



**GEANT4**  
A SIMULATION TOOLKIT  
Version 11.2



## Hadronic Physics 2

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11<sup>th</sup> International Geant4 Tutorial in Korea,

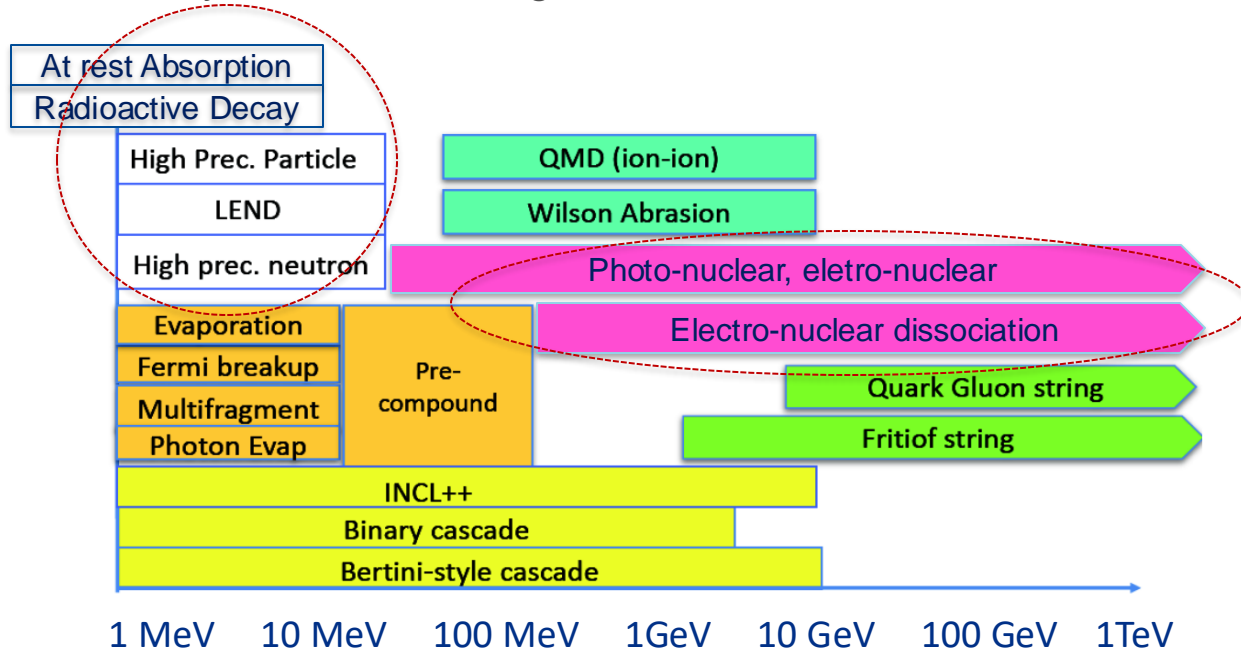
Aug 19-23, 2024@YonSei Univ., Wonju

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- Low energy hadronic models
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- Radioactive decay, capture, stopping and fission
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- Special topics
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  - Variation of model parameters
  - Validation portal (geant-val)

# Low Energy Hadronic Models

- High precision neutron packages (thermal energies to ~20 MeV)
- Radioactive decay at rest and in-flight

