PHYSICS CONTENT OF GEANT4

"AN OVERVIEW"

Geant4 PHENIICS & IN2P3 Tutorial,
12 - 16 May 2025,
Orsay

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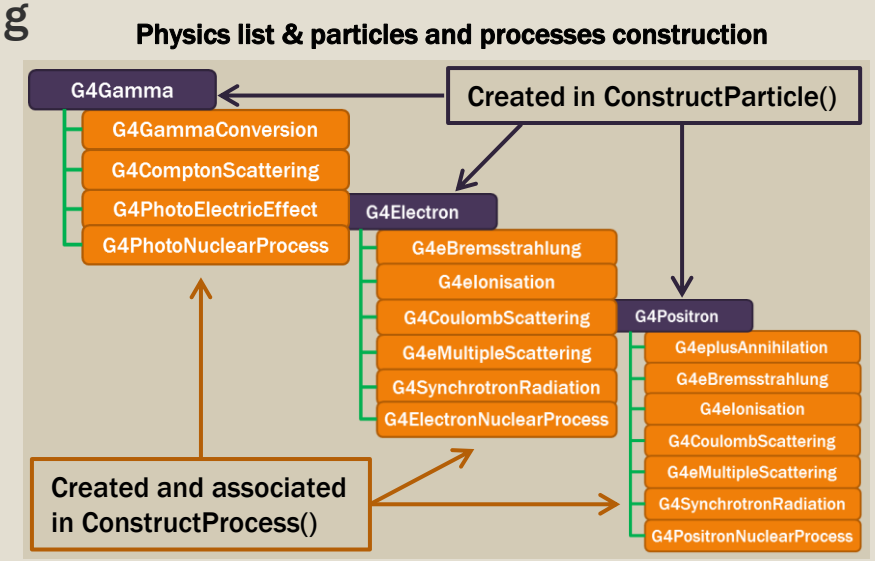
INTRODUCTION

- 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 give more details to the physics content(s) of (some !) processes
  - Eg : what is there in G4ionIonisation ?

OUTLINE

I. Generalities
II. EM physics
III. Optical Physics
IV. Decay Physics
V. Hadronic Physics
    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)
- What physics list to use ?

I. GENERALITIES

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
- But share similar approaches on:
  - Physics quantities calculations (cross-sections, stopping powers, final states), based on either:
    - 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 and to leave no "holes" in coverage

PHYSICS DATASETS (GEANT4 V11.3.2)

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
G4EMLOW8.6.1	G4LEDATA	data files for low energy electromagnetic processes	314
G4PhotonEvaporation6.1	G4LEVELGAMMADATA	data files for photon evaporation (from ENSDF)	9.6
G4RadioactiveDecay6.1.2	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
G4PARTICLEXS4.1	G4PARTICLEXSDATA	data files for evaluated particle XS on natural composition of elements	11.7
G4ABLA3.3	G4ABLADATA	data files for nuclear shell effects in INCL/ABLA hadronic model	0.105
G4INCL1.2	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
G4ENSDFSTATE3.0	G4ENSDFSTATEDATA	Data files for nuclides properties	0.284
G4TENDL1.4	G4PARTICLEHPDATA	Optional data files for incident particles	870
G4CHANNELINGDATA1.0	G4CHANNELINGDATA	Optional crystal data files for channeling	3.7
G4NUDEXLIB1.0	G4NUDEXLIBDATA	Optional data for NuDEX nuclear de-excitation hadronic model	8.6
G4URRPT1.1	G4URRPTDATA	Optional data for Unresolved Resonance Region via Probability Table	288

LAST GENERAL PAPER

- Last published paper published in 2016.
  - Provides a full overview of Geant4,
  - including physics options,
  - All this in one single paper

- *Available in open access*
- Plans in Geant4 to go for a new general paper in 2025 - 2026

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

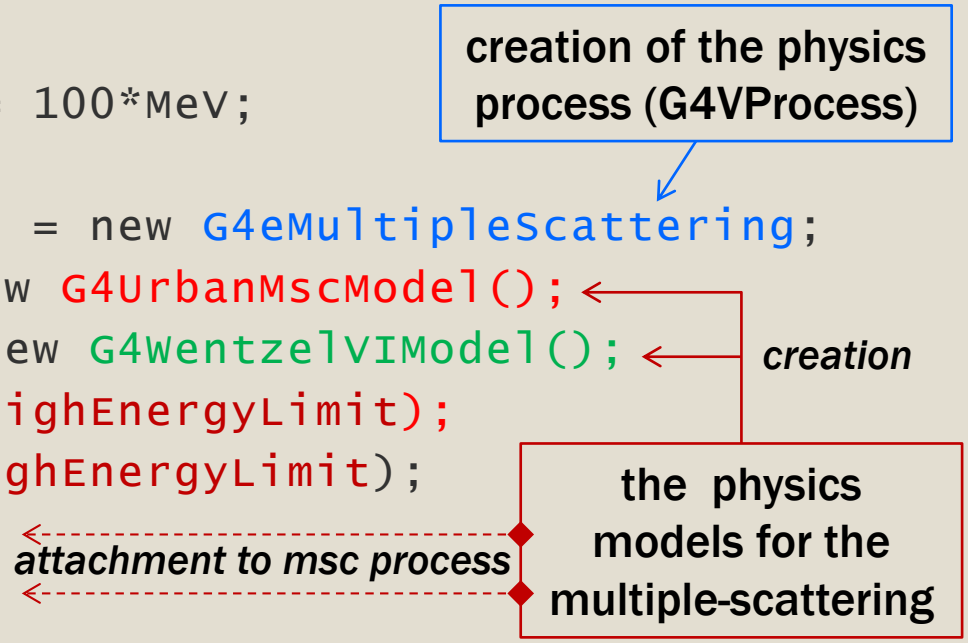
PROCESSES & MODELS IN EM

- A **physics process** is described by a **process class (G4VEmProcess)**:
  - Naming scheme : « G4**ProcessName** »
  - For example: **G4Compton**
- A physics process can be hold **several models**, each model being described by a **model class (G4VEmModel)**:
  - Naming scheme : G4**ModelName**ProcessNameModel or G4**ModelName**Model …
    - For example: **G4LivermoreComptonModel**
  - Models are valid in certain **energy ranges** and can be assigned to **G4Regions**
    - → **EM physics level description** can be adapted to the regions
- Models implement the **physics contents** :
  - 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:

