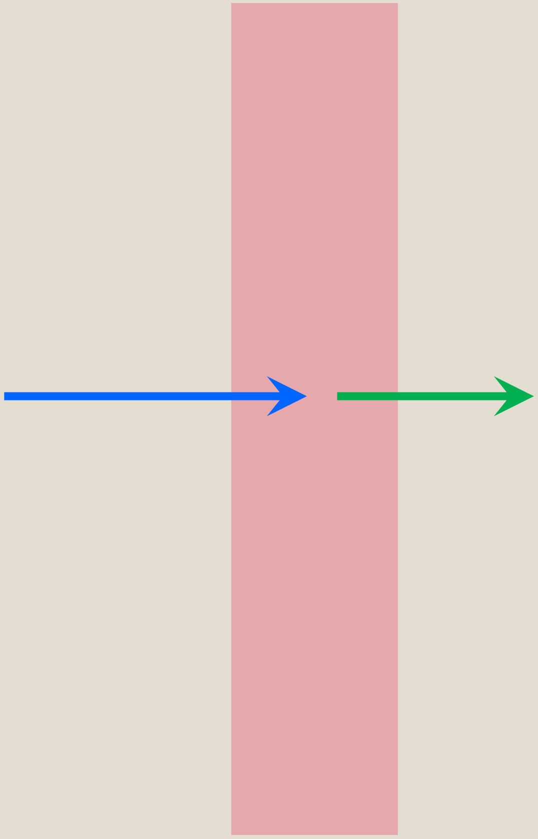
BOUNDARY PROCESSES

- G4OpBoundaryProcess
  - Reflection
  - Refraction
- User must supply surface properties using G4OpticalSurfaceModel
  - In the detector construction
- Boundary properties
  - Dielectric-dielectric
  - Dielectric-metal
  - Dielectric-black material
- Surface properties
  - Polished
  - Ground
  - Front- or back-painted, etc…



WAVELENGTH SHIFTING

- G4OpWLS:
  - Simulates wavelength shifting of photons crossing material.
  - Initial photon is killed, and a “daughter” photon is created with new energy.
- User must supply:
  - Absorption length as function of photon energy
  - Emission spectra parameters as function of energy
  - Time delay between absorption and re-emission



BULK PROCESS & RAYLEIGH

- G4OpAbsorption:
  - Uses photon attenuation length from material properties to sample path length before absorption
  - Photon is simply killed after sampled path length

- G4OpRayleigh:
  - Optical photon version of Rayleigh scattering
    - G4Gamma's have their Rayleigh version too
  - Elastic scattering including polarization of initial and final photons

IV. DECAY PHYSICS

PARTICLE DECAYS

- Applies to all unstable long-lived particles
  - In flight, or at rest
  - Not used for radioisotopes (handled by G4RadioactiveDecay)
- Specificity of decay process:
  - Mean free path is $\lambda = \beta\gamma c\tau$
  - While it is $\lambda = (\mathcal{N}\rho\sigma/A)^{-1}$ for other processes
- Same process used for all eligible particles
  - Retrieves branching ratio and decay modes from decay table stored for each particle
  - No such data provided by Geant4 for heavy flavor particles
    - eg: B mesons
    - In what case user must supply "pre-assign" decay
      - Specifying lifetime, decay modes, decay products
    - Or delegate to an external generator, using the G4ExtDecayer interface

DECAY MODES AVAILABLE

- **Phase space:**
  - 2-body: $\pi^0 \to \gamma\gamma$
  - 3-body: $K_L^0 \to \pi^0\pi^+\pi^-$
  - Many body
- **Dalitz decay:**
  - $\pi^0 \to \gamma l^+ l^-$
- **V-A:**
  - For muon and tau decays
  - No radiative corrections, mono-energetic neutrinos
- **Semi-leptonic kaon decay:**
  - $K \to \pi l \nu$

SPECIALIZED PARTICLE DECAYS

- G4DecayWithSpin
  - Produces Michel electron/positron spectrum with first order radiative corrections
  - Initial muon spin is required
  - Propagates muon spin in magnetic field (precession)

- G4UnkwonDecay
  - For not yet discovered particles
    - Eg : SUSY
  - For in-flight decays only
  - User must supply pre-assigned decay, or interface to generator

THAT'S ALL FOR TODAY !

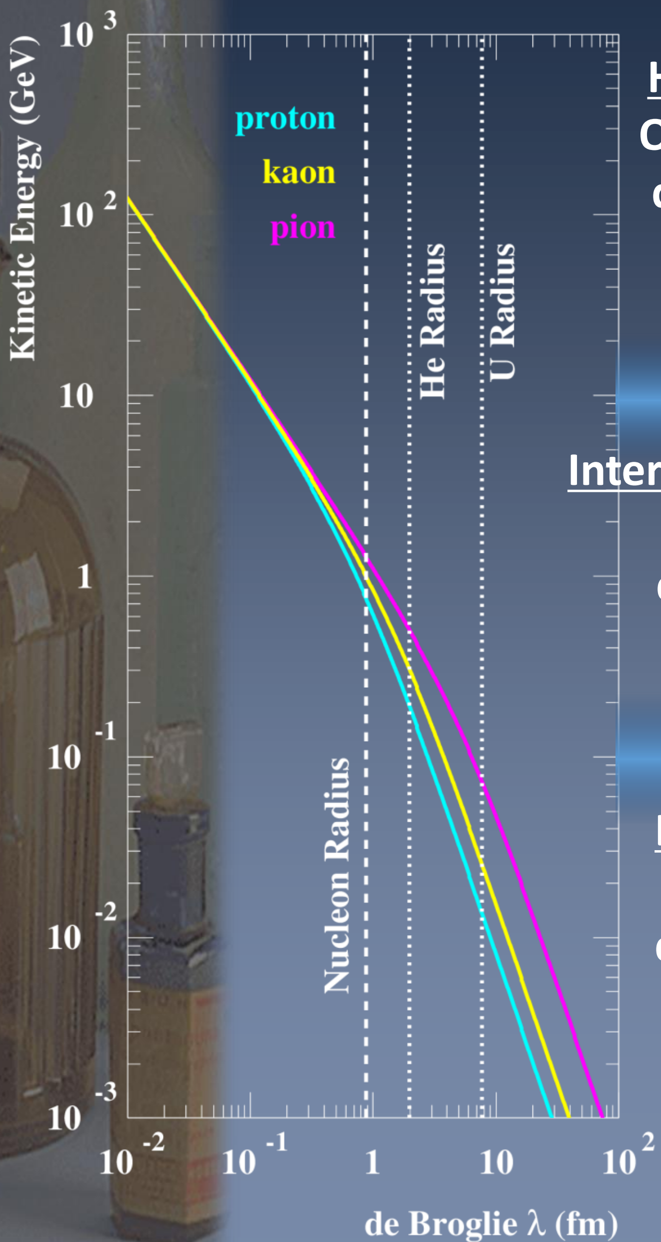
V. HADRONIC PHYSICS

OVERVIEW

1. Generalities
2. The Hadronic Framework
3. Hadron Elastic
4. High Energy : String Models
5. Intermediate Energies : Intra-nuclear cascades
6. Nucleus “Cooling Down” Models
7. Low Energies : Capture, Stopping, Fission
8. Low Energy (< 20 MeV) Particle Transport, including Neutrons
9. Radioactive Decays
10. Ion-ion Physics
11. Gamma-, Lepto-Nuclear

V.1 - GENERALITIES

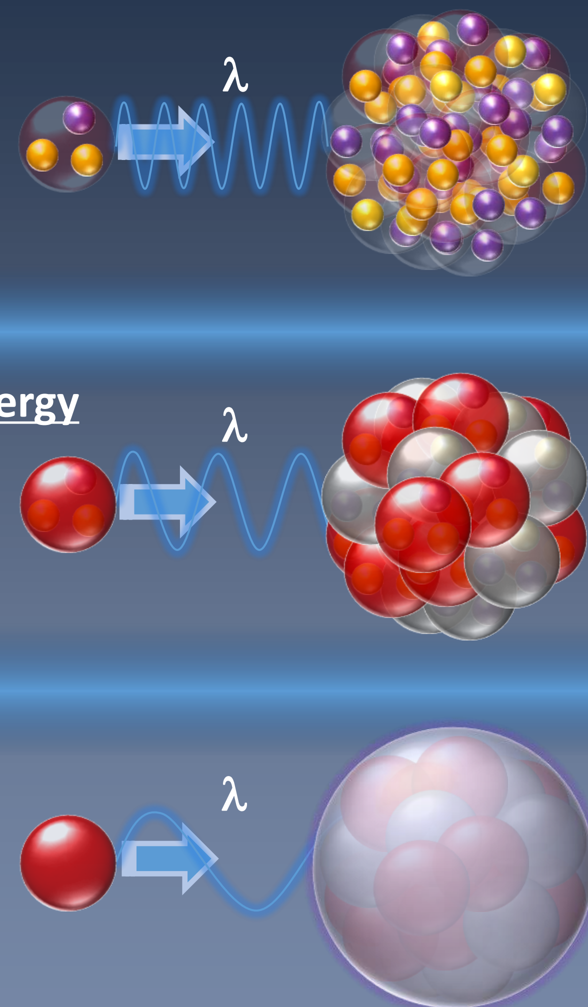
Variety of Hadronic Physics Models



High Energy
Quark/gluon dominating behavior

Intermediate Energy
Nucleon dominating behavior

Low Energy
Nucleus dominating behavior



Main Models

String Models: Quark Gluon String, Fritiof

Intra-Nuclear Cascade Models: Binary, Bertini, INCL++

Precompound

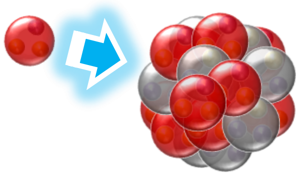
Fission / evaporation

γ evaporation

Radioactive decay

Capture at rest

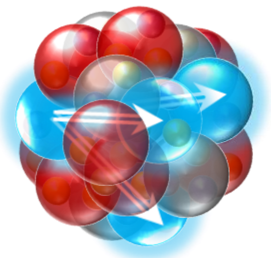
<u>One</u> hadronic collision = sequence of many hadronic interaction<u>s</u>



Projectile hitting
a target nucleus

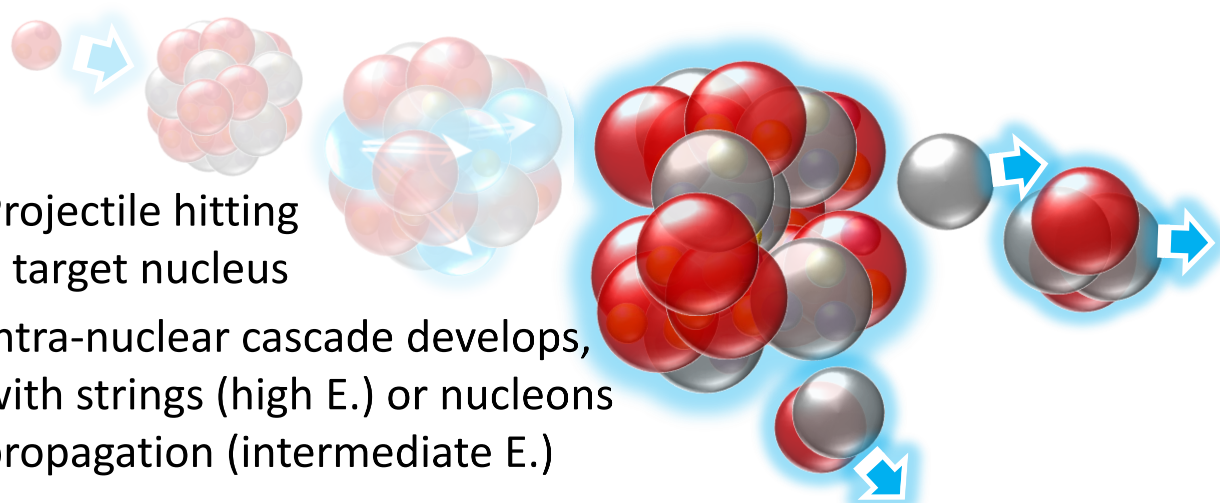
One hadronic collision = sequence of many hadronic interactions

Projectile hitting
a target nucleus



Intra-nuclear cascade develops,
with strings (high E.) or nucleons
propagation (intermediate E.)