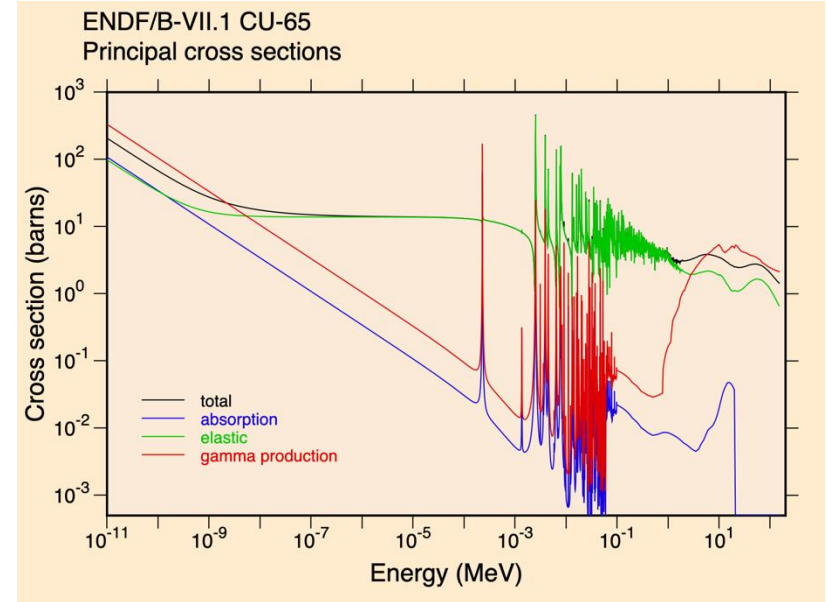


- $\gamma$  and  $e^\pm(\mu^\pm)$  induced nuclear reactions (~10 MeV - ~TeV)

# Low Energy Hadronic Models

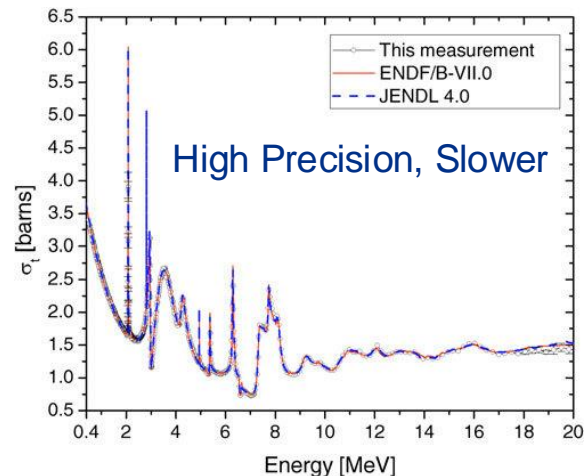
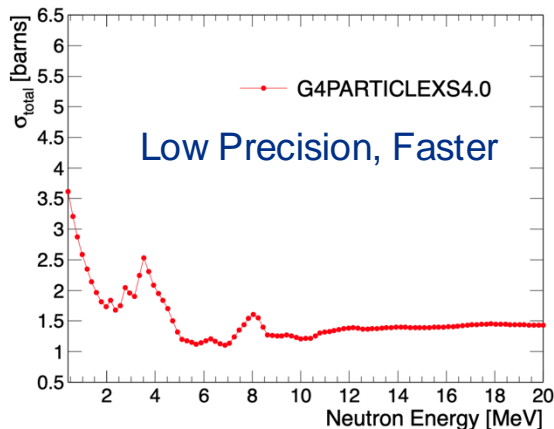
- Geant4 provides several low energy hadronic models, especially for treating neutron interactions in detail
  - At energies below 20 MeV, cross sections are sensitive to nuclear structure and specific isotope
  - Neutrons are dominant at low energy and undergo mostly elastic scattering until they are thermalized or capture by a nucleus,  $n + X(A, Z) \rightarrow X(A+1, Z) + \gamma$ 's
- Low energy models for elastic, inelastic, capture and fission (mostly depends on ENDF/B-VII data)
  - High precision neutron (Neutron HP)
  - Low energy neutron data (LEND/Livermore)
  - Low energy charged particles (Particle HP)