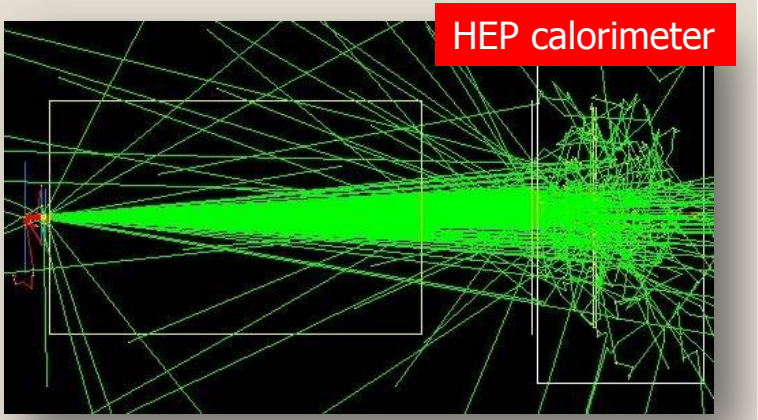
```
…
G4double highEnergyLimit = 100*MeV;
…
G4eMultipleScattering* msc = new G4eMultipleScattering;
G4UrbanMscModel* msc1 = new G4UrbanMscModel();
G4WentzelVIModel* msc2 = new G4WentzelVIModel();
msc1->SetHighEnergyLimit(highEnergyLimit);
msc2->SetLowEnergyLimit(highEnergyLimit);
msc->AddEmModel(0, msc1);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

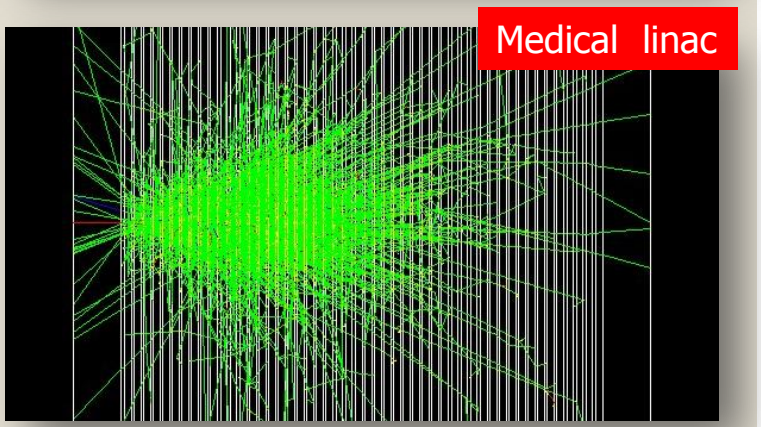


II.1 - OVERVIEW OF EM STANDARD PHYSICS

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⁻ ($e < e_{cut}$)

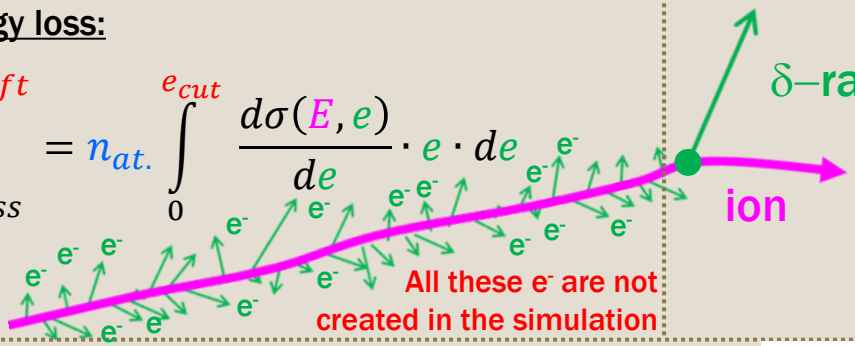
Mean energy loss:

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

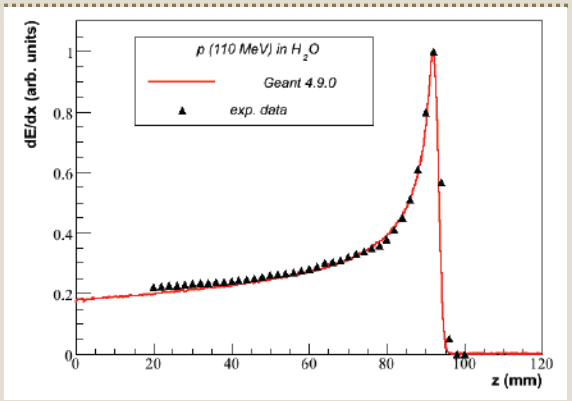
Discrete loss from hard e⁻ ($e > e_{cut}$)

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
    - G4BragglonModel



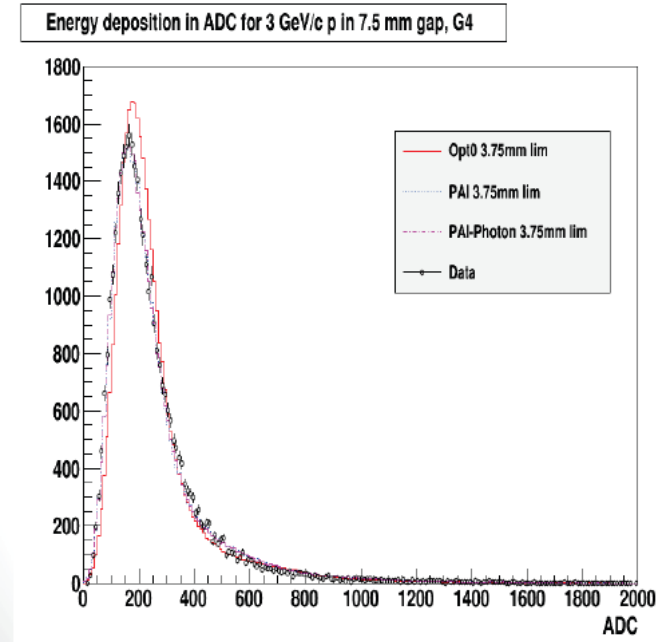
FLUCTUATION ON (MEAN) IONIZATION

- **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 available:**

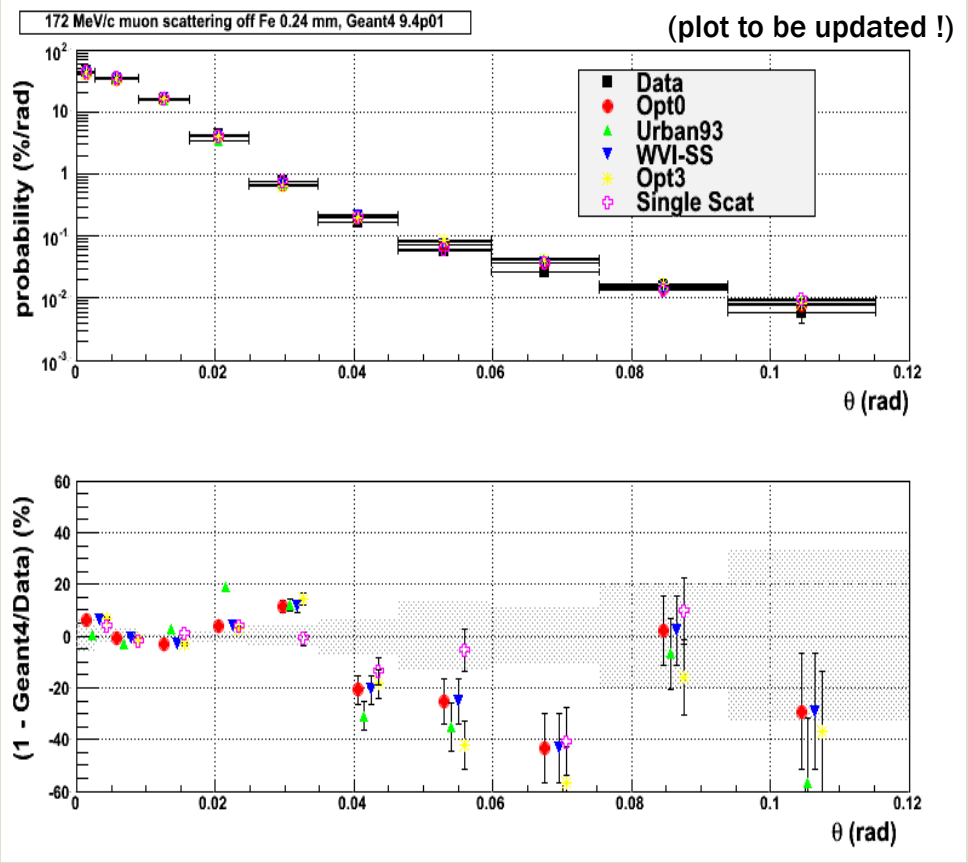
  - **Urban Modelling:**
    - Based on simplified atomic model:
      - Assumed only two levels E_1, E_2
    - Particle-atom interactions can be:
      - An excitation of atom with energy loss $E = E_1 - E_2$
      - An ionization, with energy loss distribution $\sim 1/E^2$
    - G4UniversalFluctuation 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)



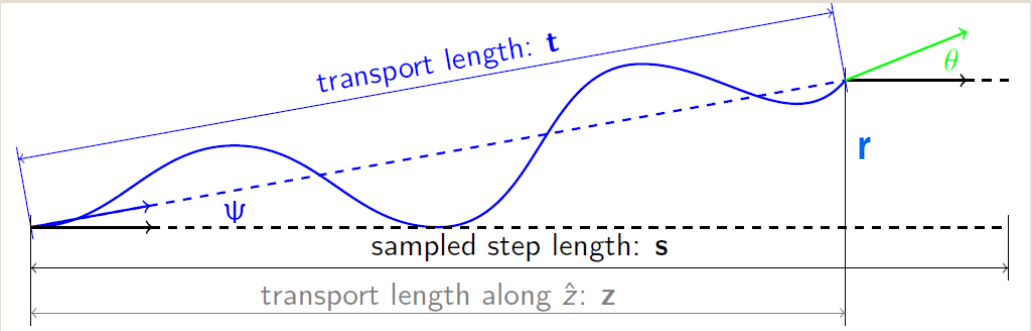
MULTIPLE COULOMB SCATTERING (MSC)

- 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)



- **MSC & tracking logic:**
  - The physics processes and the geometry select the step length;
  - MSC performs the true path length ↔ z transformation to compare with geometry
  - The track is moved to the end of the step
  - Scattering angles (θ, ψ) are sampled
  - Lateral displacement is calculated, particle is moved accordingly

- **Several models provided in Geant4** (depending on incident particle type, energy, calculation of effects [recoil or not], screening effect [simulated or not]).
  - Most used one is the so-called **Urban model**

MSC CLASSES

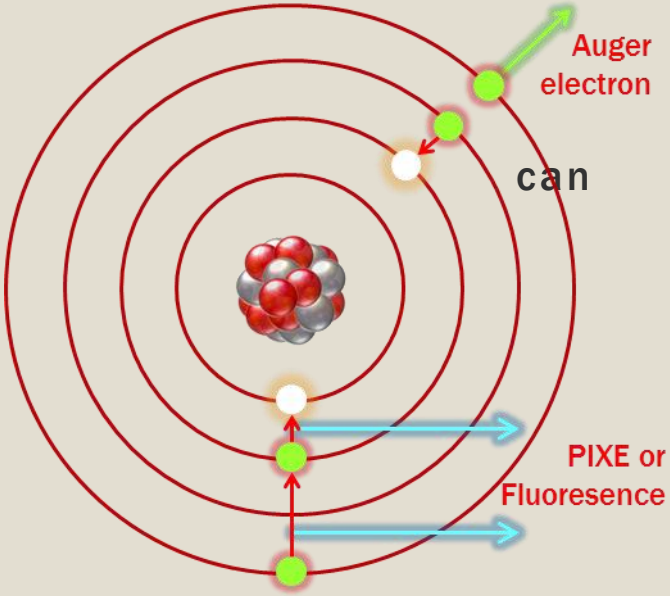
- Processes per particle type are available
  - G4eMultipleScattering for e+/e-
  - G4MuMultipleScattering for μ+/μ-
  - G4hMultipleScattering for hadrons and ions
- L. Urban model
  - G4UrbanMscModel :
    - The most established Geant4 scattering model
- Combined multiple and single scattering model: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

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 : $\beta^{\pm}$, α, electronic capture)
    - Nuclear evaporation, etc.
- Atomic relaxation follows and atom can de-excite through:
  - Fluorescence
  - Auger
  - PIXE (Particle Induced X-Ray Emission)
- Detailed atomic structure required:
  - radiative: fluorescence
  - non-radiative:
    - Auger (initial & final vacancies in ≠ sub-shells)
    - Coster-Kronig (same sub-shells)
  - EADL transition probability database used (Livermore)



- Reference physics lists include atomic deexcitation
  - Fluo. (inactive with EM std) Auger, PIXE (de)activable & per region by command lines
  - Beware of cuts and do /process/em/deexcitationIgnoreCut true !

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
- Existing packages in Geant4:
  - 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]
- More CPU intensive than “standard EM”
  - To be used for proper purposes

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

- Based on public **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

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

- Include elements from **Z=1 to Z=100**

- Data tables contain:
  - Total cross sections: photoelectric, Compton, Rayleigh, pair production, brem.
  - Shell integrated cross sections: photo-electric, ionization
  - Energy spectra: secondary e- processes
  - Atomic effects (fluorescence, Auger)
  - Atomic relaxation : Z > 5 (EADL transition data)
- Validity range (recommended) : **250 eV - 100 GeV**
  - Acceptable down to 100 eV (reduced accuracy)
  - In principle, down to ~10 eV

- **Polarized photon interactions provided too**

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

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

- 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 ?

PHYSICAL STAGE
step-by-step modelling of **physical interactions** of incoming & secondary ionising radiation with biological medium (liquid water)

- Excited **water molecules**
- Ionised **water molecules**
- **Solvated electrons**

PHYSICO-CHEMICAL / CHEMICAL STAGE
- **Radical** species production
- Diffusion
- Mutual chemical interactions

GEOMETRICAL MODELS
DNA strands, chromatin fibres, chromosomes, whole cell nucleus, cells...
for the prediction of damage resulting from direct and indirect hits