One hadronic collision = sequence of many hadronic interactions

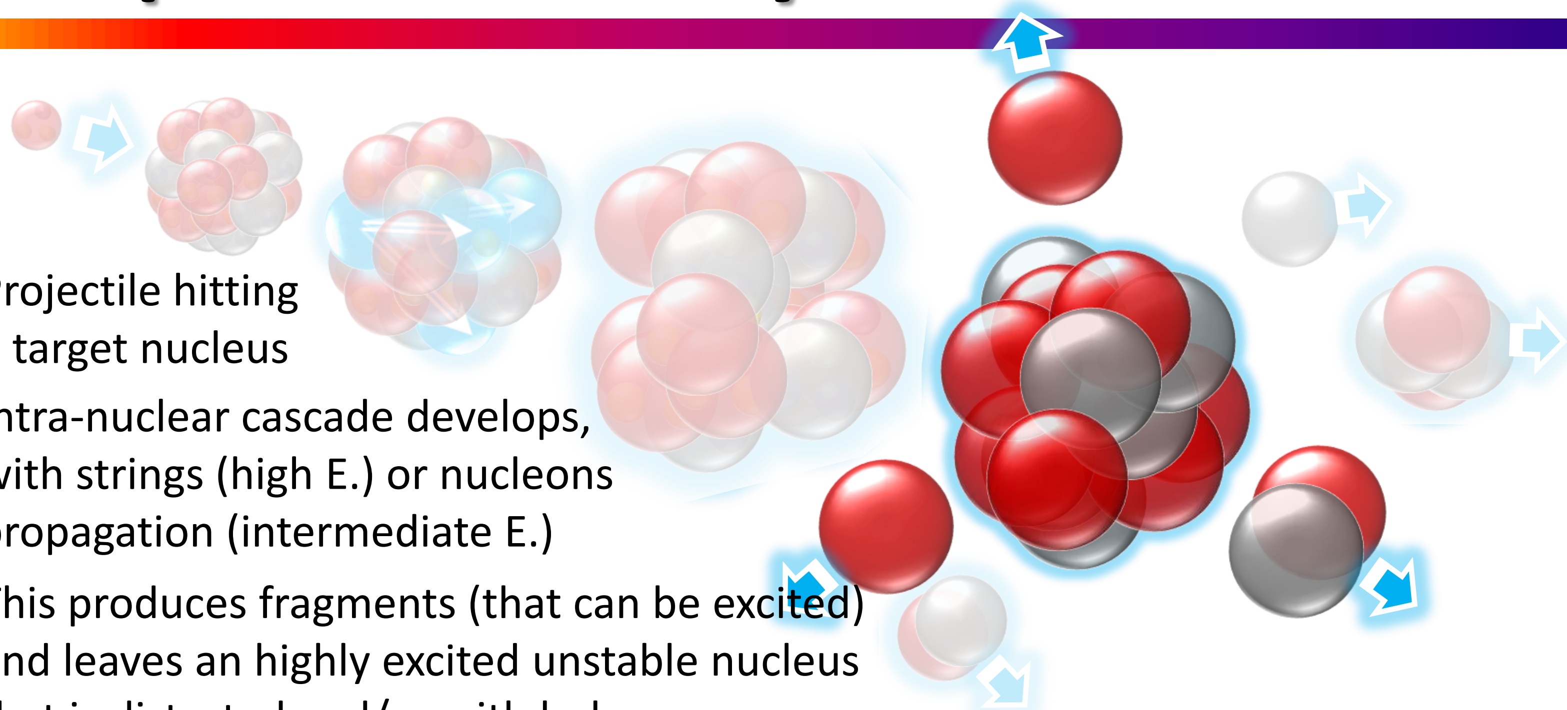


Projectile hitting a target nucleus

Intra-nuclear cascade develops, with strings (high E.) or nucleons propagation (intermediate E.)

This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.

<u>One</u> hadronic collision = sequence of many hadronic interaction<u>s</u>



Projectile hitting a target nucleus

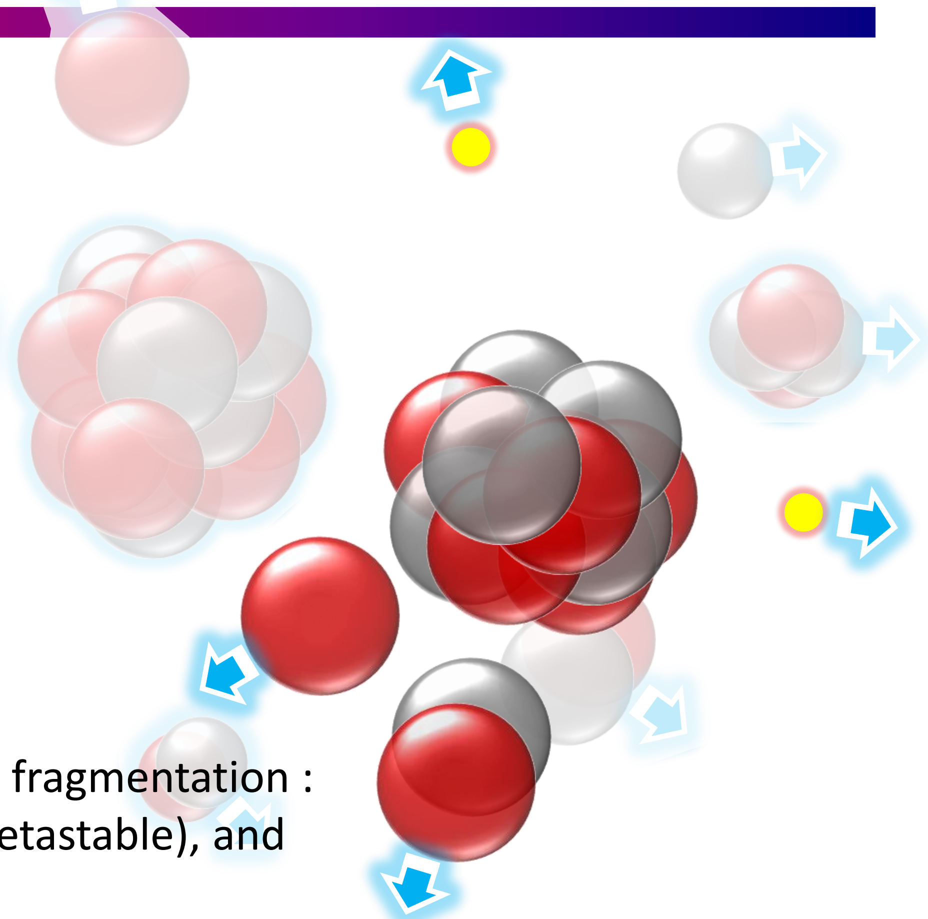
Intra-nuclear cascade develops, with strings (high E.) or nucleons propagation (intermediate E.)

This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.

Nucleus rearranges itself by evaporation* and/or fragmentation : this leads to a still excited nucleus, but stable (metastable), and with no memory of the collision history.

(*) **Evaporation** = de-excitation by emission of light nuclei ∈ {n, p, d, t, 3He, a} or photon

One hadronic collision = sequence of many hadronic interactions



Projectile hitting a target nucleus

Intra-nuclear cascade develops, with strings (high E.) or nucleons propagation (intermediate E.)

This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.

Nucleus rearranges itself by evaporation* and/or fragmentation : this leads to a still excited nucleus, but stable (metastable), and with no memory of the collision history.

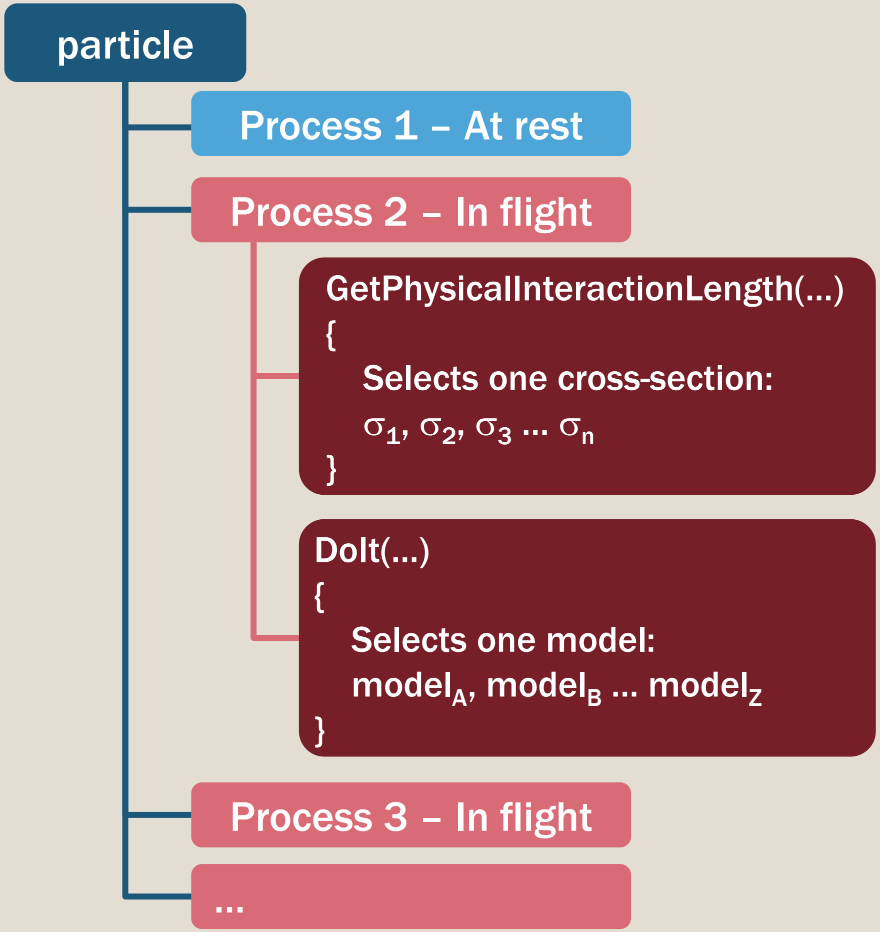
The nucleus undergoes final de-excitation by evaporation* or fission and ends-up in its ground state. In case of fission, further de-excitation of fragments may occur.

(*) **Evaporation** = de-excitation by emission of light nuclei $\in$ {n, p, d, t, 3He, α} or photon