- Cross sections: neutron + Cu from ENDF/B-VII data base



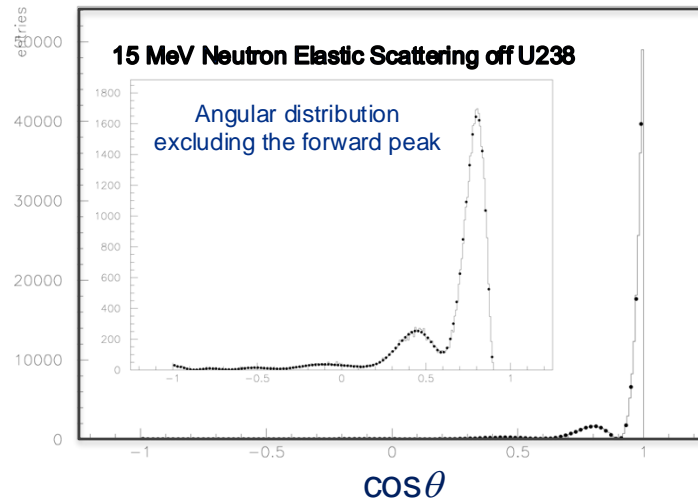
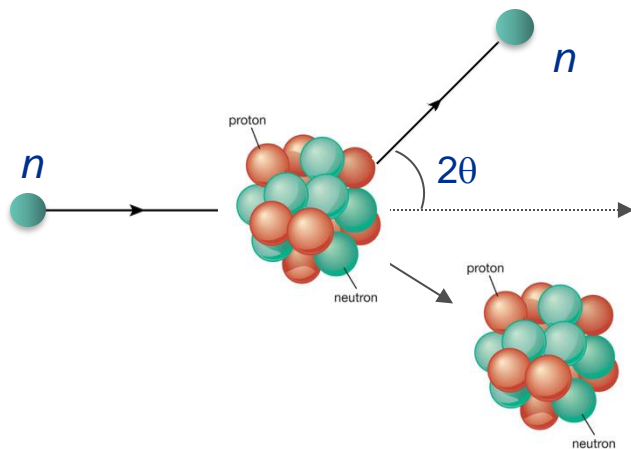
# NeutronHP: High Precision Neutron

- Data (G4NDL) driven model which includes both **cross sections** and **final states**
  - **Isotope dependent data** for elastic, inelastic, capture and fission with the G4NDL format
  - Including models that handle thermal scattering from chemically bounded atoms
  - G4NDL (Geant4 Neutron Data Library) based on ENDF/B-VII database: in Geant4 11.2 export `G4NEUTRONHPDATA=${G4DATA}/G4NDL4.7`
  - Cross section comparison between Bertini and neutron HP



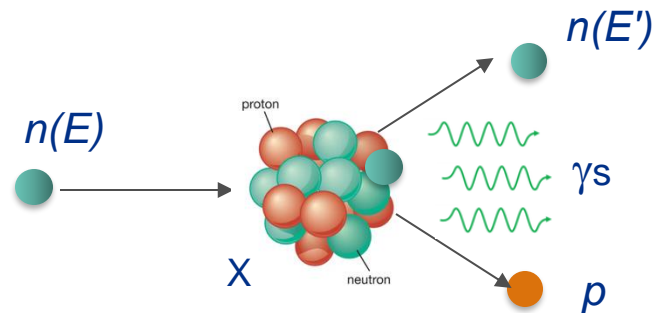
- G4NeutronHPElastic handles sampling differential cross section,  $d\sigma(E, \cos\theta)/d\Omega$  for elastic scattering of neutrons and recoiled nucleus generated as the final state
  - Interpolates between points in cross section tables as a function of **energy** or interpolates between Legendre polynomial coefficients to get the **angular distribution** as a function of energy

$$\frac{2\pi}{\sigma(E)} \frac{d\sigma}{d\Omega}(\cos\theta, E) = \sum_{l=0}^{n_l} \frac{2l+1}{2} a_l(E) P_l(\cos\theta)$$



- Currently supports 34 inelastic final states and gammas (discrete and continuum)

- $n + X(A, Z) \rightarrow X(A, Z) + n \gamma$ s
- $n + X(A, Z) \rightarrow X(A-1, Z-1) + n p$
- $n + X(A, Z) \rightarrow X(A-3, Z) + n n n n$
- $n + X(A, Z) \rightarrow X(A-4, Z-2) + d t$
- ...