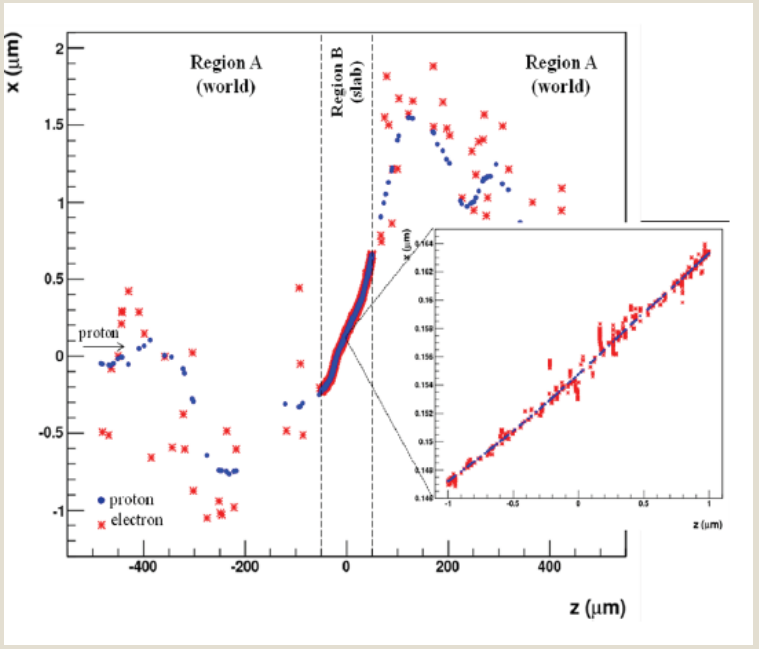
DIRECT DNA DAMAGE

INDIRECT DNA DAMAGE

t=0 $t=10^{-15}$s $t=10^{-6}$s

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

<table>
<tr><th>Particles</th><th>e-</th><th>p</th><th>H</th><th>He^{++}, He^{+}, He^{0}</th><th>C, N, O, Fe,...</th></tr>
<tr><td>Elastic scattering</td><td>> 9 eV – 1 MeV
Screened Rutherford
>7.4 eV – 1 MeV
Champion</td><td>-</td><td>-</td><td>-</td><td>-</td></tr>
<tr><td>Excitation</td><td>9 eV – 1 MeV
Born</td><td>10 eV – 500 keV
Miller Green
500 keV – 100 MeV
Born</td><td>10 eV – 500 keV
Miller Green</td><td rowspan="3">Effective charge scaling from same models as for proton

1 keV – 400 MeV</td><td>-</td></tr>
<tr><td>Charge Change</td><td>-</td><td>100 eV – 100 MeV
Dingfelder</td><td>100 eV – 100 MeV
Dingfelder</td><td>-</td></tr>
<tr><td>Ionisation</td><td>11 eV – 1 MeV
Born</td><td>100 eV – 500 keV
Rudd
500 keV – 100 MeV
Born</td><td>100 eV – 100 MeV
Rudd</td><td>Effective charge scaling
0.5 MeV/u – 10^{6} MeV/u</td></tr>
<tr><td>Vibrational excitation</td><td>2 – 100 eV
Michaud et al.</td><td colspan="4" rowspan="2">-</td></tr>
<tr><td>Attachment</td><td>4 – 13 eV
Melton</td></tr>
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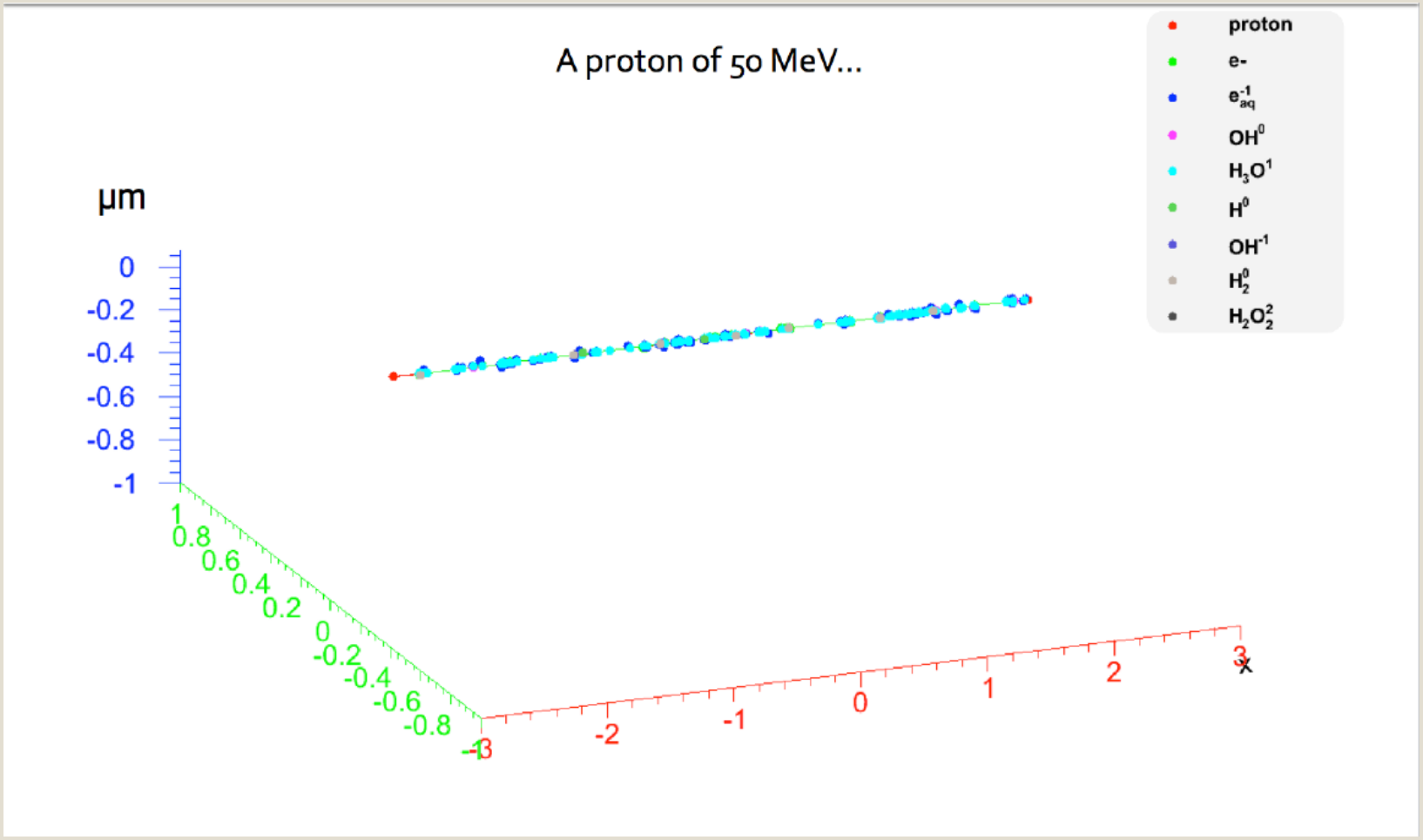
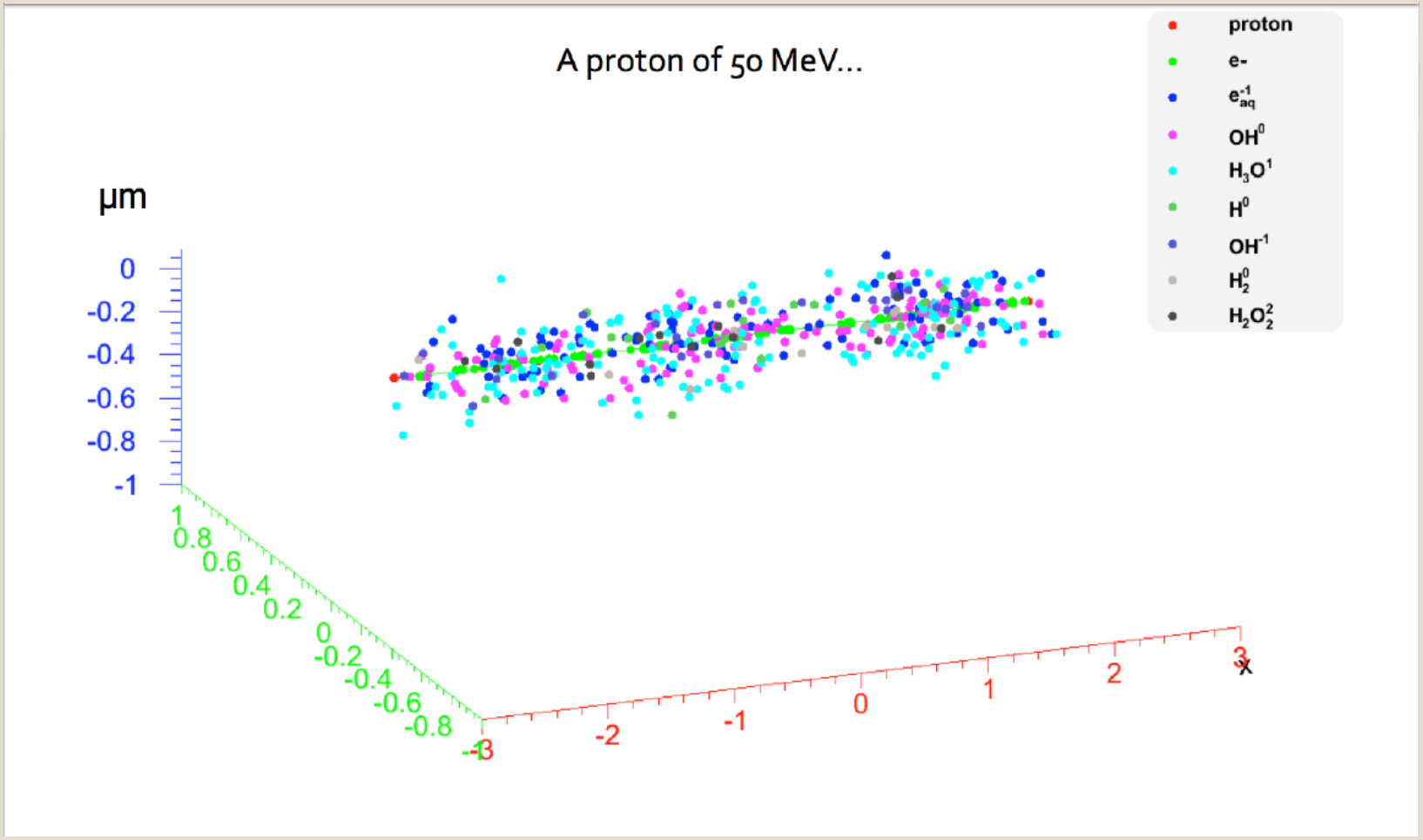
1 PICOSECOND AFTER IRRADIATION…

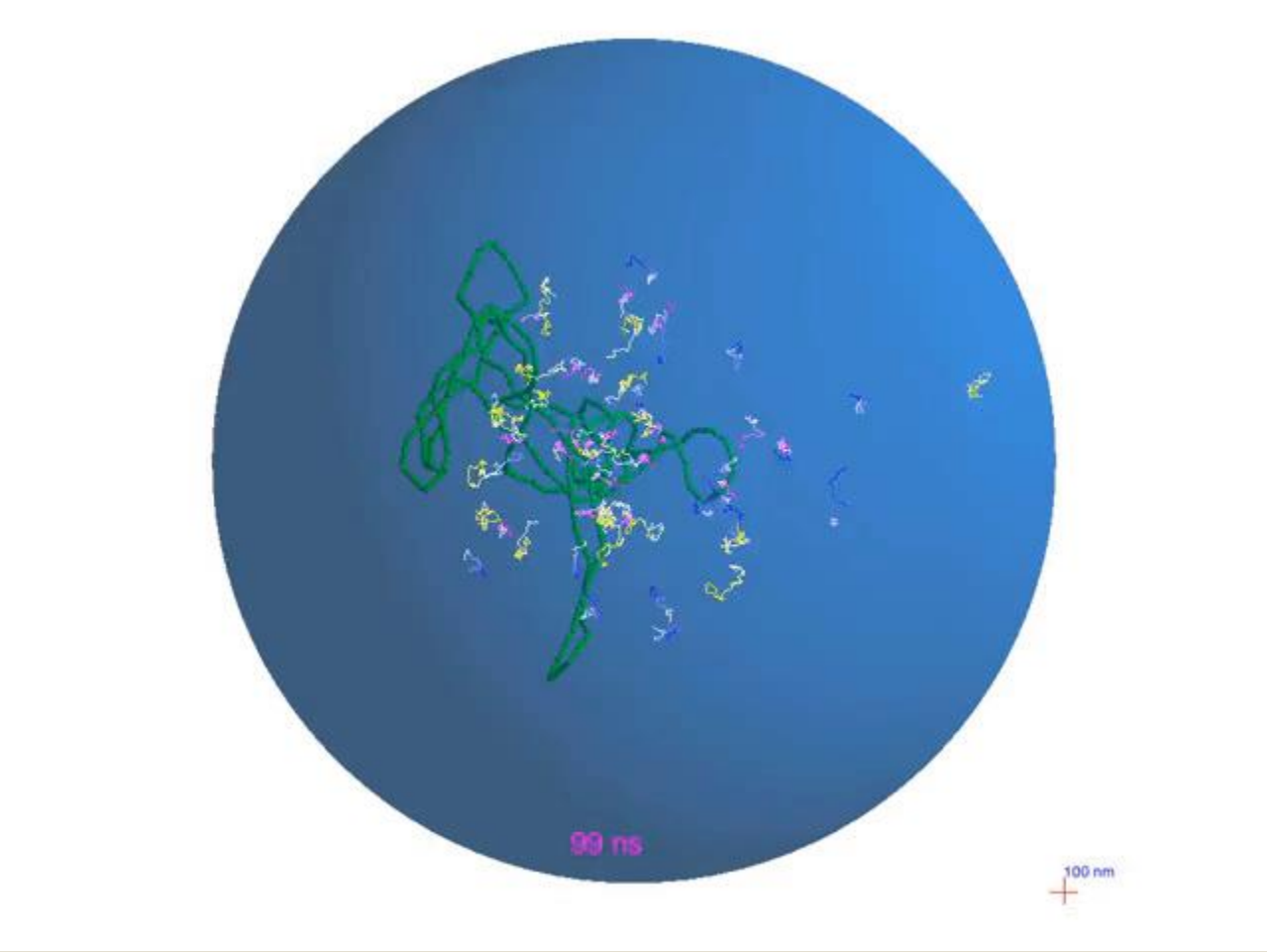


1 MICROSECOND AFTER IRRADIATION…



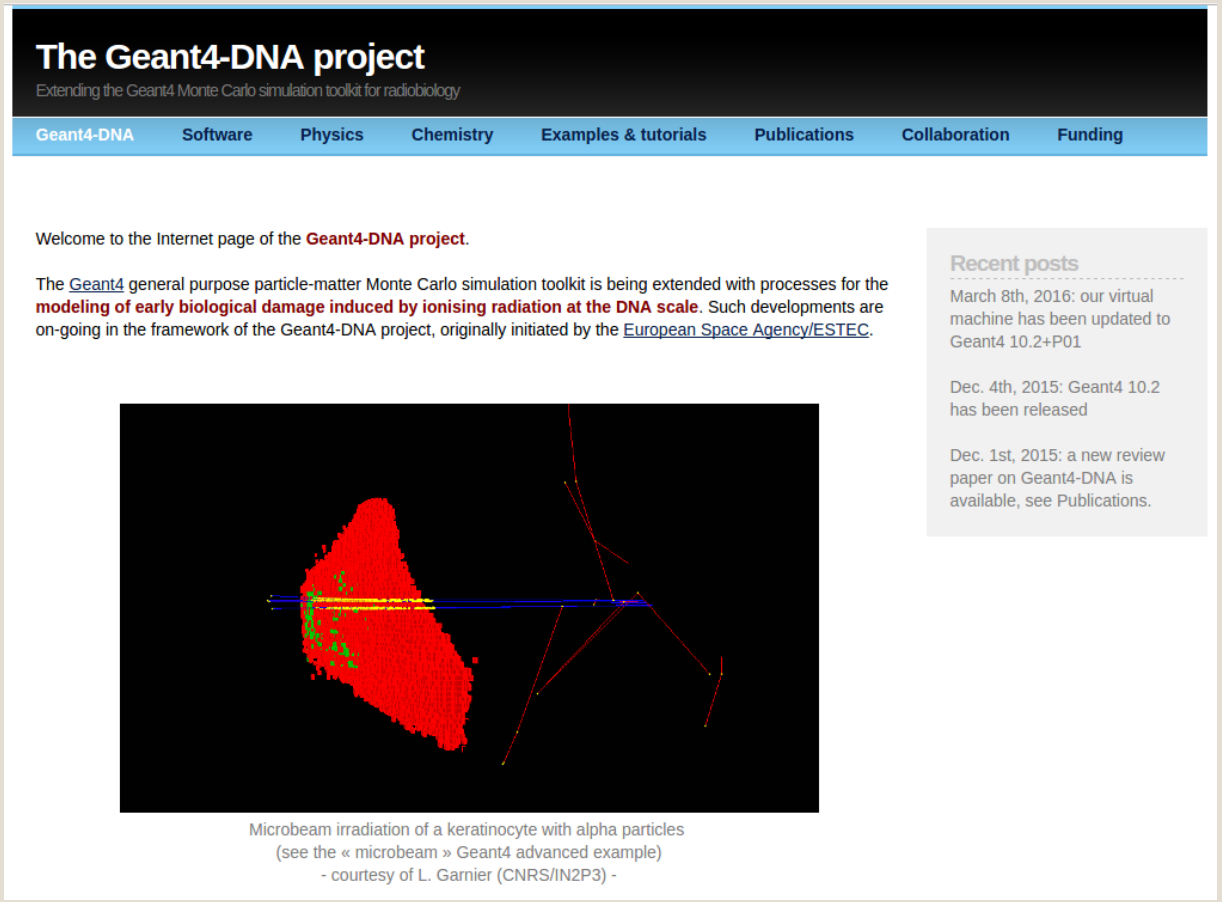
IRRADIATION OF A PBR322 PLASMID, INCLUDING RADIOLYSIS

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



DEDICATED WEB SITE

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



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 & EXAMPLES

USER INTERFACES AND HELPER CLASSES

- Physics configuration and control:
  - G4EmParameters
    - C++ interface to EM options alternative to UI commands
  - G4EmConfigurator
    - add models per energy range and geometry region
- Physics calculations:
  - Very useful classes to compute physics quantities !
    - Are the classes used for calculations in G4 EM packages (cross-sections, etc.)
    - Propose further calculations (Birks, ionisation clusters)
  - 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
  - G4NIELCalculator
    - Allows computation of NIEL (Non Ionizing Energy Loss) at a step

EXAMPLE FOR CROSS-SECTION

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

auto material =
     G4NistManager::Instance()->FindOrBuildMaterial(matName);
auto density = material->GetDensity();
auto 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.

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 !

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 Aka “”	Default: nothing or _EMO (QGSP_BERT, FTFP_BERT,...)	for ATLAS and other HEP simulation applications
G4EmStandardPhysics_option1 Aka “EMV”	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 Aka “EMX”	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 Aka "EMY"	Urban MSC model for all particles	proton/ion therapy
G4EmStandardPhysics_option4 Aka "EMZ"	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 Aka "LIV"	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 Aka "PEN"	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

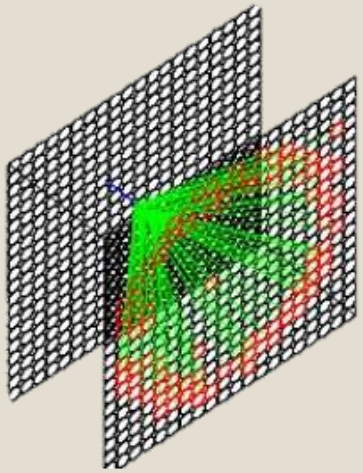
- Primarily meant for developers and model validations

Constructor	Components	Comments
G4EmStandardPhysicsGS Aka “GS”	standard EM physics and the GS MSC model for $e^{\pm}$ with HEP settings	may be considered as an alternative to EMO i.e. for HEP
G4EmStandardPhysicsWVI Aka “WVI”	WentzelWVI + Single Scattering mixed simulation model for Coulomb scattering	high and intermediate energy applications
G4EmStandardPhysicsSS Aka “SS"	single scattering (SS) model description of the Coulomb scattering	validation and verification of the MSC and mixed simulation models
G4EmLowEPPhysics Aka “LE”	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

III. OPTICAL PHYSICS

OPTICAL PHOTON
ASSUMPTIONS & LIMITATIONS

- G4OpticalPhoton is the class representing optical photons, with "opticalphoton" as particle name



- Treated as "point-like" objects:
  - Simulation of "point like" interactions ✓
    - Scattering, absorption, reflection…
  - No simulation of "wave-like" behaviors ✘
    - No phase treatment ⇒ no interferences simulated !
- Optical photons treated separately from EM processes:
  - Wavelengths are much larger than atomic spacing
  - G4OpticalPhoton ≠ G4Gamma; no smooth transition defined.
- Energy/momentum generally not conserved in G4 optics

OPTICAL PHOTON PROCESSES

- **Production processes:**
  - G4Cerenkov
  - G4Scintillation
    - Large production of photons !
    - Trick used : If N photons produced → suspend primary → track photons → resume tracking of primary
- **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(…):