V.2 - THE HADRONIC FRAMEWORK

CROSS-SECTIONS & MODELS

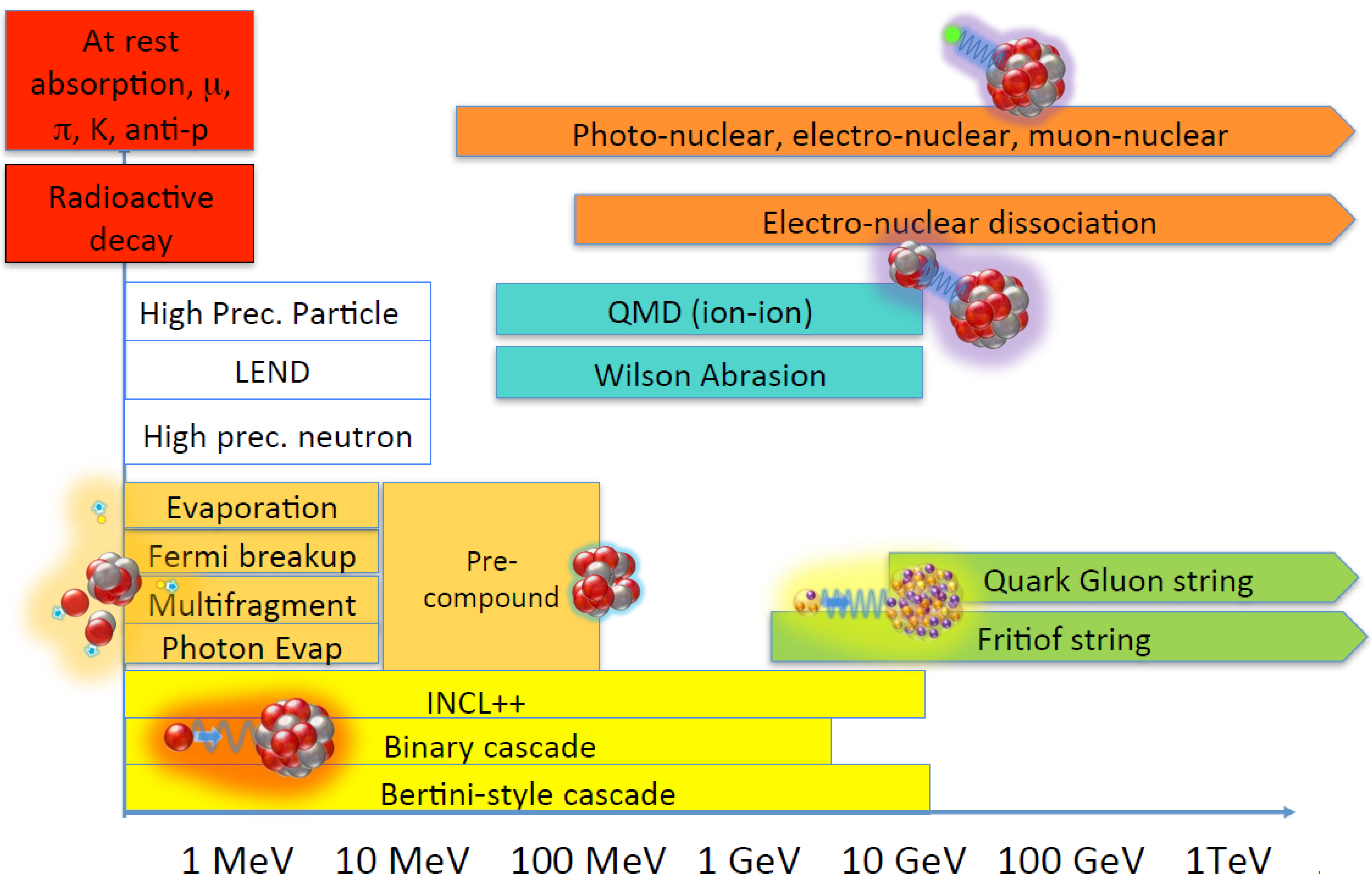
- Hadronic interactions are all “point-like”:
  - Either at-rest (AtRest processes)
  - Or in flight (PostStep processes)
- Hadronic processes usually need:
  - Several cross-sections
    - To cover a wide range of energy
    - GetPhysicalInteractionLength(…) selects one of these, valid at proper energy
    - Cross-sections are inclusive
    - Elastic, inelastic, fission, capture
  - Several final-state models
    - To again cover a wide range of energy
    - “final-state models” simply called “models” by hadronic people
    - Used in “DoIt(…)”
- Hadronic framework designed to handle these sets of cross-sections and models
  - Default ones, overlay some, etc.



Available Inelastic Hadronic Cross Sections

- Low-energy neutron cross sections (below 20 MeV)
  - G4NDL available as Geant4 distribution files
  - Livermore database (LEND) also available
  - Available with or without thermal cross sections
- Medium-energy neutron- and proton-nuclear reaction cross sections
  - 14 MeV < E < 20 GeV
  - Barashenkov cross sections; Glauber-Gribov-Grichine extension at high energies
- Nucleus-nucleus reaction cross sections
  - Tripathi, Shen, Kox : good for E/A < 10 GeV
  - Glauber-Gribov-Galoyan-Uzhinskiy : all energies; also for anti-baryons
- Pion-nuclear reaction cross sections
  - Barashenkov cross sections; Glauber-Gribov-Grichine extension at high energies
- Kaon- , hyperon- and anti-hyperon - nuclear cross sections
  - Kossov cross sections (extracted from CHIPS)

Partial Model Inventory



V.3 - HADRON ELASTIC

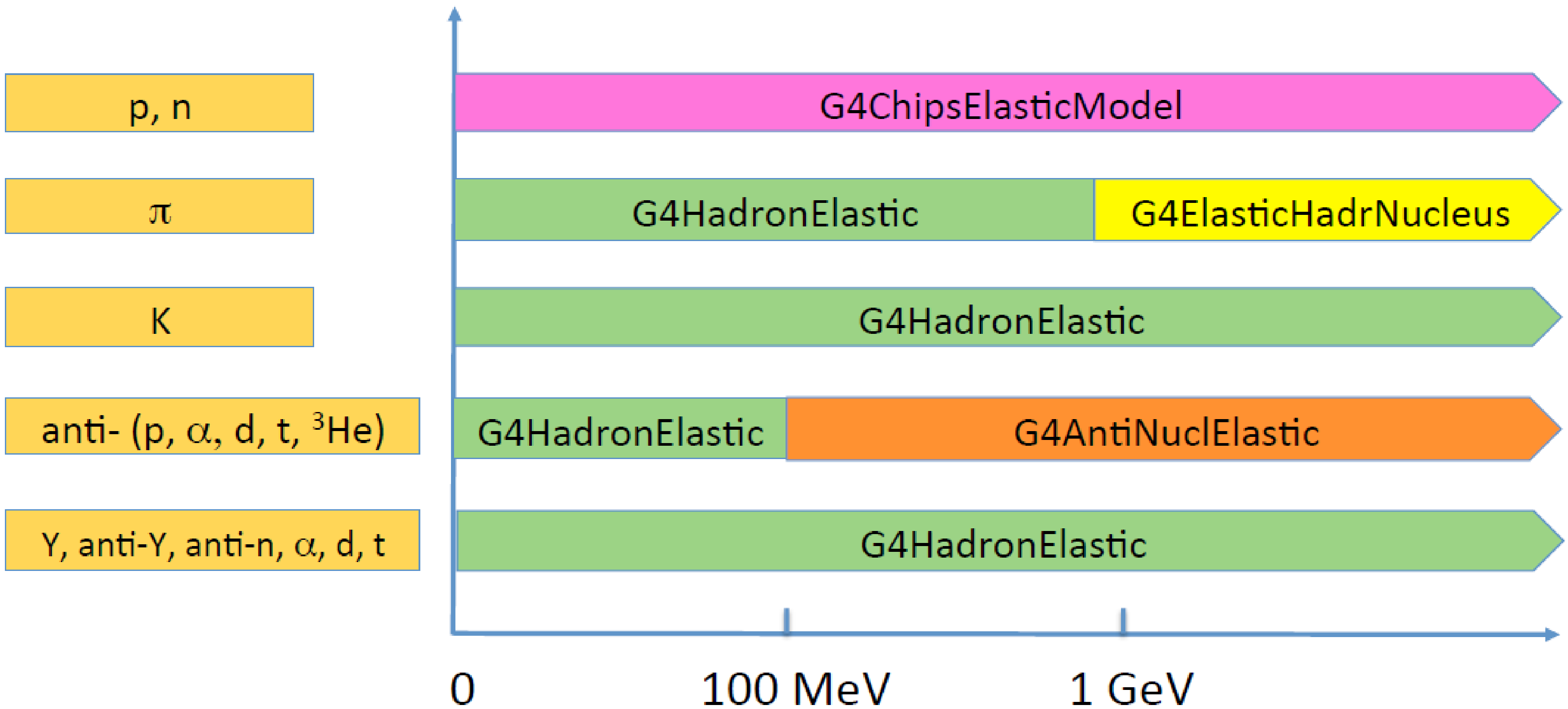
Elastic Process

- **G4HadronElasticProcess**
  - Class name of that process
  - Displayed as « **hadElastic** » in « /tracking/verbose »
- The **proton production cut is applied to recoil nucleus** for all type of projectile hadrons
  - Ie : applied to protons and all nucleus, using proton cut value
  - Threshold is:

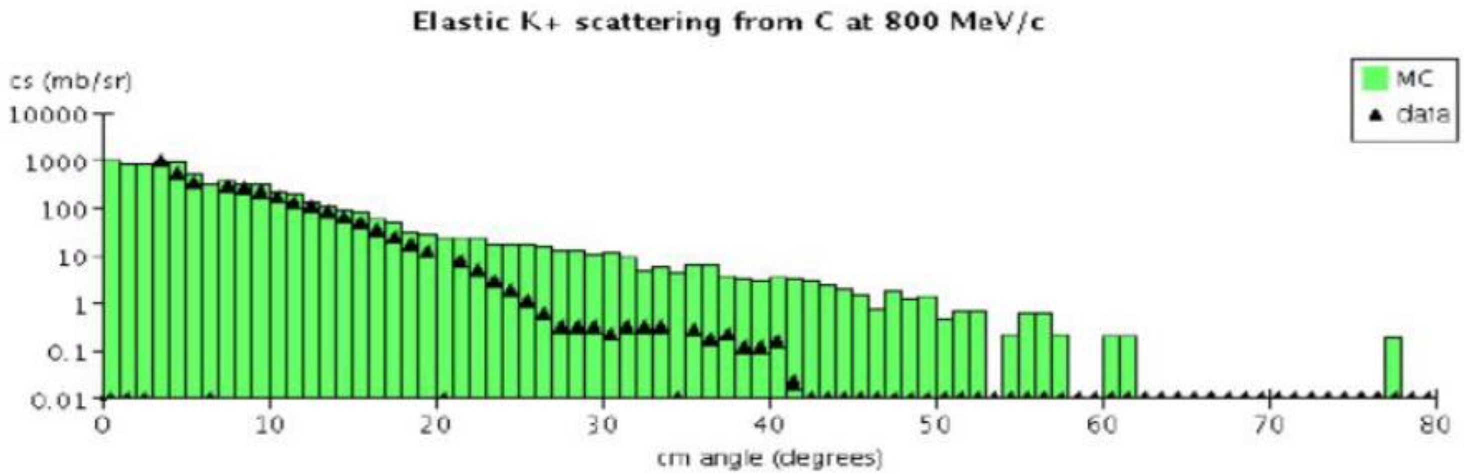
    (100*keV)*proton_production_cut_in_mm
  - Above this value, recoil nucleus is explicitely tracked

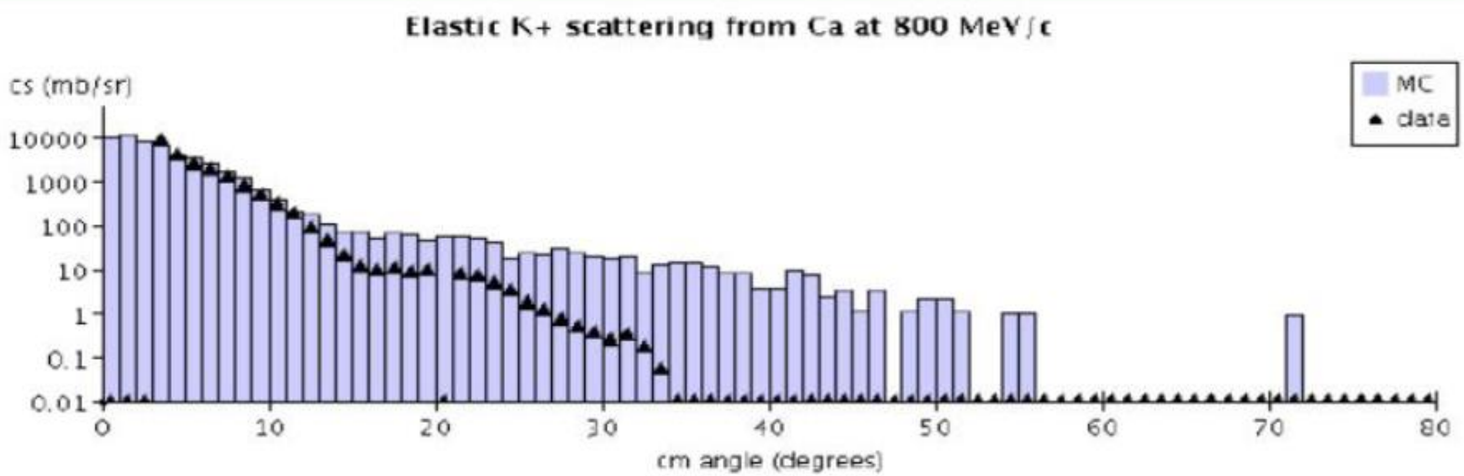
- **Cross-section:**
  - Geisha (parameterization) by **default** except for:
  - **protons & neutrons** : CHIPS (CHIral Invariant Phase Space)
  - **pions** : Barashenkov-Glauber-Gribov
  - **nuclei** : Barashenkov parameterization below 91 GeV and Glauber-Gribov above
  - **anti-nucleons and light anti-nucleus** : Glauber
- **Model (final state)** has similar pattern
  - (next slide)