- Production cross section for  $n$ : 
$$\sigma_n(E, E', \cos(\theta)) = \sigma(E) Y_n(E) p(E, E', \cos(\theta))$$

- $Y_n(E)$  is the product multiplicity,  $p(E, E', \cos(\theta))$  is the distribution probability

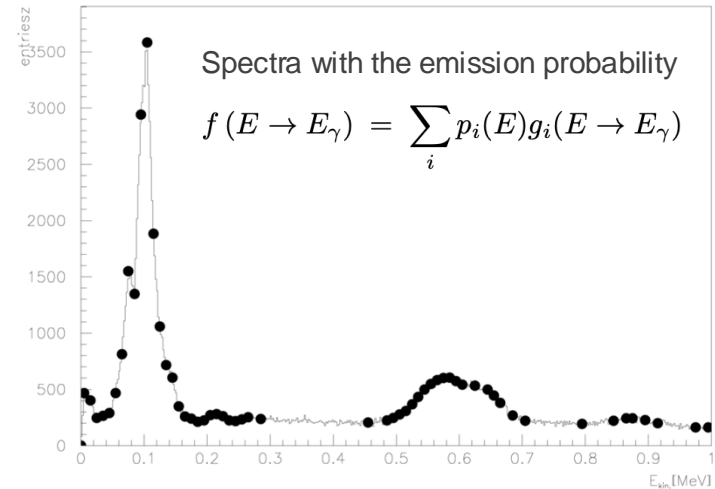
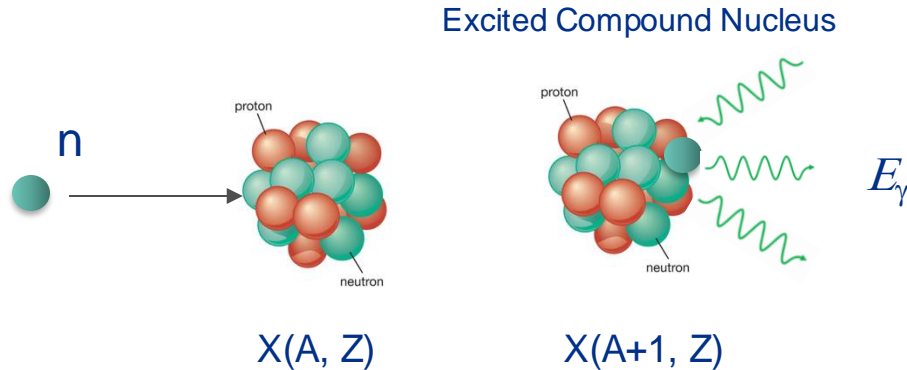
- Secondary distribution probabilities

- Isotropic emission
- Discrete two-body kinematics and N-body phase space
- Continuum energy-angle distributions (in lab and CM)

# NeutronHP: Radiative Capture

- Neutrons are captured by a nucleus and emit gamma rays (unique for each isotope)
  - Can turn stable materials into radioactive ones, neutrons can be used to create certain important radionuclides such as molybdenum-99, used in medical imaging, or cobalt-60, used in cancer treatment.
- The final state of radiative capture (unique for each isotope) is described by
  - Photon multiplicities,
  - Photon energy spectra
  - Angular distributions of the emitted photons

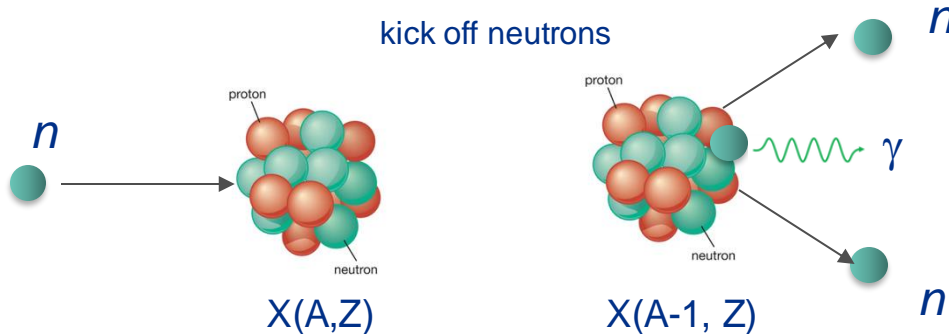
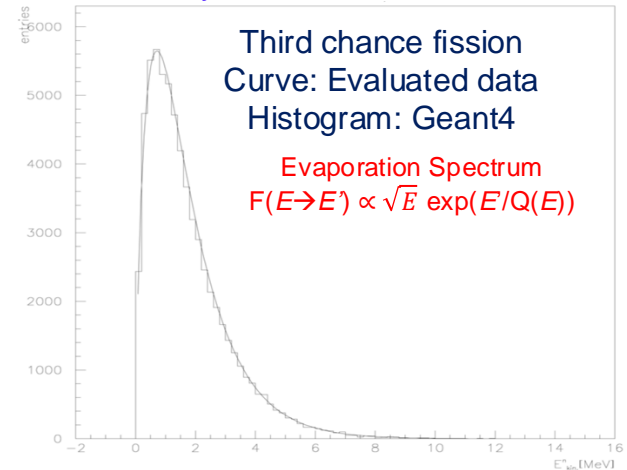
Photon energy distributions for radiative capture of 15 MeV neutrons on U238