```
auto 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)

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

- Decay modes:
  - Phase space, Dalitz decay, V – A and semileptonic are available
  - As well as decay with spin
  - User pre-assigned decay is possible (in primary generator action)
    - branching ratio and decay modes retrieved from decay table stored for each particle
  - The G4ExtDecayer interface allows to treat decays from heavy flavor physics, like B meson decays

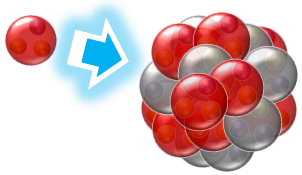
V. HADRONIC PHYSICS

OVERVIEW OF HADRONIC PHYSICS PART

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)

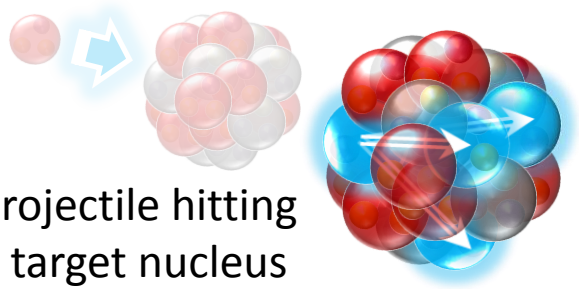
V.1 - GENERALITIES

One hadronic collision = sequence of many hadronic interactions



Projectile hitting
a target nucleus

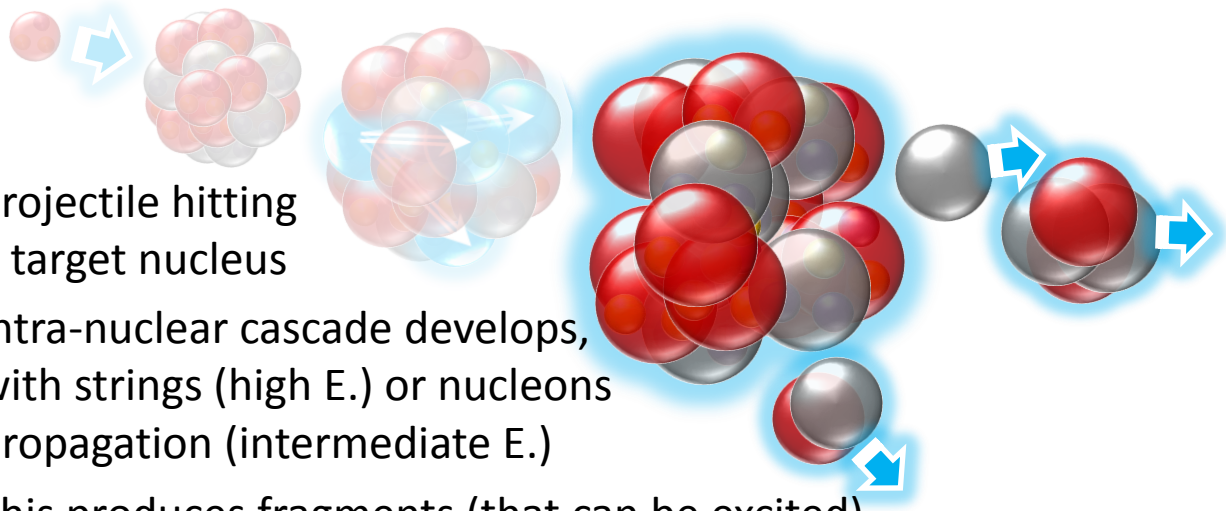
One hadronic collision = sequence of many hadronic interactions



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

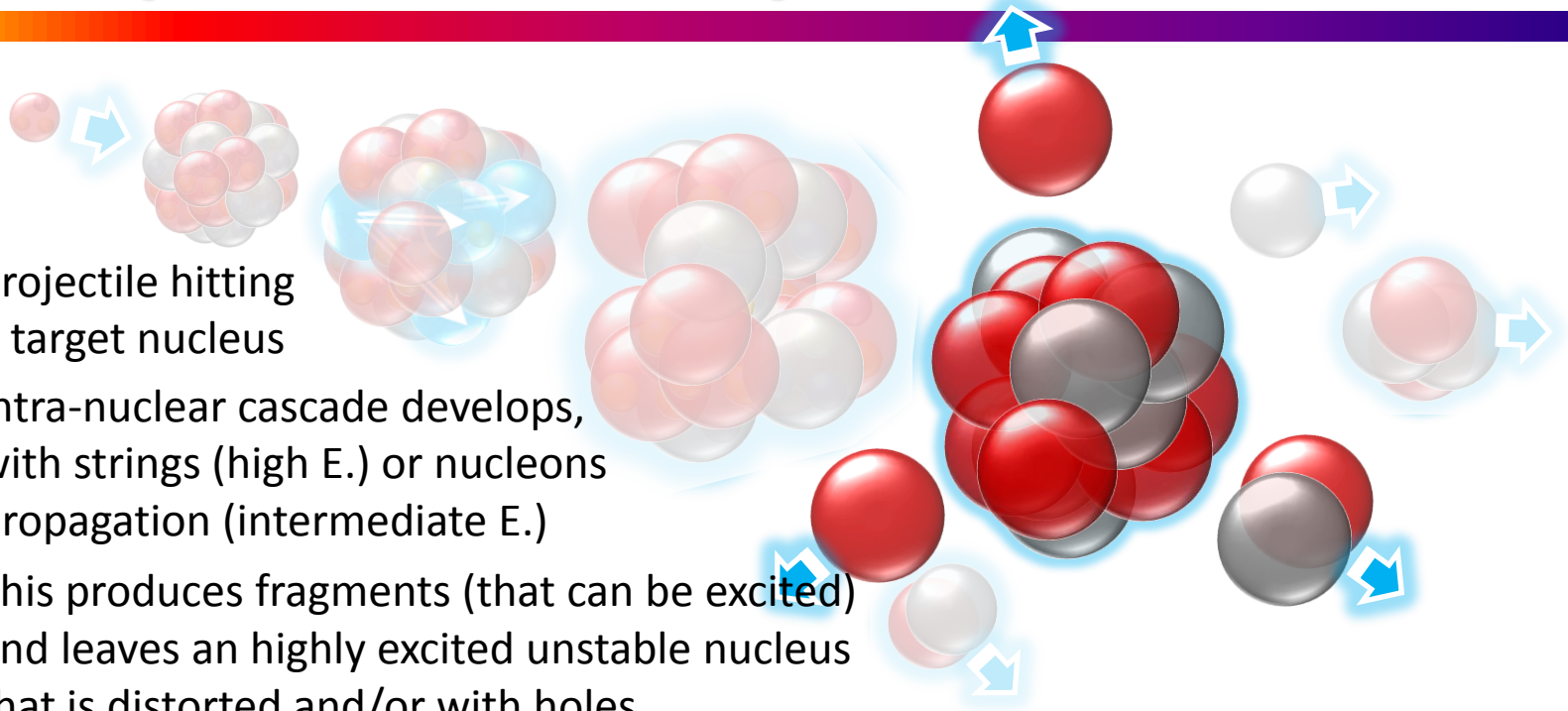


Projectile hitting a target nucleus

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.

One hadronic collision = sequence of many hadronic interactions



Projectile hitting a target nucleus

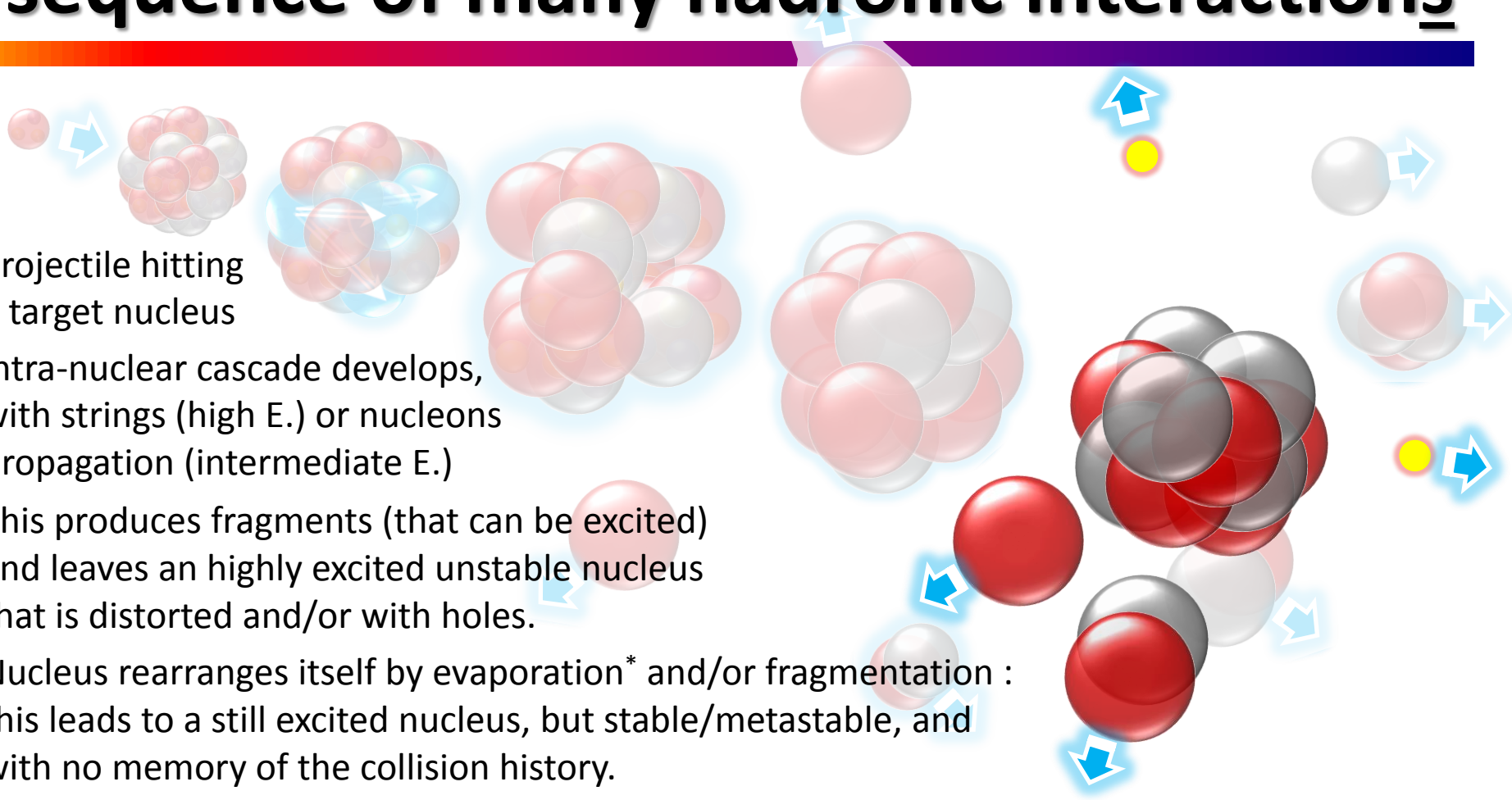
Intra-nuclear cascade develops, with strings (high E.) or nucleons propagation (intermediate E.)