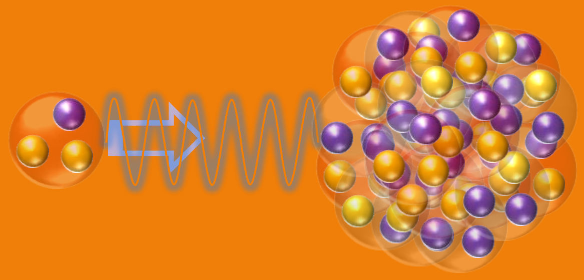
Hadronic Models Implementing G4HadronElasticProcess



Elastic Scattering Validation (G4HadronElastic)

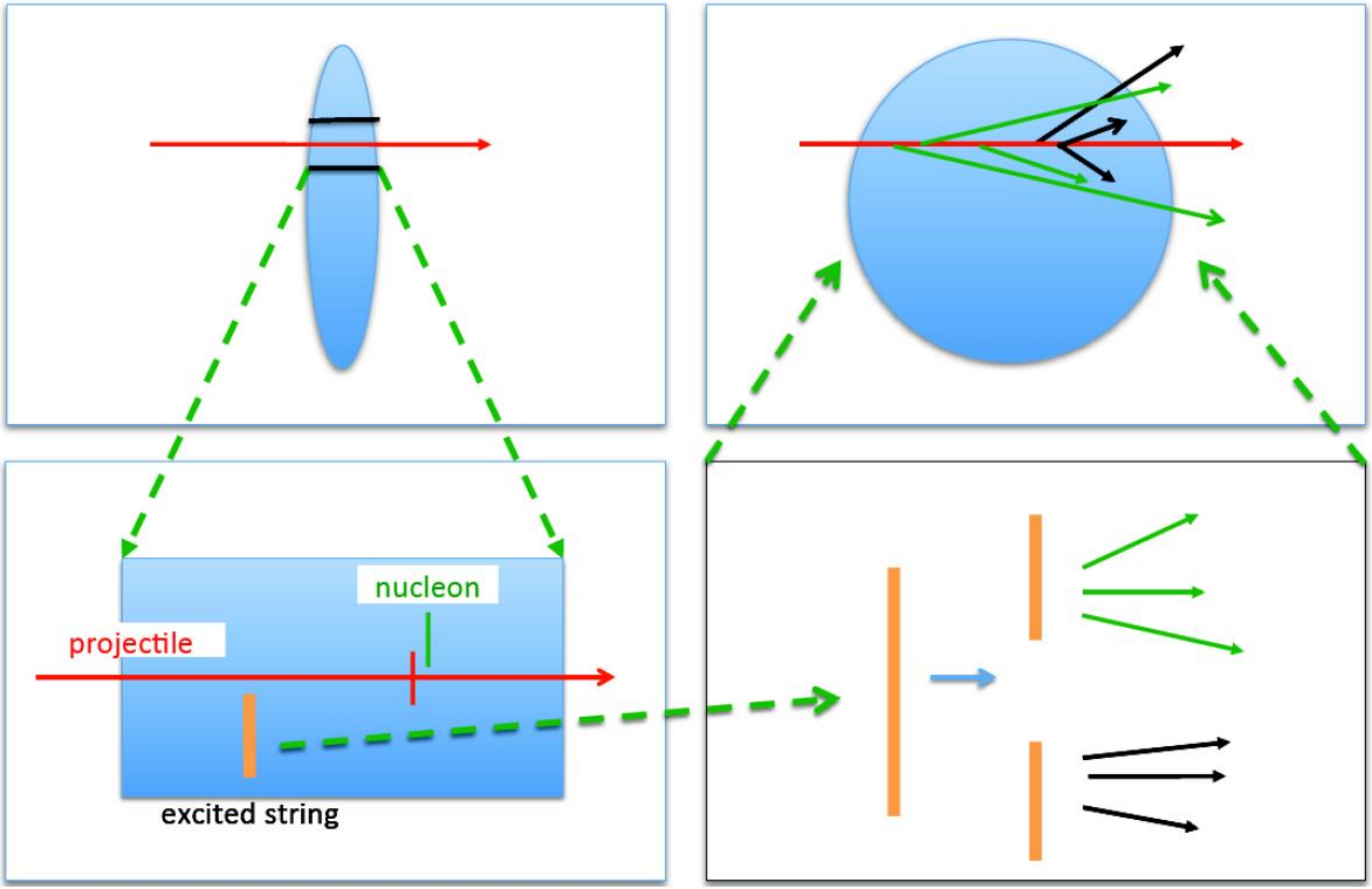






V.4 - HIGH ENERGIES : STRING MODELS

High-Energy Nuclear Reaction



How the String Model Works (FTF Model)

- Lorentz contraction turns nucleus into pancake
- All nucleons within 1 fm of path of incident hadron are possible targets
- Excited nucleons along path collide with neighbors
  - n + n → nΔ, NN, ΔΔ, NΔ, …
  - essentially a quark-level cascade in vicinity of path → Reggeon cascade
- All hadrons treated as QCD strings
  - projectile is quark-antiquark pair or quark-diquark pair
  - target nucleons are quark-diquark pairs

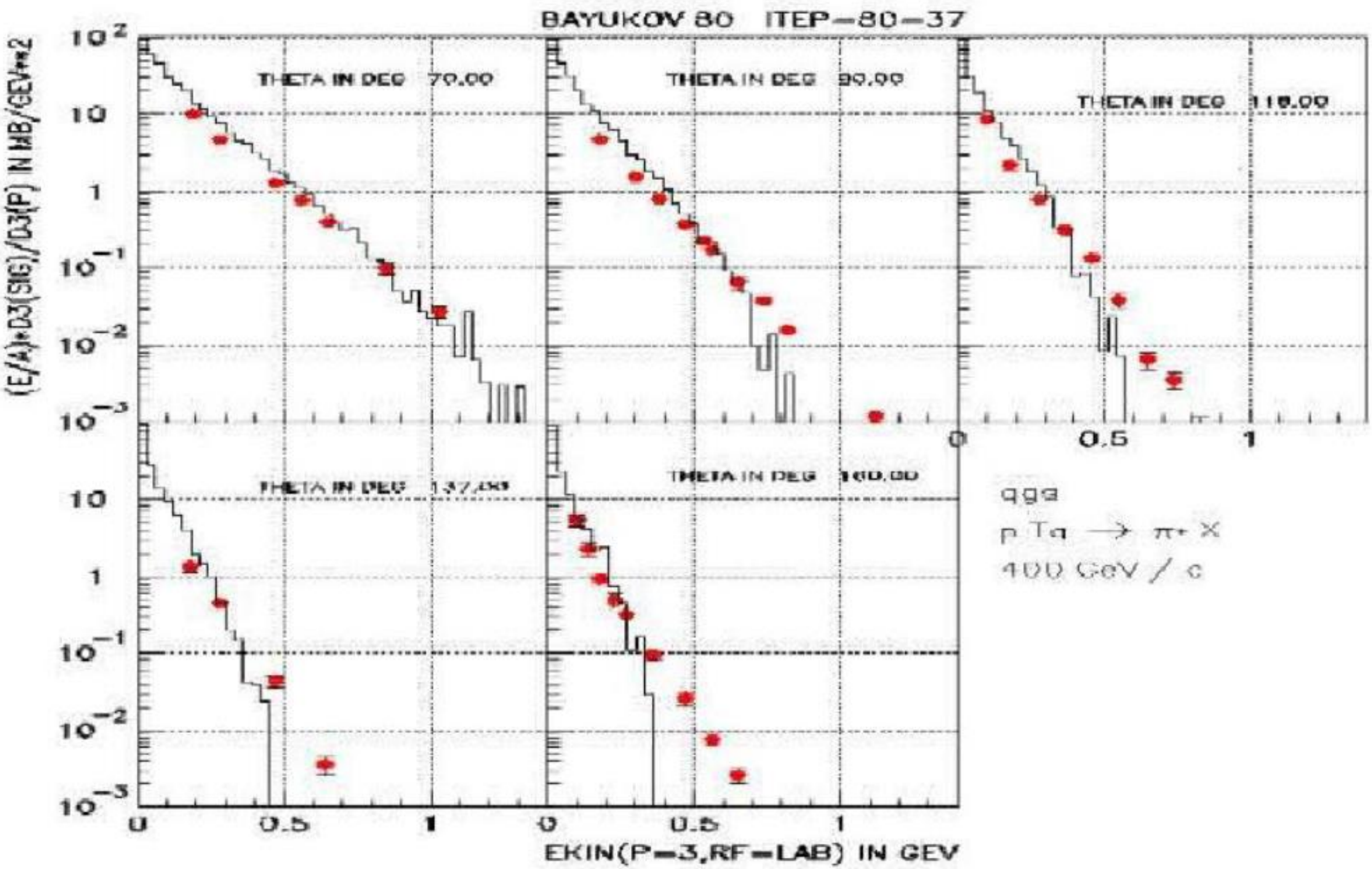
How the String Model Works (FTF Model)

- Hadron excitation is represented by stretched string
  - string is set of QCD color lines connecting the quarks
- When 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
- Resulting hadrons can then interact with nucleus in a traditional cascade