# NeutronHP Fission (Neutron induced fission)

- $n + X(A, Z) \rightarrow X(A-i) + (i+1) n + \Delta m$  where  $\Delta m \rightarrow \Delta E \rightarrow$  gamma rays  $\rightarrow$  evaporation spectrum  
 $\Delta E = f(E \rightarrow E') = f(E'/Q(E))$  where  $Q$  is the effective temperature (tabulated function of  $E$ )
- High Precision model based on Evaluated Nuclear Data Files (ENDF) for induced fission reaction of neutrons below 20 MeV (cross sections, final states)  $\rightarrow$  G4NDL
- Emits neutrons and gammas but no nuclear fragments
  - Neutron multiplicities and evaporation spectra (gamma energy)
  - Angular distributions of the emitted photons and neutrons

Neutron energy distribution of induced fission by 15 MeV neutrons on U238



# Neutron Thermal Scattering

- To describe scattering of thermal neutrons (kinetic energy  $< 4$  eV)
  - Coherent (directional)
  - Incoherent (uniform)
  - Inelastic
- G4NDL4.7 (JEFF-3.3 and ENDF/B-VIII-0) includes thermal neutron scattering data (cross sections and final states for ~30 materials)
- Geant4 description is based on the Thermal Scattering Law (TSL) and relies both on experimental measurements and molecular dynamics calculations
  - see examples/extended/hadronic/Hadr04
- HP physics lists by default do **not** include thermal scattering models. To enable

```
G4VModularPhysicsList *physicsList = new FTFP_BERT_HP();  
physicsList->RegisterPhysics(new G4ThermalNeutrons());  
runManager->SetUserInitialization(physicsList);
```

# LEND (Low Energy Neutron Data) Models

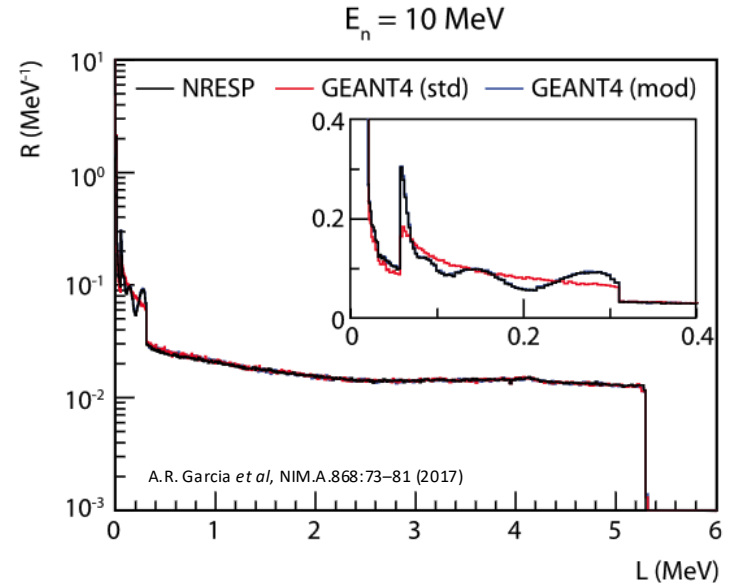
- The Livermore neutron models as an alternative to the HP models (hadronic/models/lend)
  - Use Generalized Nuclear Data (GND) which is a modern format for storing nuclear data (faster)