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.

(*) **Evaporation** = de-excitation by emission of light nuclei $\in$ {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.

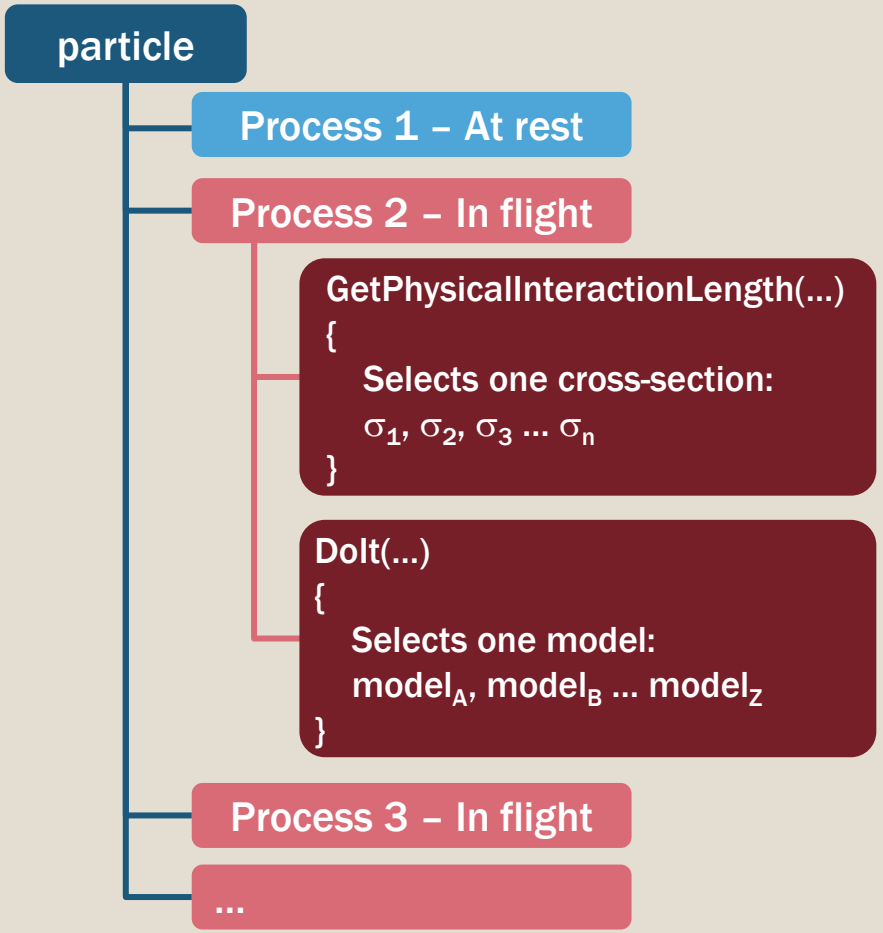
The nucleus undergoes final de-excitation by evaporation* or fission and ends-up in its ground state. In case of fission, further de-excitation of fragments may occur.

(*) **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.

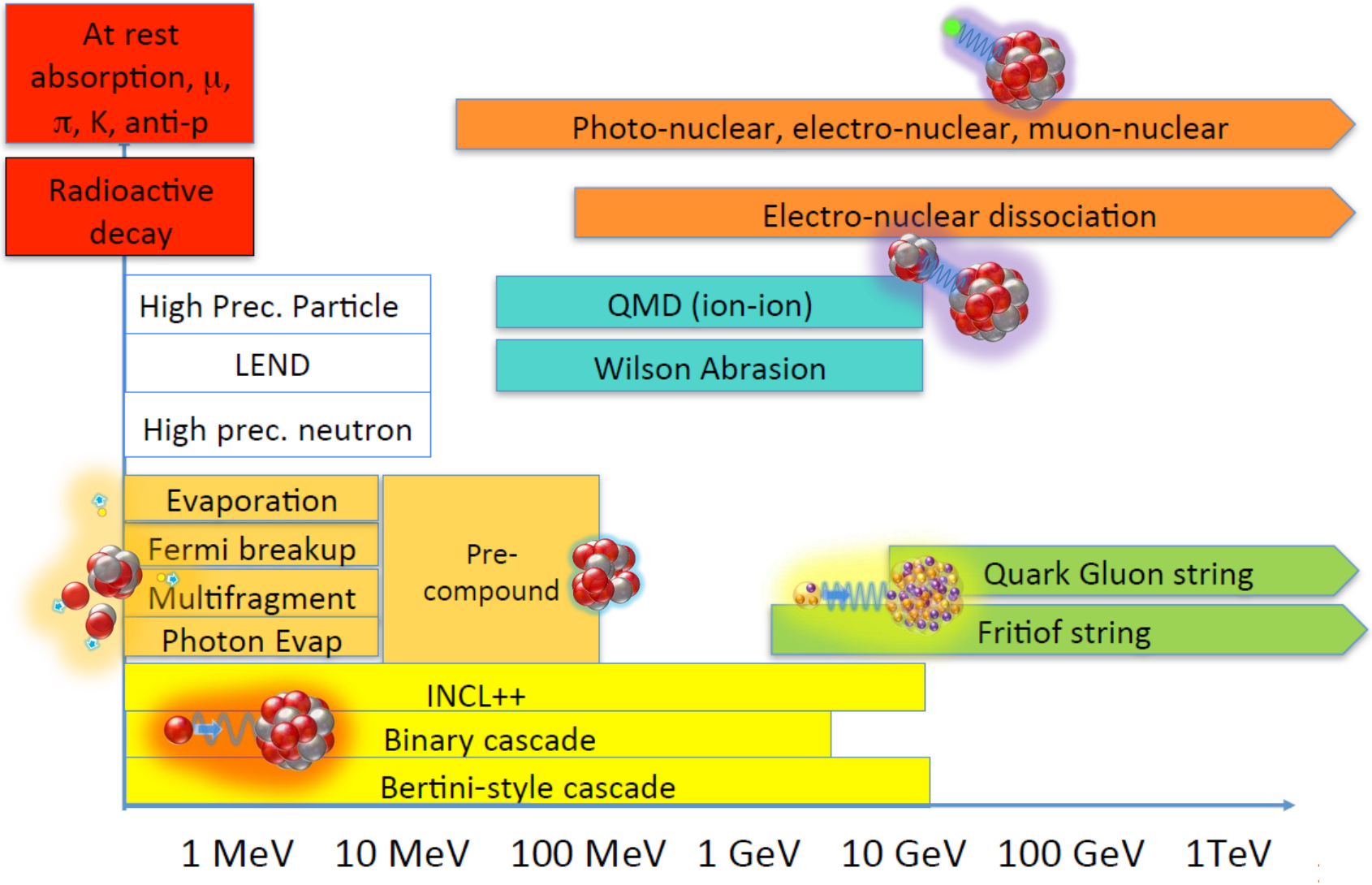


Available Inelastic Hadronic Cross Sections

- 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)

9

Partial Model Inventory



V.3 - HADRON ELASTIC

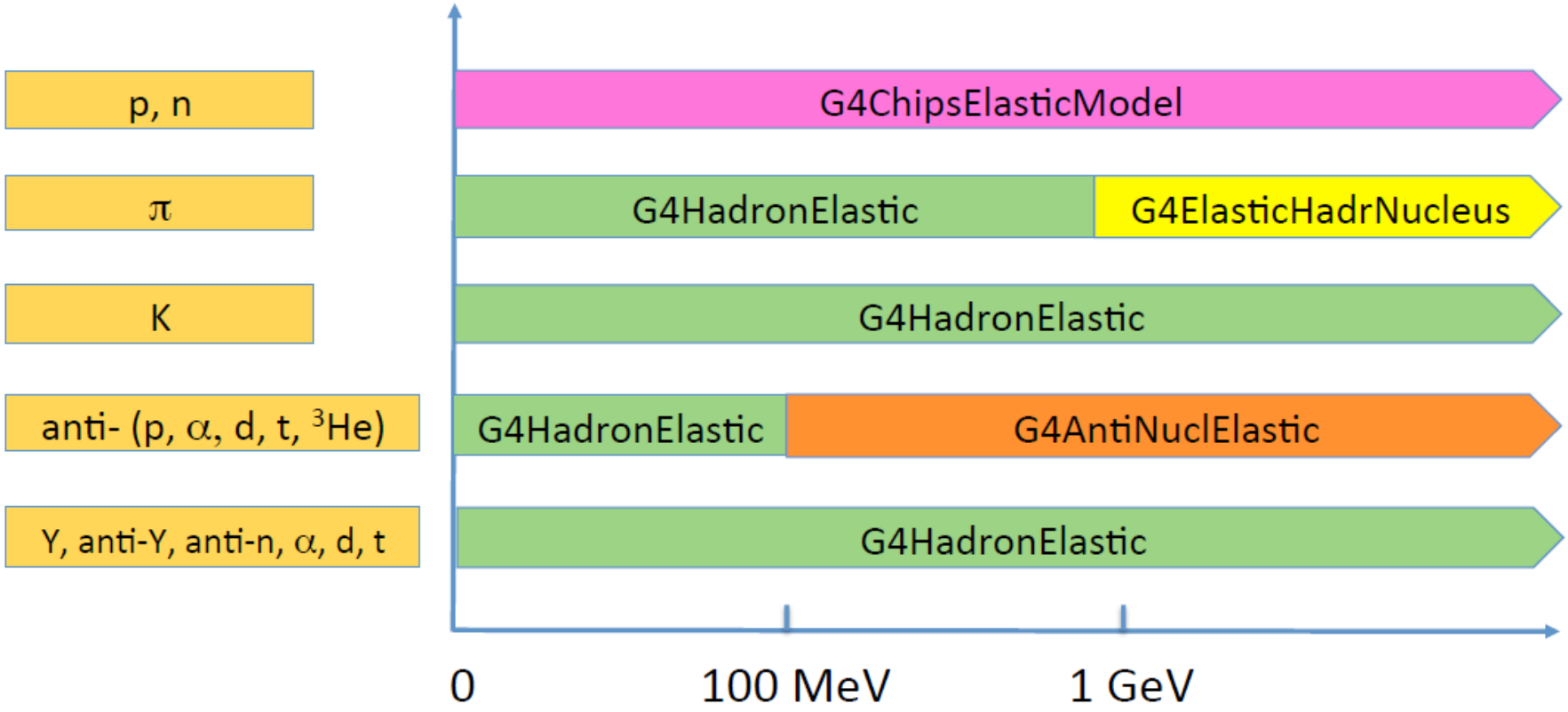
Elastic Process

- **G4HadronElasticProcess**
  - Displayed as « **hadElastic** » in « /tracking/verbose »
- **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:

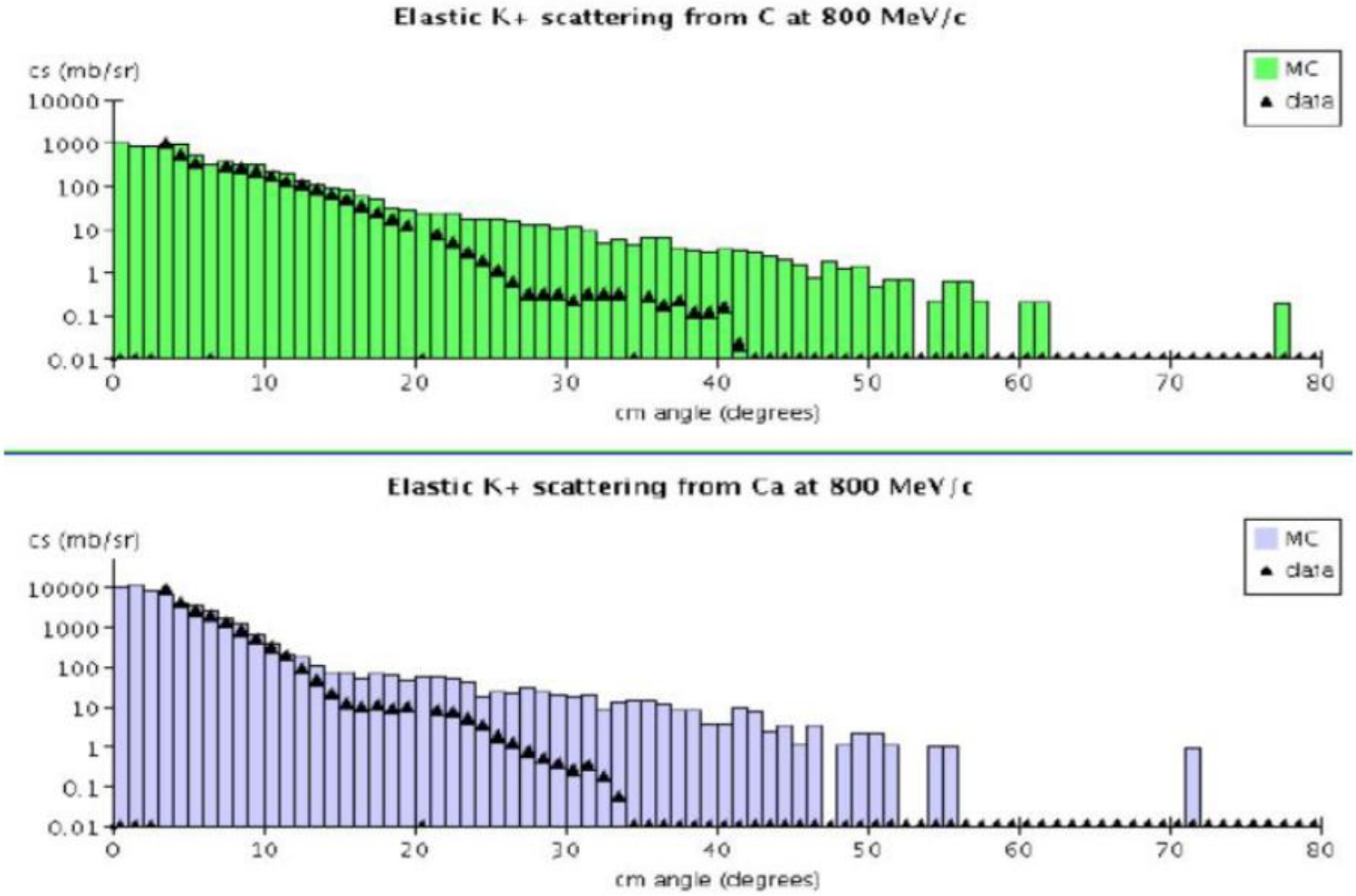
    (100*keV)*proton_production_cut_in_mm
  - Above this value, recoil nucleus is explicitely tracked

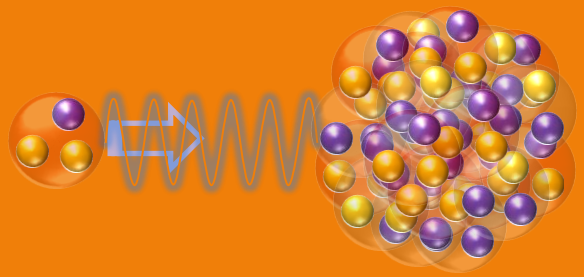
- **Cross-section:**
  - Geisha (parameterization) by **default** except for:
  - **protons & neutrons** : CHIPS (CHIral Invariant Phase Space)
  - **pions** : Barashenkov-Glauber-Gribov
  - **nuclei** : Barashenkov parameterization below 91 GeV and Glauber-Gribov above
  - **anti-nucleons and light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

Hadronic Models Implementing G4HadronElasticProcess



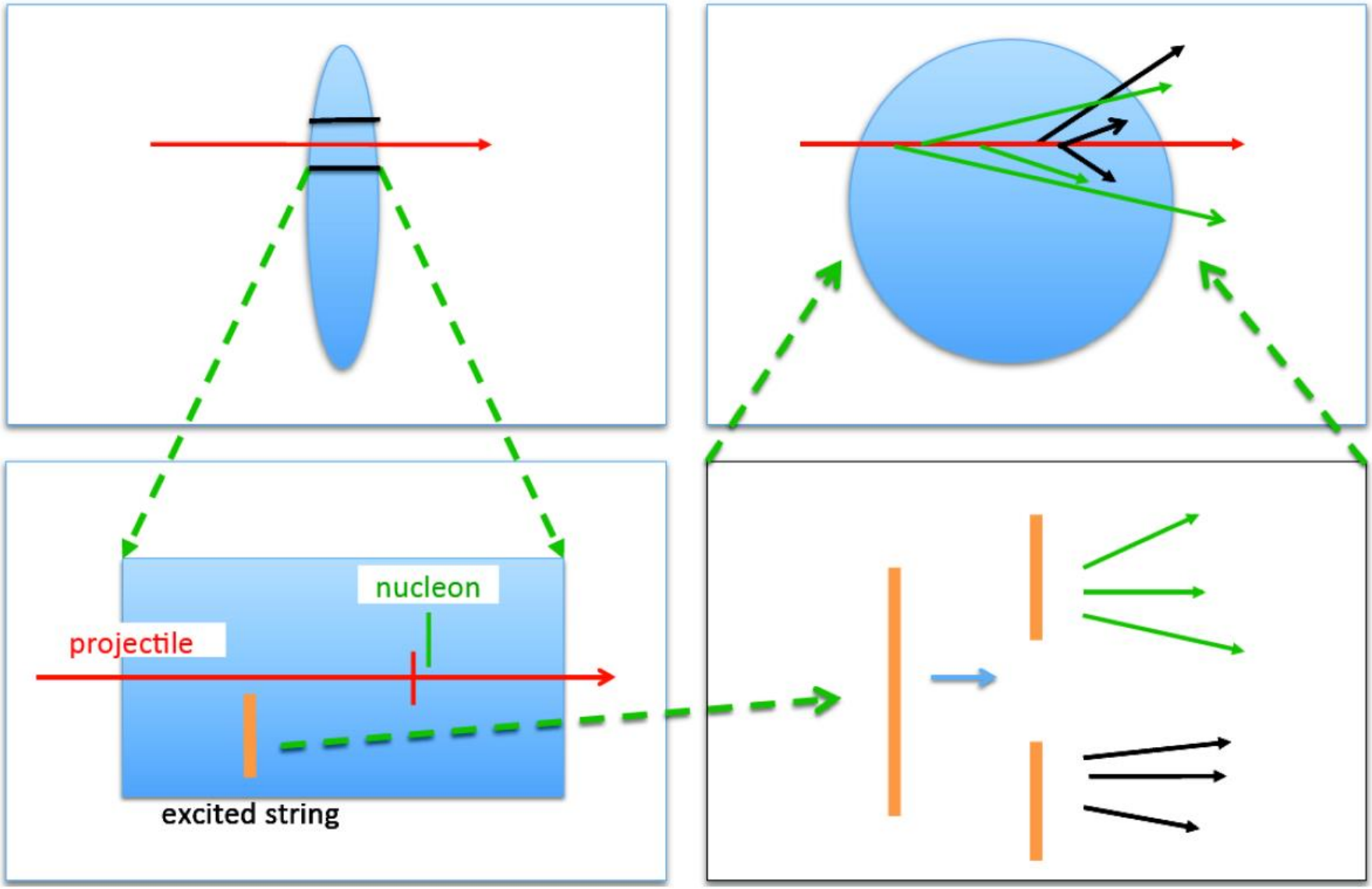
Elastic Scattering Validation (G4HadronElastic)





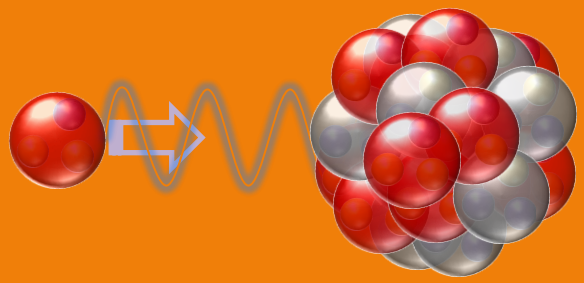
V.4 - HIGH ENERGIES : STRING MODELS

High-Energy Nuclear Reaction



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



V.5 - INTERMEDIATE ENERGIES : INTRA-NUCLEAR CASCADES

INTRA-NUCLEAR CASCADE MODELS

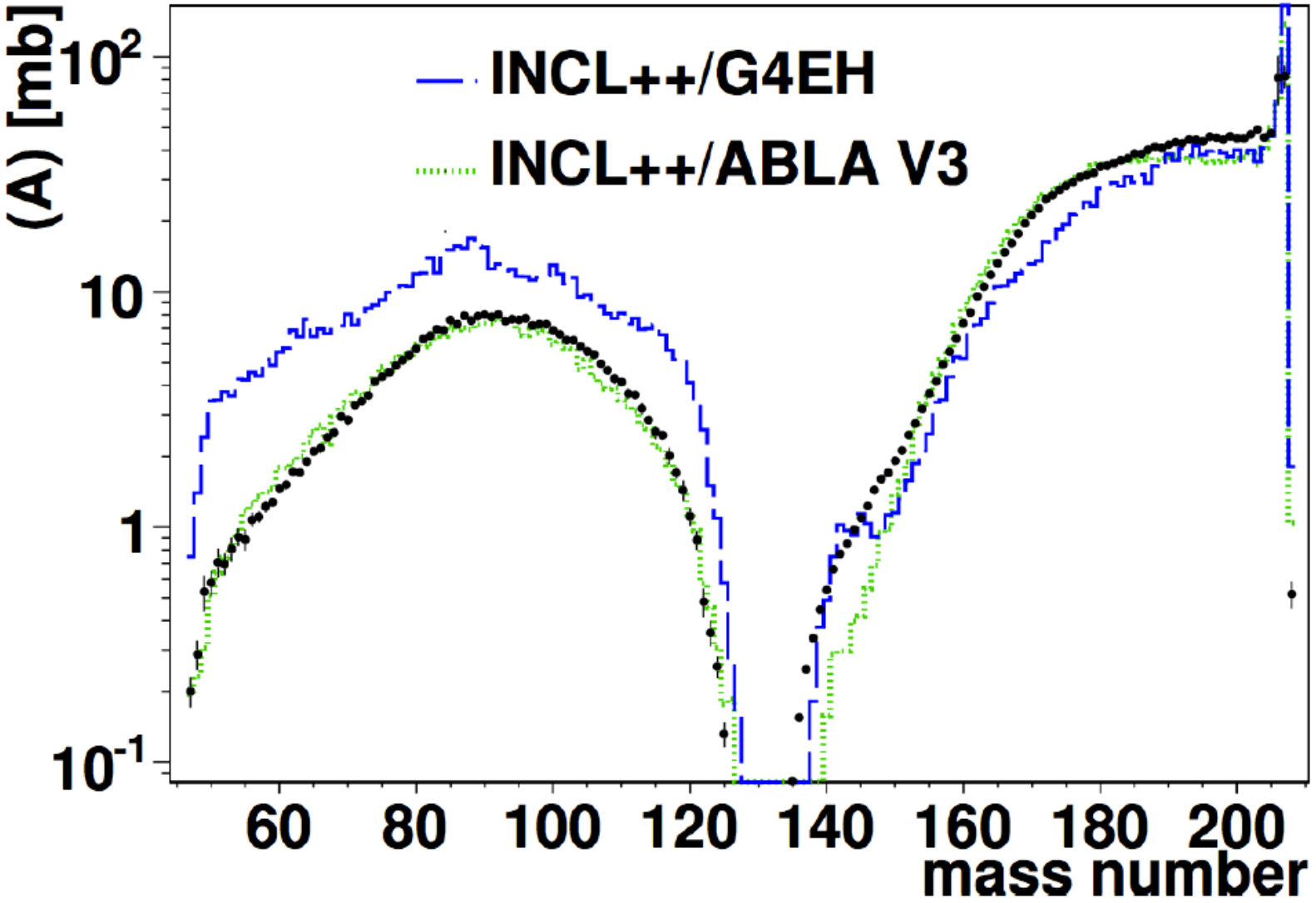
- Energies at which intra-nuclear cascade models are used are:
  - Too high for nuclear physics treatments
  - Too low for QCD
- Intra-nuclear cascade models use Monte Carlo techniques to propagate hadrons within the target nucleus
  - A “Monte Carlo within a Monte Carlo”
  - Indeed, one of the first application of Monte Carlo methods to nuclear interaction !
- Specific channels not produced:
  - No way to select a priori, in such a complicated treatment, a specific final state.
- The gross features of this modeling are:
  - The nucleus is a “bag of nucleons”, with ~ no binding energies
  - The incident particle (and descendants) interacts with these nucleons as if they were independent
- Then there are variations / modulations depending on the model