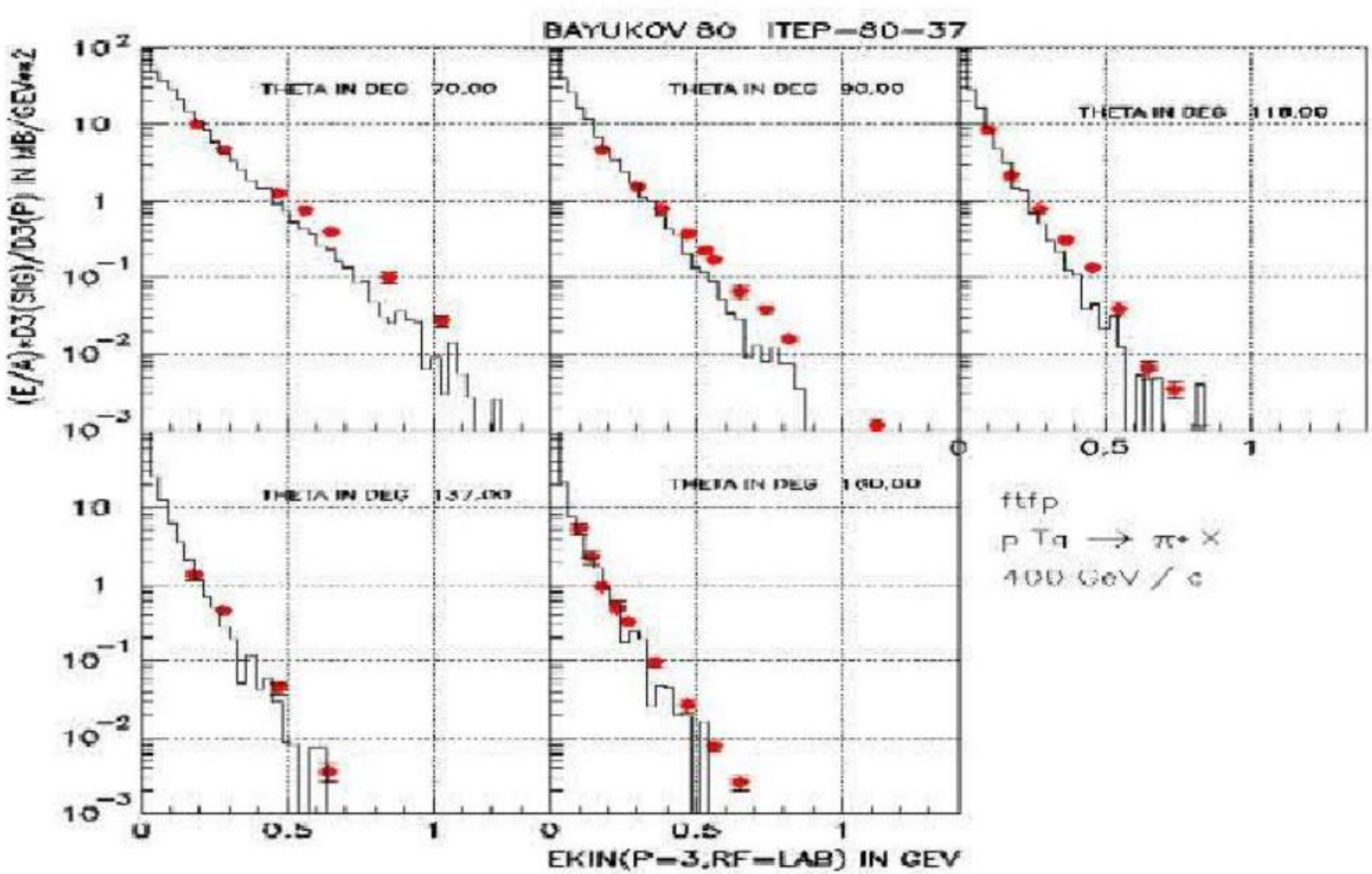
Two QCD String Models Available

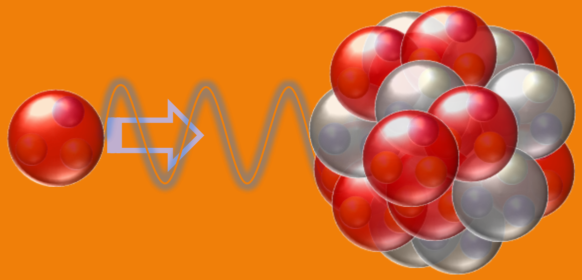
- Fritiof (FTF) valid for
  - p, n, π, K, Λ, Σ, Ω from 3 GeV to ~TeV
  - anti-proton, anti-neutron, anti-hyperons at all energies
  - anti-d, anti-t, anti-^{3}He, anti-α with momenta between 150 MeV/nucleon and 2 GeV/nucleon
- Quark-Gluon String (QGS) valid for
  - p, n, π, K from 15 GeV to ~TeV
- Both models handle:
  - building 3-D model of nucleus from individual nucleons
  - splitting nucleons into quarks and di-quarks
  - formation and excitation of QCD strings
  - string fragmentation and hadronization

QGS Validation



FTF Validation





V.5 - INTERMEDIATE ENERGIES : INTRA-NUCLEAR CASCADES

Intra-nuclear Cascade Models

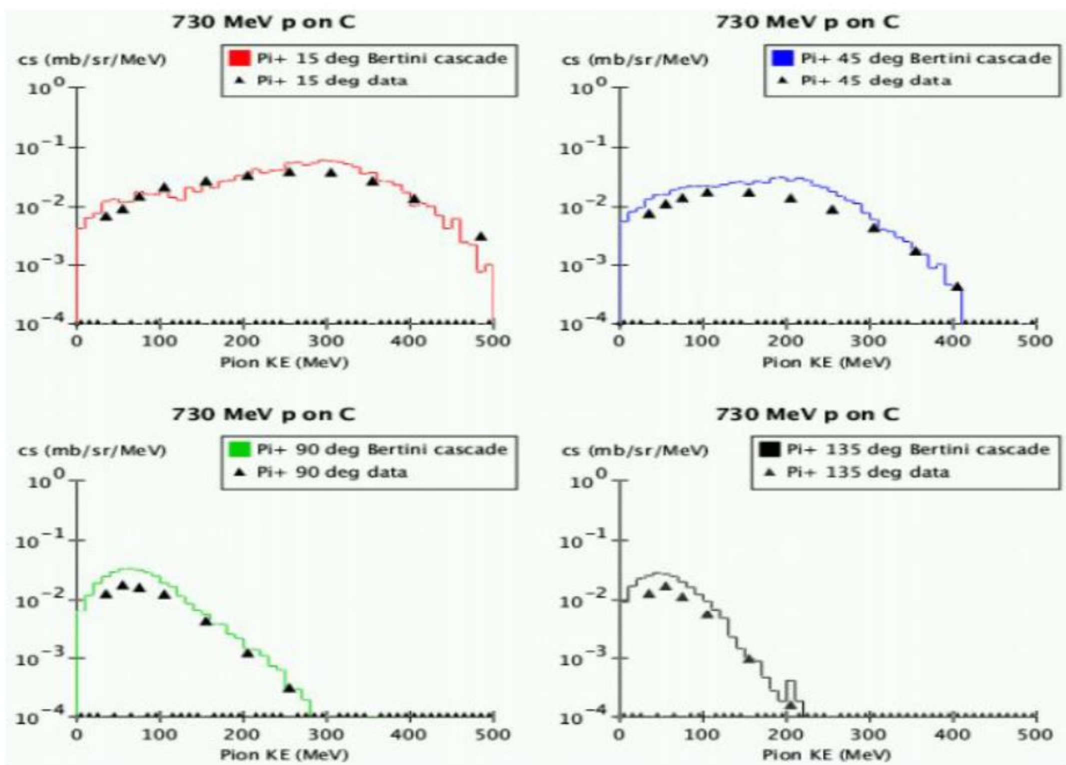
- Typical intra-nuclear cascade energies are inconvenient
  - too high for nuclear physics treatments
  - too low for QCD
- Must use Monte Carlo techniques to propagate hadrons within the target nucleus in order to produce a final state
  - "Monte Carlo within a Monte Carlo"
  - one of the first applications of Monte Carlo methods to nuclear interactions
  - time-consuming
- Specific channels not produced
  - do not use data to produce, for example $^{14}N(p,n)^{14}O$

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



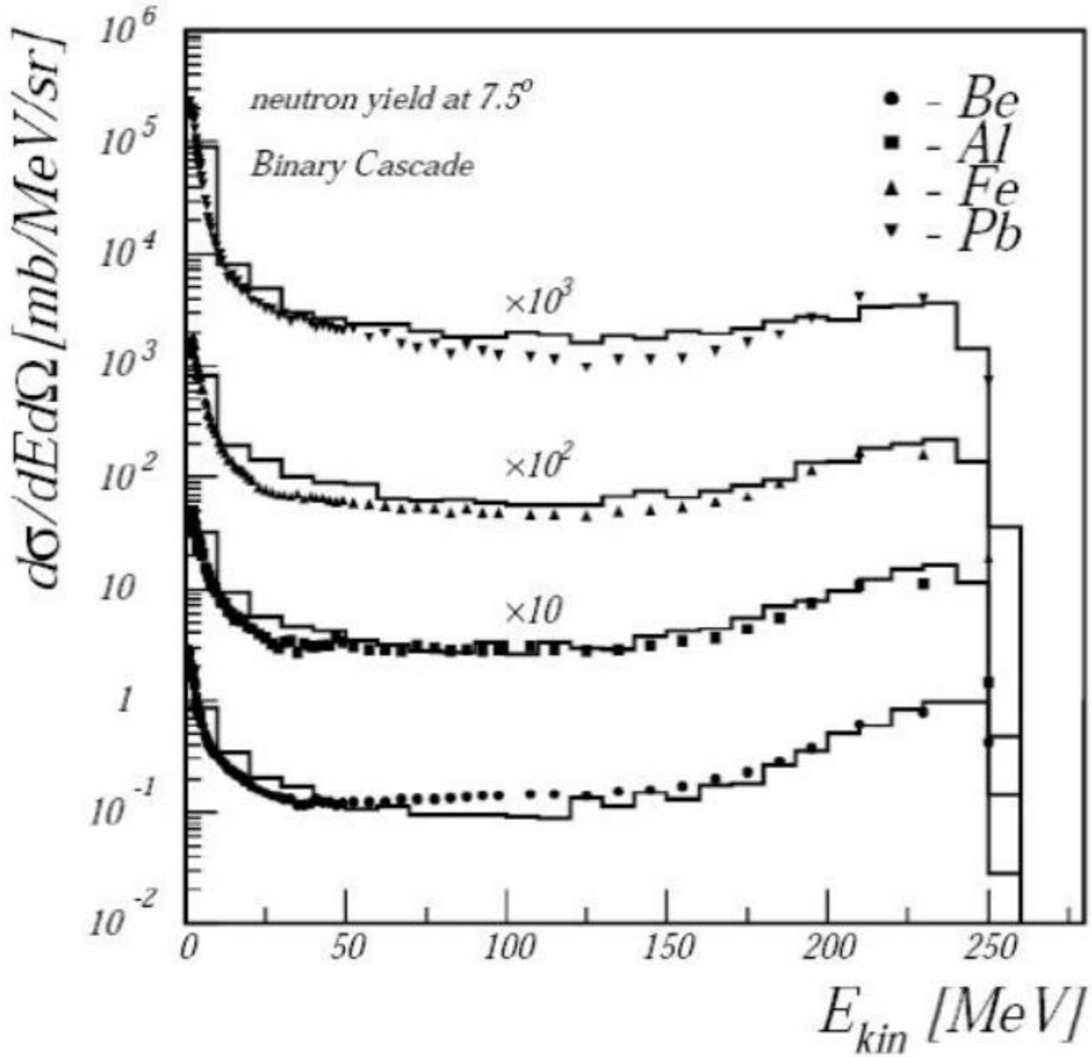
Binary Cascade Model

- Modeling sequence similar to Bertini, 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)

Validation of Binary Cascade 256 MeV protons

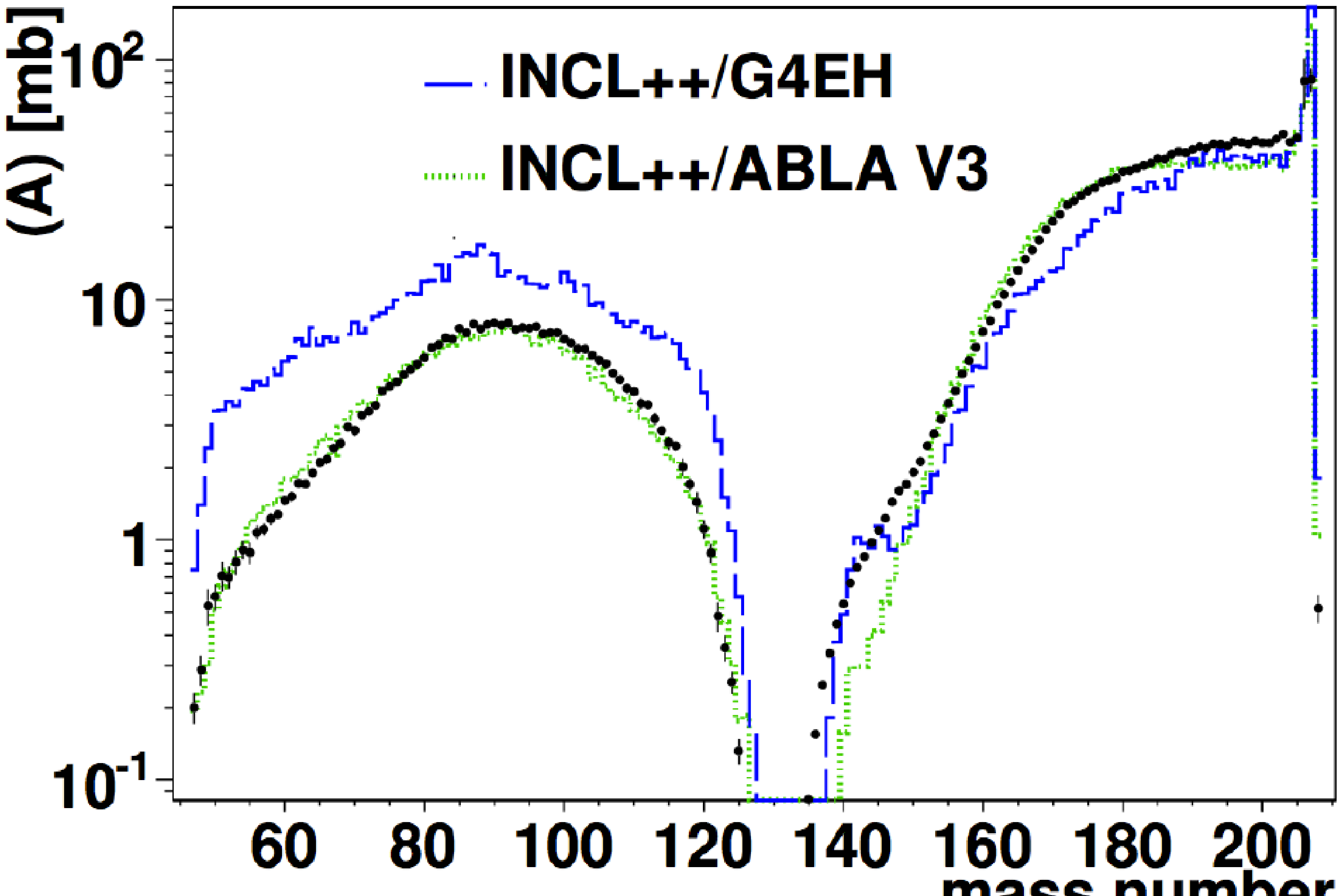


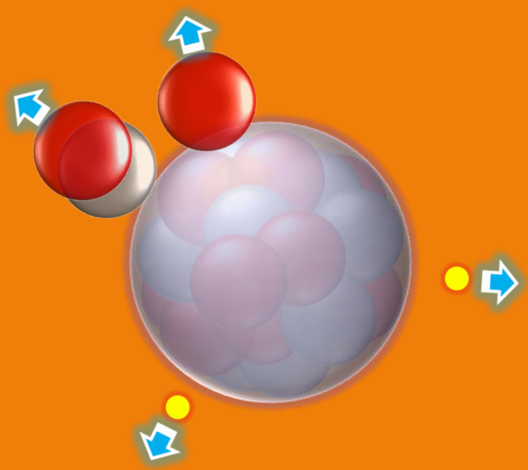
INCL++ Cascade Model

- 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 10 GeV
  - also works for projectiles up to A = 18
  - targets must be 17 < 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++ Model