	Model Name	Cross Section
Capture	G4LENDCapture	G4LENDCaptureCrossSection
Elastic	G4LENDElastic	G4LENDElasticCrossSection
Inelastic	G4LENDInelastic	G4LENDInelasticCrossSection
Fission	G4LENDFission	G4LENDFissionCrossSection

- How to get and use the G4LENDATA dataset (neutrons and gammas):
  - go to <ftp://gdo-nuclear.ucllnl.org> and select G4LEND\_GND1.3, then LEND\_GND1.3\_ENDF.BVII.1.tar.gz
  - export G4LENDATA=/path/to/LEND\_GND1.3\_ENDF.BVII.1
- Invocation in physics list: add *G4NeutronLENDBuilder* into *G4NeutronBuilder*
  - See an example in *G4HadronPhysicsShielding*

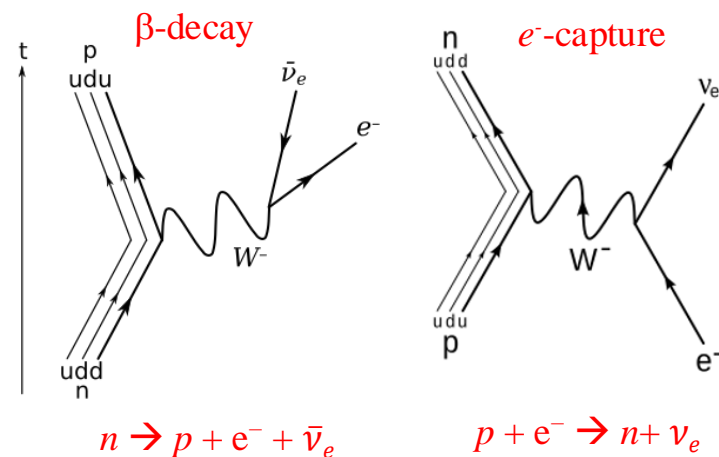
# Low Energy Charged Particles: G4ParticleHP

- G4ParticleHP models simulate the interactions of **proton, d, t, <sup>3</sup>He, α** as well as **neutrons**
  - Elastic, inelastic, capture and fission
  - Mostly below 20 MeV for *n*
  - 0 < E < 200 MeV for charged particles
  - Depends on large database (ENDF/B-VII)
  - Alternative DBs: TENDL, IAEA medical, IBANDL
- Planned to consolidate with NeutronHP
- Verification of **G4ParticleHP**
  - Good comparisons so far with MCNP
  - **G4ParticleHPInelasticCompFS**: Comparison of neutron response functions calculated with NRESP MC (two mechanisms) by the amount of scintillation light *L* produced by secondary charged particles



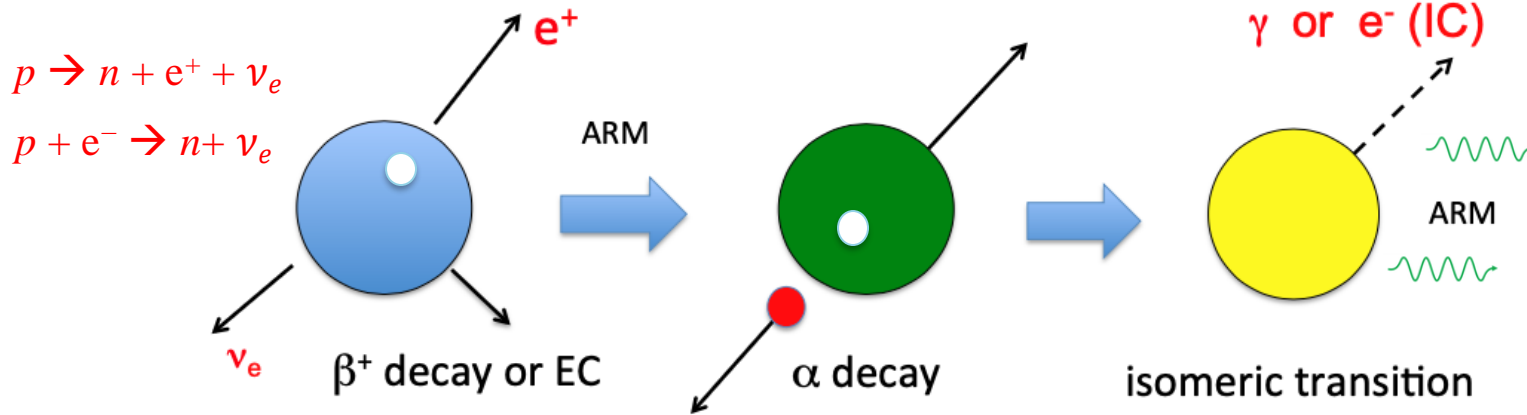
# Radioactive Decay, Capture, Stopping and Fission