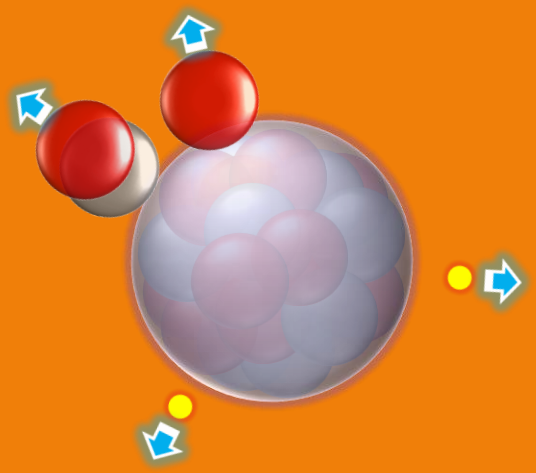
EXISTING CASCADE MODELS

- **Bertini:**
  - Earliest codes from the 1960s !
  - Non-quantum mechanical cascade
    - Average solution of particle traveling through a medium (Boltzmann equation)
  - Target nucleus modeled as 3 concentric shells
  - Valid for ~15 hadronic species, 0 – 10 GeV, and usable for gammas
- **Binary cascade model:**
  - Similar to Bertini but with improvments:
    - It's a time-dependent model
    - Hadron-nucleon collisions handled by forming resonances which decay according to their quantum numbers
    - Particles follow curved trajectories in smooth nuclear potential
  - Valid for p, n, 0 – 10 GeV, and π^+, π^-, 0 – 1.3 GeV
  - Extension to light ions
- **INCL++**
  - Similar to Binary except:
    - Smooth Woods-Saxon or harmonic oscillator potential
    - Particles travel in straight lines through potential
  - Valid for p, n, π, d, t, ^{3}He, α
    - Also works for projectile <= 12 on target 11 < A < 239
  - Good for spallation studies, and medical applications

Validation of INCL++ Model

Spallation residues from p + ^{208}Pb

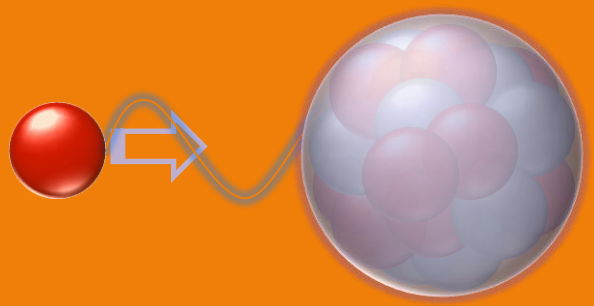




V.6 - NUCLEUS "COOLING DOWN" MODELS

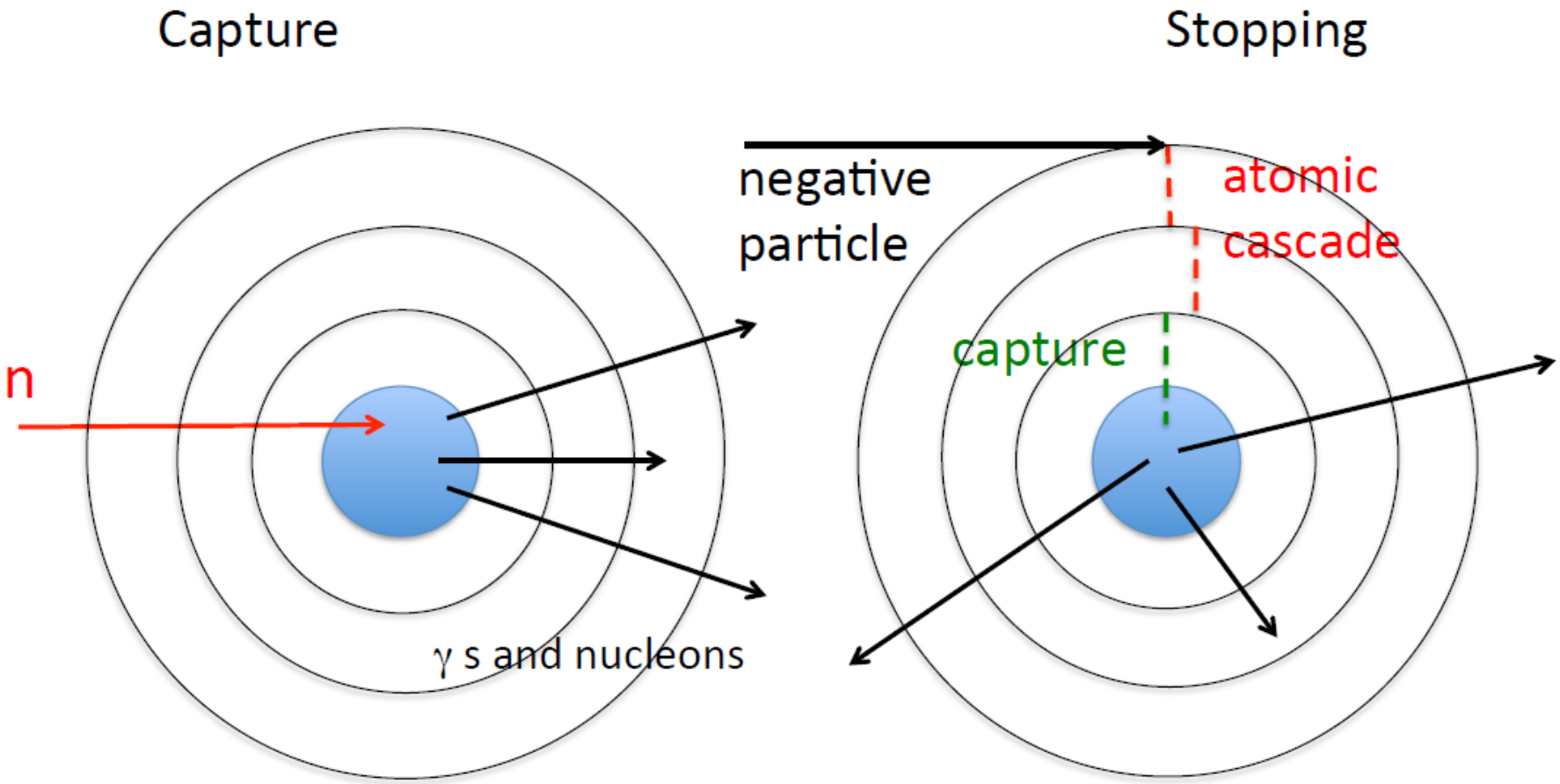
PRECOMPOUND & DE-EXCITATION MODELS

- **G4PrecompoundModel** used for:
  - Nucleon-nucleus interaction at low energy
    - Valid for p, n from 0 to 170 MeV
  - Nuclear de-excitation model in higher-energy codes
    - Takes a highly excited nucleus (set of particle-hole states) down to equilibrium energy, by emitting p, n, d, t, ^{3}He and α
    - **Once equilibrium is reached, 4 competitive de-excitation models can take over**
- **De-excitation models:**
  - Fermi break-up:
    - Full destruction of nucleus, leaving only p, n, t, α
    - Valid for A < 17 and high excitation energies
  - Multi-fragmentation:
    - Statistical breakup, with propagation of fragments in Coulomb field
    - For excitation energies E/A > 3 MeV
  - Fission:
    - Split excited nucleus, emits fission fragments + n
    - Valid for A > 65
  - Photon evaporation:
    - Usually final stage of de-excitation
    - Data-driven : uses ENSDF database
      - Up to hundreds of gamma levels for more than 2000 nuclides
    - Handles gamma cascades and electron emission



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

Capture and Stopping Models



STOPPED NEGATIVE PARTICLE MODELS

- Negative particles always end-up with a stopping process
- Stopped hadrons models:
  - Bertini cascade model used for negative pion, kaon and sigma
  - Fritiof model used for anti-proton and negative sigma
    - Usable as > 2 GeV in center of mass
  - Include atomic cascade, but no decay in orbit
- Negative muon models:
  - Atomic cascade with decay in orbit enabled
  - K-shell capture
  - Two models, which differ from de-excitation model

CAPTURE & FISSION MODELS

Capture:

- Neutrons and anti-neutrons never really stop
  - They keep having elastic scattering (“bouncing”)
    - Up to the point they are absorbed
  - Kinetic energy must be taken into account
- Models available:
  - G4NeutronRadCapture
    - All energies
  - G4ParticleHPCapture
    - For better precision below 20 MeV
  - G4AntiNeutronAnnihilationAtRest
    - Based on old GEISHA modeling

Fission processes & models:

- G4HadronFissionProcess is the process
- It can use two models:
  - G4ParticleHPFission
    - For neutrons < 20 MeV
    - Option to produce fragments or not
  - G4FissLib
    - Livermore spontaneous fission
    - Only produce neutron spectra by default
- Fragment production is an option:
  - See /example/extended/hadronic/FissionFragment

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)

Thermal Scattering

- Special treatment needed for 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));

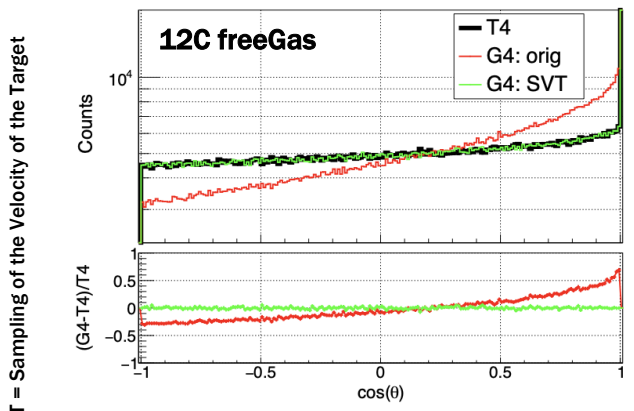
ParticleHP

- 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

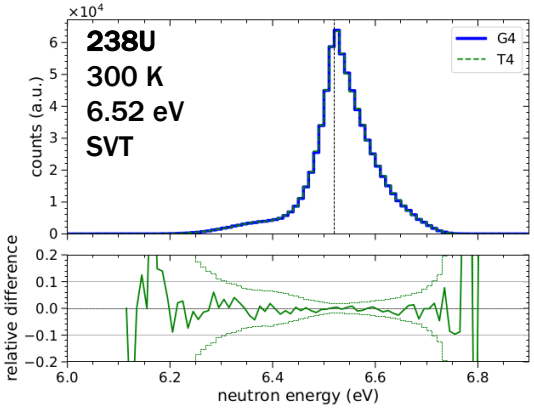
RENEWED NEUTRON TRANSPORT !

- An **in depth** revision of the low energy neutron transport was started~2-3 years ago, by neutron experts who joined Geant4
  - Revision of the existing
  - Additions in transport treatment

Doppler Broadening of elastic kernel for light & heavy nuclei



L. Thulliez, C. Jouanne, E. Dumonteil, Improvement of Geant4 Neutron-HP package: From methodology to evaluated nuclear data library, Nucl. Instrum. Meth. Phys. Res. Sec. A, Volume 1027, 2022, 166187, ISSN 0168-9002, https://doi.org/10.1016/j.nima.2021.166187 (arXiv:2109.05967)



M. Zmeškal, L. Thulliez, E. Dumonteil, Improvement of Geant4 Neutron-HP package: Doppler broadening of the neutron elastic scattering kernel, Annals of Nuclear Energy, Volume 192, 2023, 109949, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2023.109949 (arXiv:2303.07300)

- Now Geant4 is on-par with MCNP6.2 and Tripoli-4® !