Spallation residues from p + ^{208}Pb





V.6 - NUCLEUS "COOLING DOWN" MODELS

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 sub-models are called to take care of nuclear evaporation and break-up
    - these 4 models not currently callable by users

- Two Geant4 cascade models have their own version of nuclear de-excitation models embedded in them

De-excitation Model Details

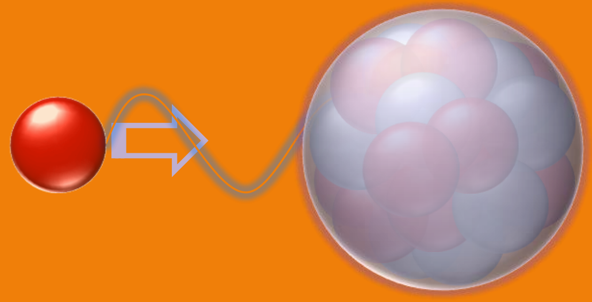
- Fermi break-up
  - remnant nucleus is destroyed – nothing left but p, n, t, a
  - valid only for A < 17 and high excitation energies

- Fission
  - splits excited nucleus and emits fission fragments + n
  - valid only for A > 65

- Multi-fragmentation
  - statistical breakup model with propagation of fragments in Coulomb field
  - for excitation energies E/A > 3 MeV

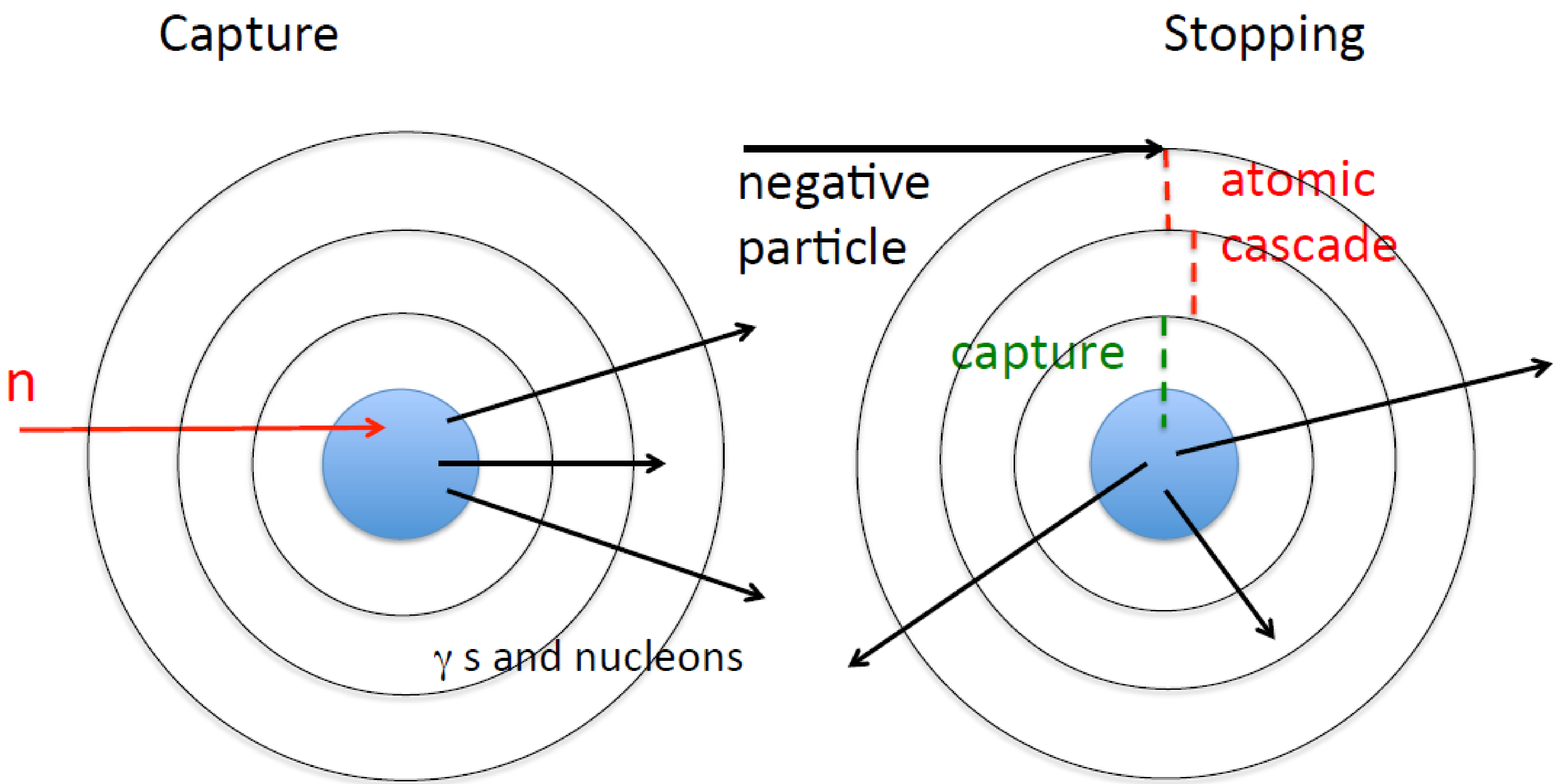
De-excitation Model Details

- Photon evaporation
  - usually final stage of nuclear de-excitation
  - data-driven: uses ENSDF database
    - Uses ENSDF files with all known gamma levels for ~3000 isotopes (in total ~ 25500 levels with half-life > 10^{-23} s)
  - handles gamma cascades, does electron emission in case of internal conversion
  - currently no correlation when more than one gamma emitted (but that's coming)



V.7 - LOW ENERGIES: CAPTURE, STOPPING, FISSION

Capture and Stopping Models



Stopped Hadron Models

- G4PiMinusAbsorptionBertini, G4KaonMinusAbsorptionBertini, G4SigmaMinusAbsorptionBertini
  - at rest process implemented with Bertini cascade model
  - G4Precompound model used for de-excitation of nucleus
  - includes atomic cascade but not decay in orbit

- G4AntiProtonAbsorptionFritiof, G4AntiSigmaPlusAbsorptionFritiof
  - FTF model used because > 2 GeV available in reaction
  - G4Precompound model used for de-excitation of nucleus
  - includes atomic cascade but not decay in orbit

Stopped Muon Models

- G4MuonMinusCapture
  - atomic cascade, with decay in orbit enabled
  - K-shell capture and nuclear de-excitation implemented with Bertini cascade model
  - used in most physics lists

- G4MuonMinusCaptureAtRest
  - atomic cascade, with decay in orbit enabled
  - K-shell capture uses simple particle-hole model
  - nuclear de-excitation handled by G4ExcitationHandler

Capture Models

- Neutrons, anti-neutrons never really stop, they just slow down from elastic scattering or are absorbed
  - kinetic energy must be taken into account
- G4HadronCaptureProcess
  - in-flight capture for neutrons
  - model implementations:
    - G4ParticleHPCapture (below 20 MeV)
    - G4NeutronRadCapture (all energies)
- G4AntiNeutronAnnihilationAtRest
  - implemented by GHEISHA parameterized model

Fission Processes and Models

- G4HadronFissionProcess can use two models
  - G4ParticleHPFission
    - specifically for neutrons below 20 MeV
    - fission fragments produced if desired
  - G4FissLib: Livermore Spontaneous Fission
    - handles spontaneous fission as an inelastic process
    - no fission fragments produced, just neutron spectra

V.8 - LOW ENERGY (<20 MEV) PARTICLE TRANSPORT

Neutron High Precision (**HP**)

- **H**igh **P**recision 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 very 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(LEND)

Notes about NeutronHP

- Geant4 Neutron Data Libraries:
  - The most recent one, G4NDL4.6, 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 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(α , β)** approach
    - Also known as "Thermal Scattering Law (TSL)", based on both experimental measurements and molecular dynamics calculations
  - Thermal neutron scattering files from ENDF/B-VII thermal data
    - There are **~ 20 materials** : al_metal, be_metal, be_beo, benzen, d_heavy_water, d_ortho_d2, d_para_d2, fe_metal, graphite, h_l_ch4, h_ortho_h2, h_para_h2, h_polyethylene, h_s_ch4, h_water, h_zrh , o_beo, o_uo2, u_uo2, zr_zrh
  - Can be activated with the elastic constructor **G4ThermalNeutrons**

```
physicsList → RegisterPhysics( new G4ThermalNeutrons(0) );
```

ParticleHP

- Extension of NeutronHP for : **p , d , t , 3He , α**
  - For high-precision elastic & inelastic interactions < **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-VII.1**
    - 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

V.9 – RADIOACTIVE DECAYS

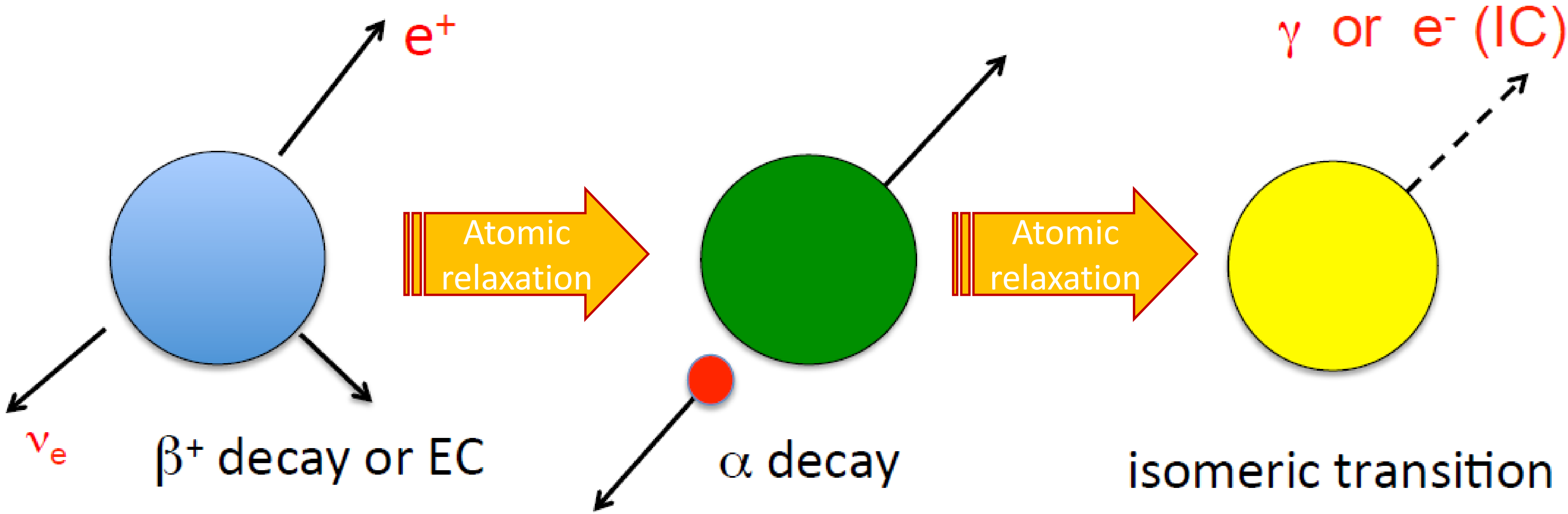
RADIOACTIVE DECAY

- Process to simulation radioactive decay of nuclei
  - At rest
  - In flight
- Decay modes implemented (and those not yet implemented):
  - **α, β^+, β^-, γ, electron capture (EC), p , n , t, spontaneous-fission**
  - Not yet implemented : pp , nn , β-delayed p , β-delayed n , ββ-- , ββ++ , etc.
- Empirical and data driven:
  - Data files from the Evaluated Nuclear Structure Data Files (ENSDF)
  - Geant4 knows **~ 6500 nuclides with half-life > 1 ns**
    - **~3000 ground states + ~3500 meta-stable states (isomers)**
- Two ways to have unstable nuclides in Geant4:
  - **Primary particle:**

```
/gun/particle ion
/gun/ion 11 24 0 472. keV # Z A Q E ; makes a Na24m nuclide
```