- Simulation of radioactive nuclei decays by  $\alpha$ ,  $\beta$  emission or electron capture based on ENSDF (Evaluation of Nuclear Structure Data File  $\rightarrow$  [G4RADIOACTIVEDATA](#)) which provides
  - Half lives, nuclear level structure for parent and daughter nuclides, decay branching ratios, energy of decay process
  - Currently 2830 nuclides (A, Z), including meta-stable states (isomers,  $\sim 3500$ ) with lifetime  $> 1$  ns
  - export `G4RADIOACTIVEDATA=${G4DATA}/RadioactiveDecay5.6`
- Processes to simulate radioactive decays of nuclei
  - In-flight
  - At rest
- Alpha Decay:  $N(Z, A) \rightarrow \alpha + N(Z-2, A - 4)$
- Beta Decay:  $N(Z, A) \rightarrow \beta + \bar{\nu}_e + N(Z+1, A)$
- Electron Capture:  $N(Z, A) + e^- \rightarrow N(Z-1, A) + \bar{\nu}_e$



# Radioactive Decay Chains

- Nuclides with lifetime  $< 1$  ps decay immediately
- Typically, the radioactive decay process triggers a chain of decays, as, for instance



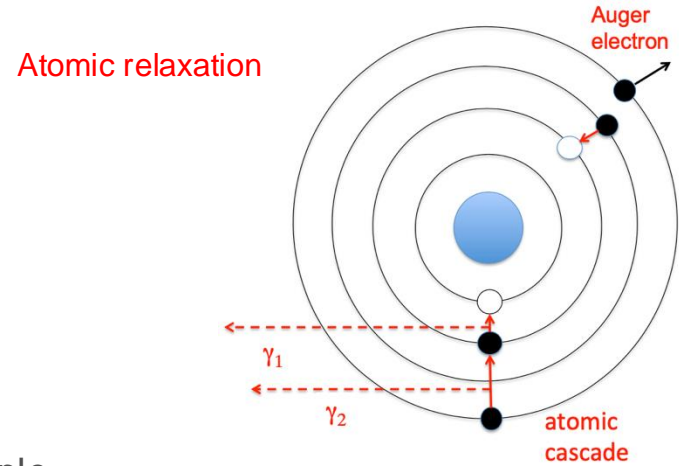
(EC: Electron Capture, IC: Internal Conversion, ARM: Atomic Relaxation Model)

- If daughter of nuclear decay is an isomer, deexcitation is done by using [G4PhotonEvaporation](#)
  - Uses ENSDF files with all known gamma levels for 3110 nuclides (PhotonEvaporation5.7)
  - Internal conversion is enabled as a competing process to gamma de-excitation

# Atomic Relaxation and Gamma (or Electron) Emission

- Electron shell configuration may change after decay → Atomic relaxation model
- Option to enable atomic relaxation after decay
  - Atomic cascade (Inner holes filled by atomic cascade)
  - Auger
  - Fluorescence
- Using `G4RadioactiveDecay`
  - Can be accessed with messengers (biasing options, etc.)
  - How to put `G4RadioactiveDecay` in your physics list: example

```
G4RadioactiveDecay* rDecay = new G4RadioactiveDecay;  
G4PhysicsListHelper* plh = G4PhysicsListHelper::GetPhysicsListHelper();  
rDecay->SetICM(true); // internal conversion  
rDecay->SetARM(true); // atomic relaxation  
plh->RegisterProcess(rDecay, G4GenericIon::G4GenericIon());
```