V.9 – RADIOACTIVE DECAYS

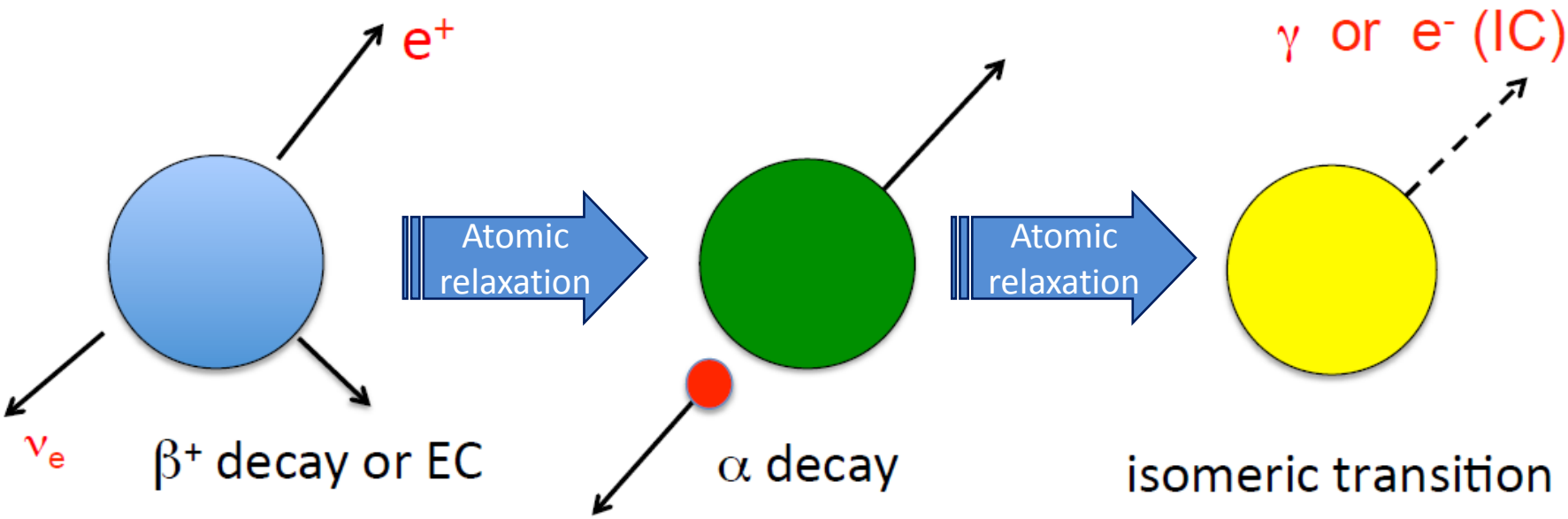
RADIOACTIVE DECAY

- Process to simulation radioactive decay of nuclei
  - At rest
  - In flight
- Decay modes implemented / 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 + 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

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

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 );
```

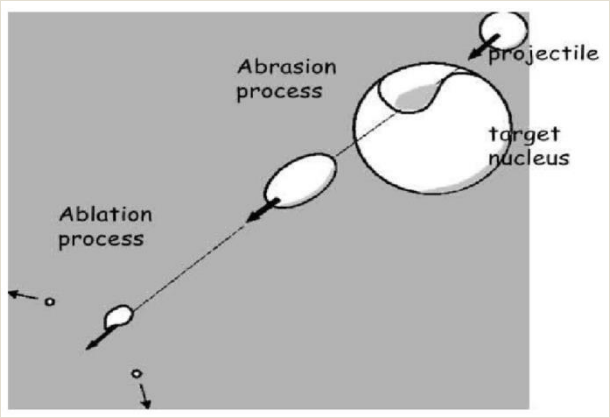
  - Or code in in your own physics list (more for experts):

```
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 MODELS [1/2]

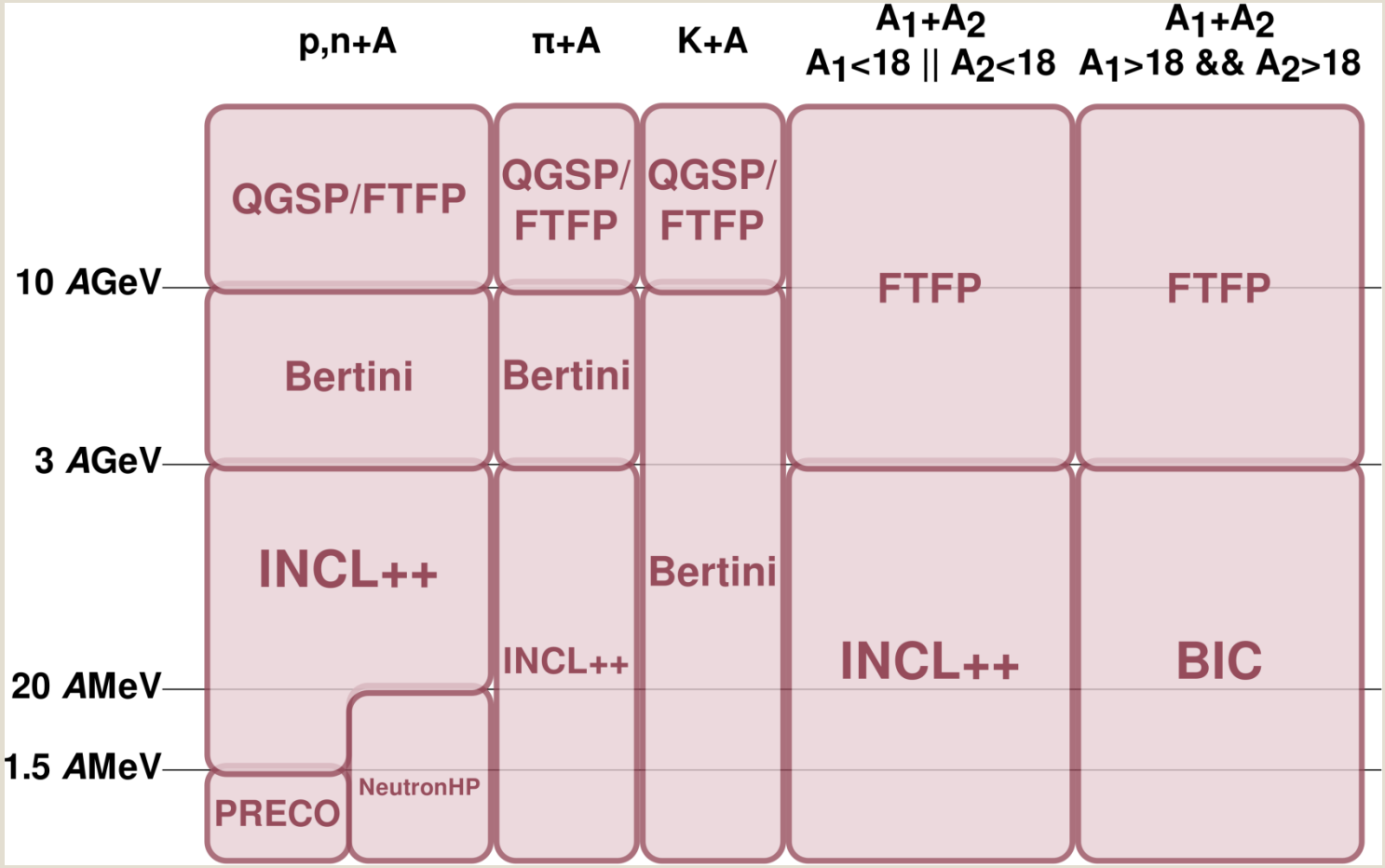
- G4BinaryLightIon
  - Same G4BinaryCascade, extended to light ions
- G4WilsonAbrasion & G4WilsonAblation
  - Simple model of nucleus-nucleus collisions
  - Largely based on geometrical arguments
  - Faster than binary and QMD, but less detailed
  - Based on NUCFRG2 model (NASA TP 3533)
  - Valid up to 10 GeV/nucleon



- G4EMDissociation
  - When two high-Z nuclei get close, the EM field can be so strong that nucleus fragments are ejected
  - Useful in relativistic nucleus-nucleus collision with high Z
  - Usable up to 100 TeV
- INCL++
  - INCL++ cascade mentioned before
  - True potential used for target, not for projectile, but binding energies are taken into account
  - For projectile <= 18 on target 18 < A < 239
- FTF
  - FTF can treat ion-ion collision above 3 GEV/n

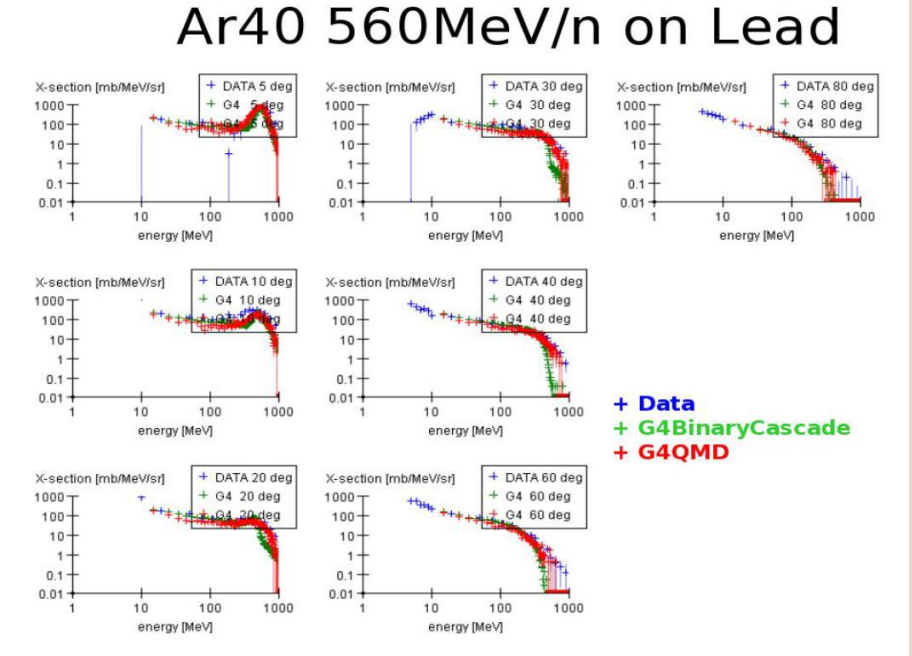
MAP OF MODELS SO FAR

COURTESY OF INCL PEOPLE



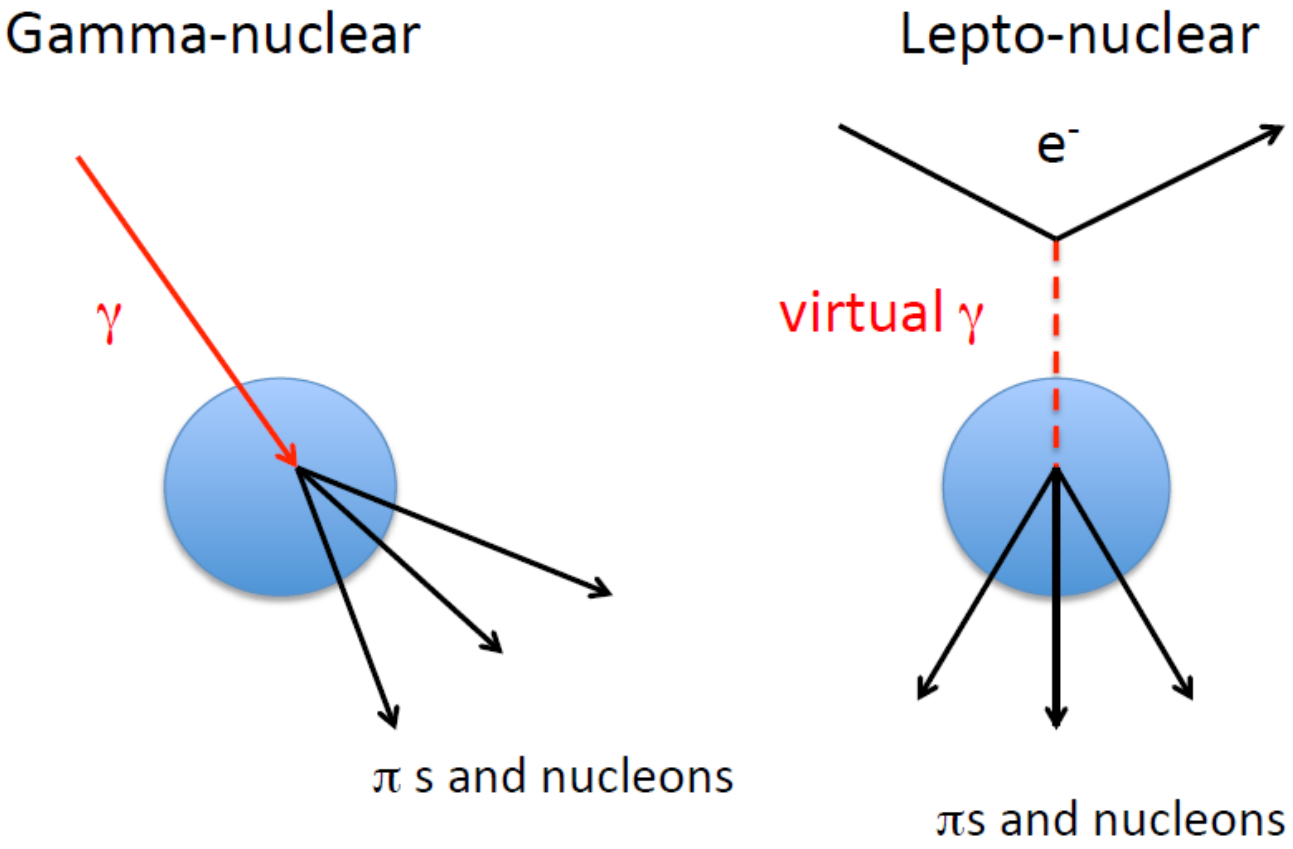
QMD MODEL

- QMD (Quantum Molecular Dynamic) Model is probably the most precise, but also most CPU intensive model
- Overcomes some of the limitations of the binary cascade:
  - Is an extension of the classical molecular dynamic model
  - Treats each nucleon as a gaussian wave packet
  - Propagation takes into account Pauli principle
  - Can be used for high energy, high Z collisions



V.11 - GAMMA- & LEPTO-NUCLEAR

Gamma- and Lepto-nuclear Models



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_γ < 10 GeV, direct interaction with nucleus using Bertini cascade
  - For E_γ > 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.