  - **Activation:**
    - Happens in some inelastic had. collisions, through the de-excitation nuclear models
    - Created as a G4Track if lifetime > 1 ns (1 μs in biased mode) and decayed by the radioactive decay module (which must then be present !)

Radioactive Decay Chain



EC: electron capture

IC: internal conversion

GAMMA (OR ELECTRON) EMISSION

- Nuclides with half-life < 1 ns are forced to decay immediately
  - This threshold can be set via UI command “/grdm/hlThreshold”
  - For biasing, the default value is 1 µs
- Prompt de-excitation is done via **G4PhotonEvaporation**
  - Uses **ENSDF** files with all known gamma levels for ~3000 isotopes (in total ~ 25500 levels with half-life > 10^{-23} s)
    - Data file pointed by the environmental variable **G4LEVELGAMMADATA**
  - Internal conversion (i.e. nuclear de-excitation via emission of atomic electrons) is enabled ads a competing process to gamma de-excitation
- Option to enable atomic relaxation after decay
  - When Radioactive Decay is activated, Fluorescence and Auger emissions are switched on by default (overriding any EM default settings).
  - Can be change by UI command

SAMPLING RADIOACTIVE DECAY : ANALOGUE MODE (DEFAULT)

- Several options available via UI commands
- Enable/disable radioactive decay in various geometry volumes
  - "/grdm/selectVolume" , "/grdm/deselectVolume"
- Limits the nuclei in which radioactive decay can be applied (useful to limit the decay chain, i.e. to avoid decays of daughters)
  - "/grdm/nucleusLimits"
- Supply a user-defined radioactive decay datafile for a given isotope (useful, for instance, to amplify rare decay branches)
  - "/grdm/setRadioactiveDecayFile"
- Supply a user-defined evaporation datafile for a given isotope
  - "/grdm/setPhotoEvaporationFile"
- Switch on/off atomic relaxation
  - "/grdm/applyARM" (default: true)

SAMPLING RADIOACTIVE DECAY : BIASED MODE (ALTERNATIVE)

- Several options exist and can be activated via UI commands
- Set all decay branch probabilities equal
  - "/grdm/BRbias" default: true
- “Splitting”: perform nuclear decay N times instead of 1
  - "/grdm/splitNuclei" default: 1
- Activation : integrate decay chain over time windows (in seconds) using **Bateman equations:**
  - "/grdm/sourceTimeProfile" ,
  - "/grdm/decayBiasProfile“,
  - "/grdm/analogueMC false" (default: true)
- Collimation of decay products :
  - "/grdm/decayDirection“
  - "/grdm/decayHalfAngle"

USING RADIOACTIVE DECAY

- Activate Radioactive Decay by one of the following 3 ways:
  - Choose one of the reference physics lists using the Radioactive Decay
    - e.g. **_HP** physics list or **Shielding**
  - 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 );
```

  - Or code in in your own physics list (for more experts):

```
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() );
```

V.10 – ION-ION PHYSICS

Ion-Ion Inelastic Scattering

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

- Also provided are several ion-ion cross section data sets
- Currently no ion-ion elastic scattering models provided

G4BinaryLightIonReaction

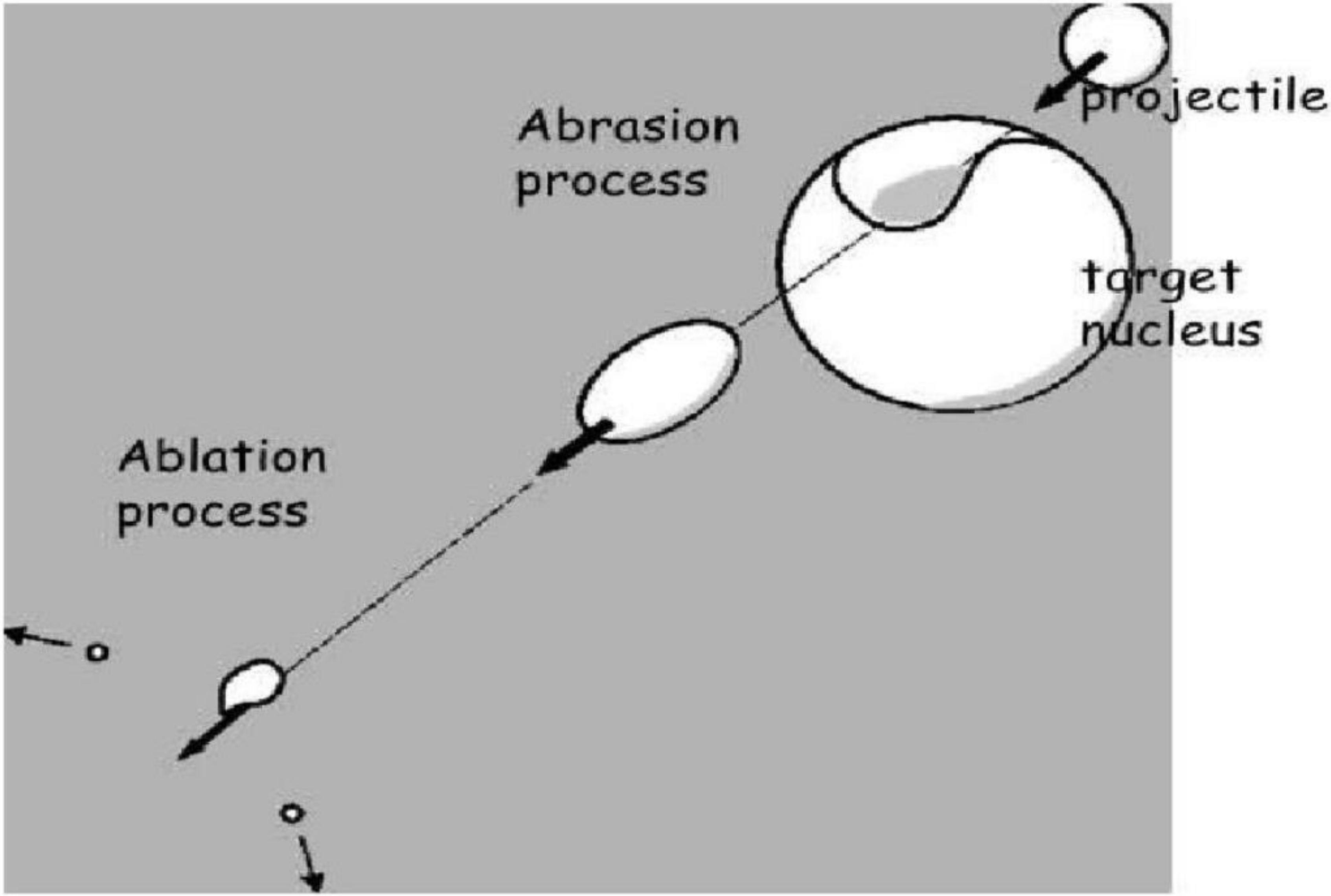
- This model is an extension of the G4BinaryCascade model
- The hadron-nuclear interaction part is identical, but the nucleus-nucleus part involves:
  - preparation of two 3D nuclei with Woods-Saxon or harmonic oscillator potentials
  - lighter nucleus is always assumed to be the projectile
  - nucleons 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

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

- The 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

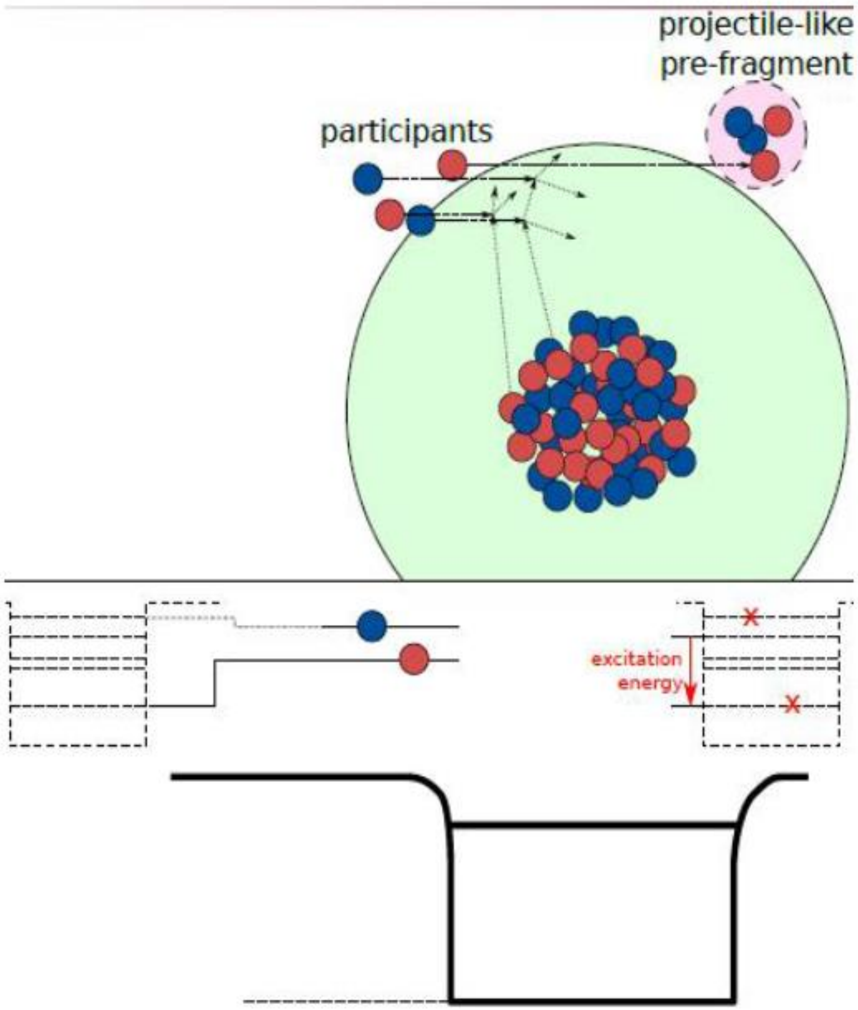


G4EMDissociation Model

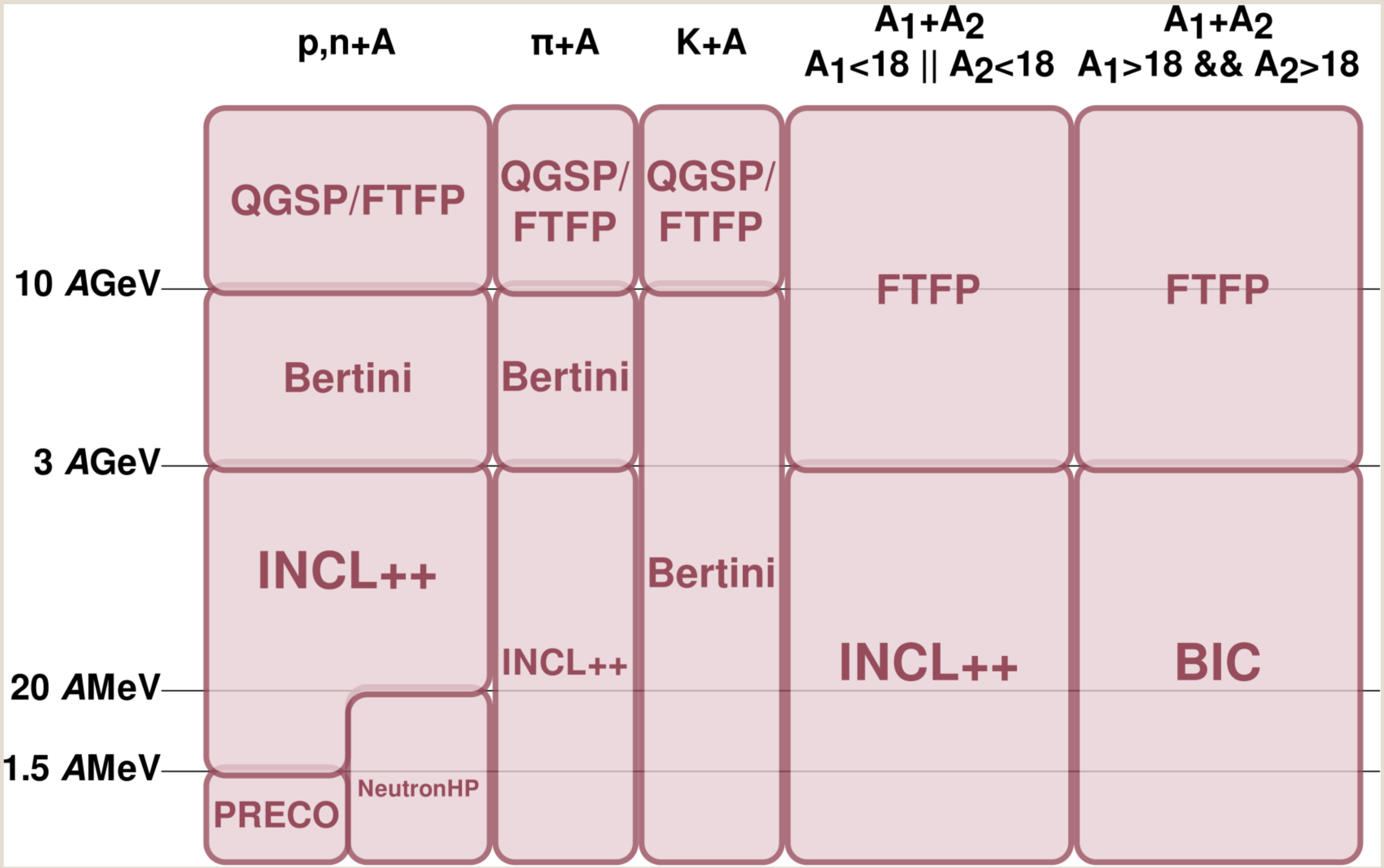
- Electromagnetic dissociation is the liberation of nucleons or nuclear fragments as a result of strong EM fields
  - as when two high-Z nuclei approach
  - exchange of virtual photons instead of nuclear force
- Useful for relativistic nucleus-nucleus collisions where the Z of the nucleus is large
- 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 target
- Projectile nucleons can pass through to form fragment or interact with nucleus



INCL VERSUS OTHER CASCADE MODELS



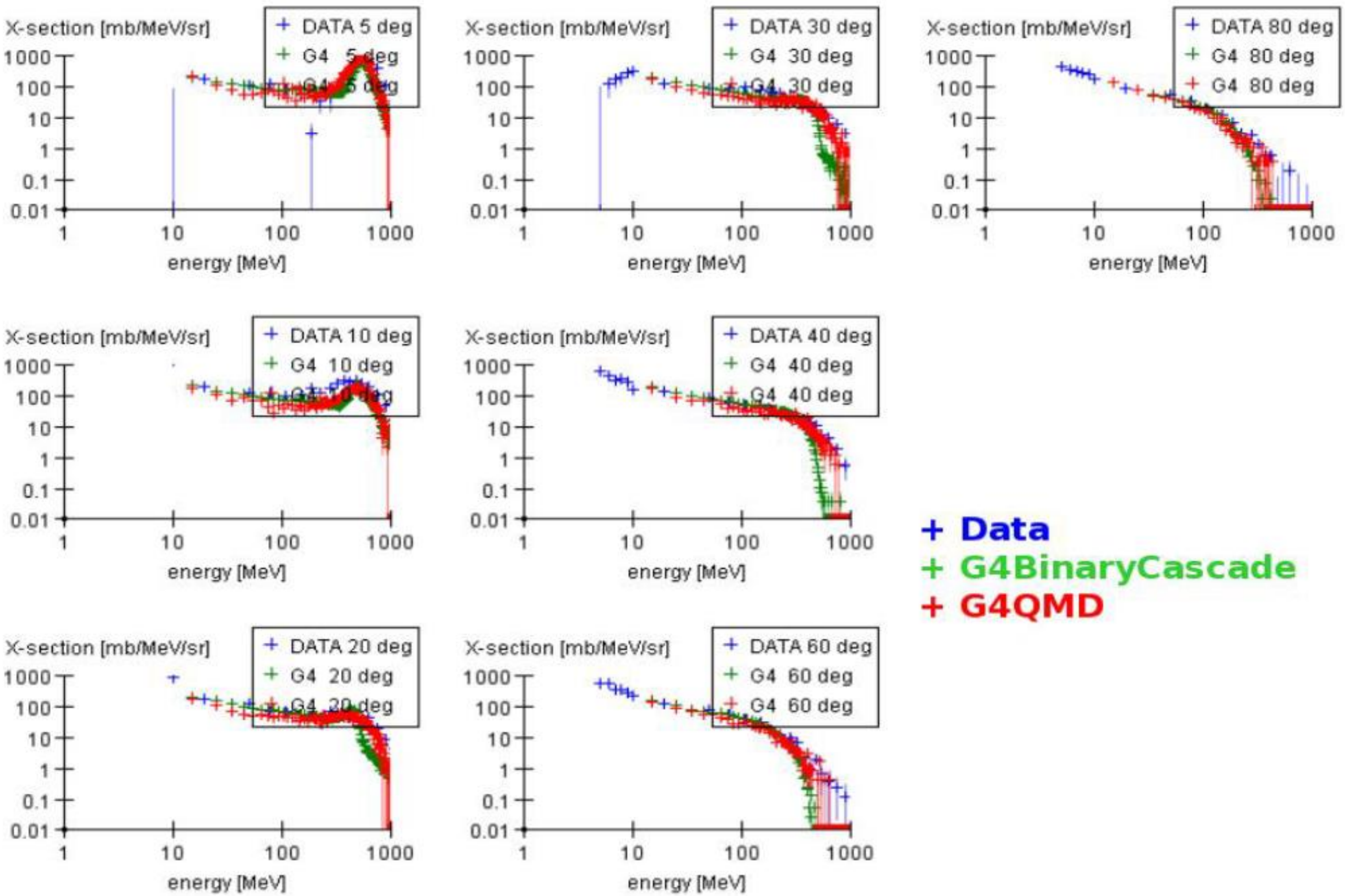
G4QMD Model

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

- Solution is QMD (quantum molecular dynamics) model
  - an extension of the classical molecular dynamics model
  - treats each nucleon as a gaussian wave packet
  - propagation with scattering which takes Pauli principal into account
  - can be used for high energy, high Z collisions

QMD Validation

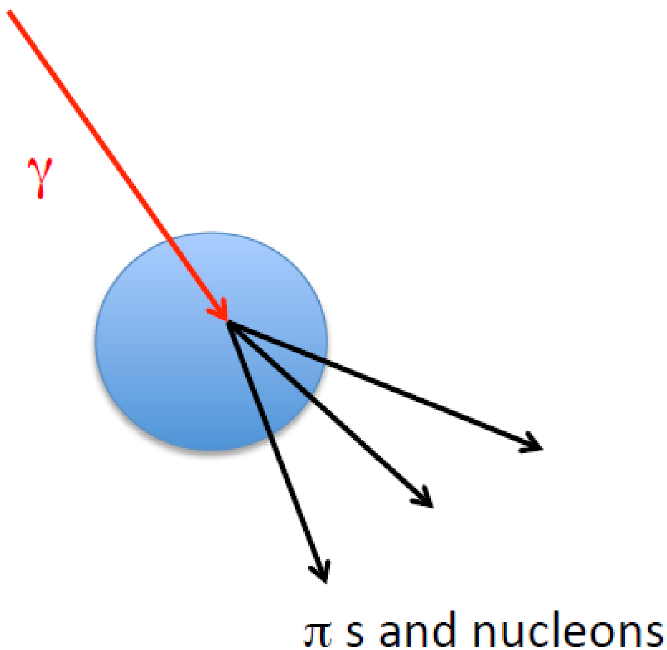
Ar40 560MeV/n on Lead



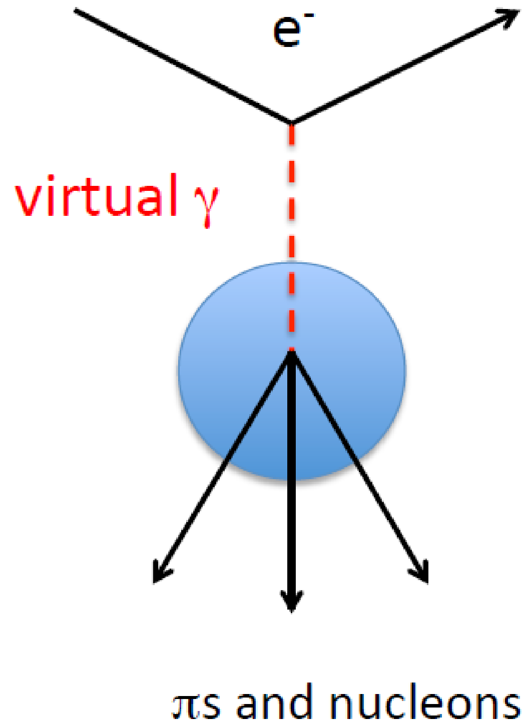
V.11 - GAMMA- & LEPTO-NUCLEAR

Gamma- and Lepto-nuclear Models

Gamma-nuclear



Lepto-nuclear



Gamma- and Lepto-nuclear Processes

- 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
  - virtual photon then interacts directly with nucleus (or nucleons within nucleus)

Gamma- and Lepto-nuclear Models

- G4MuonVDNuclearModel
  - Kokoulin model of EM cross section and virtual photon generation
  - Weizsacker-Williams conversion of virtual to real gamma
  - For $E_\gamma < 10$ GeV, direct interaction with nucleus using Bertini cascade
  - For $E_\gamma > 10$ GeV, conversion of γ to π^0, then interaction with nucleus using FTFP model

- G4ElectroVDNuclearModel
  - Kossov model of EM cross section and virtual photon generation
  - all else identical to that in G4MuonVDNuclearModel

- For gamma-nuclear reaction
  - Bertini cascade below 3.5 GeV
  - QGSP from 3 GeV to 100 TeV

SUMMARY (1/2)

- The Geant4 hadronic framework is structured to allow cross-sections and models to cooperate in various energy ranges

- Various cross-sections and models are available for elastic interactions.
- Two QCD string models are available for high energy interactions:
  - Fritiof and QGS
- The intermediate energy range is covered by intra-nuclear cascade models
  - BIC, BERT and INCLXX
- Nucleus “cooling down” after interaction by higher energy models (FTF, QGS, INCL) is handled by pre-compound and de-excitation models.

SUMMARY (2/2)

- Capture, stopping (for negative particles) and fissions are available.
- Low energy hadrons (< 20 MeV) are handled by means of databases.
- Radioactive decay module is available.
  - And covers a wide range of decays through mean of large database
- The hadronic package includes ion-ion interactions,
- And gamma- lepto-nuclear processes.