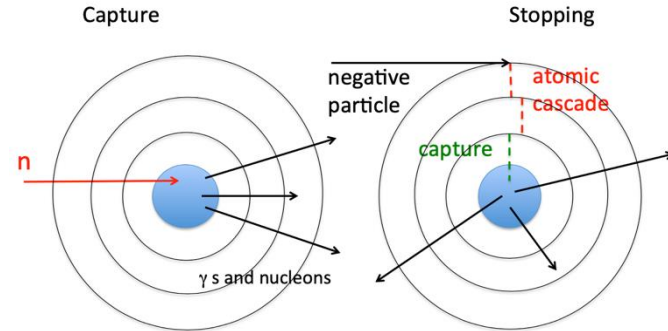
- Set environment variables to point to `RadioactiveDecay5.6` and `PhotonEvaporation5.7`

# Capture and Stopping Models

- Neutrons, anti-neutrons never really stop, they just slow down from elastic scattering or are absorbed  $\rightarrow$  kinetic energy must be taken into account

## • *G4NeutronCaptureProcess*

- In-flight capture for neutrons
- Model implementations:
  - *G4NeutronHPCapture* (below 20 MeV)
  - *G4NeutronRadCapture* (all energies)



- Negatively charged particles can be captured by a nucleus

## • *G4HadronStoppingProcess*

- *G4HadronicAbsorptionBertini* ( $\pi^-$ ,  $K^-$ ,  $\Sigma^-$ , hadronic absorption at rest using the Bertini cascade)
- *G4HadronicAbsorptionFritiof* ( $\bar{p}$ ,  $\bar{\Sigma}^+$ , hadronic absorption at rest using FTF/Preco)
- *G4MuonMinusCapture* (atomic cascade with decay in orbit, nuclear capture with the Bertini cascade)

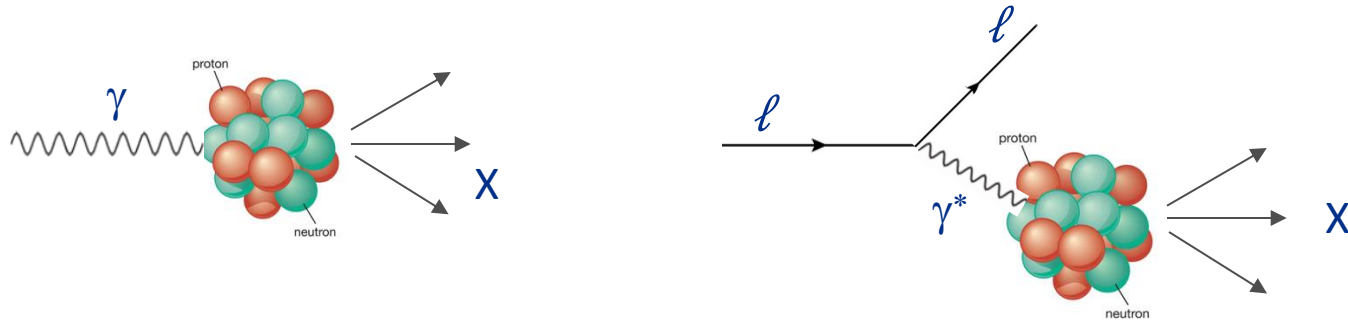
# Fission Processes and Models

- Many hadronic models already include fission implicitly
  - Included in nuclear de-excitation code
  - In that case, don't add fission process to physics list → double counting
  - Usually only needed in special cases
- *G4NeutronFissionProcess* handles neutron-induced fission of nuclei
  - *G4NeutronHPFission* (*G4ParticleHPFission*)
    - Specifically for neutrons below 20 MeV
    - Fission fragments produced if desired
  - *G4FissionLibrary*: Livermore Spontaneous Fission (*G4LLNLFission*)
    - Handles spontaneous fission as an inelastic process
    - No fission fragments produced, just neutron spectra
  - *G4LENDFission*: Low Energy Neutron Data Fission (*G4LENDModel*)

# Gamma- and Lepto-nuclear Processes

# Gamma- and Lepto-nuclear Processes

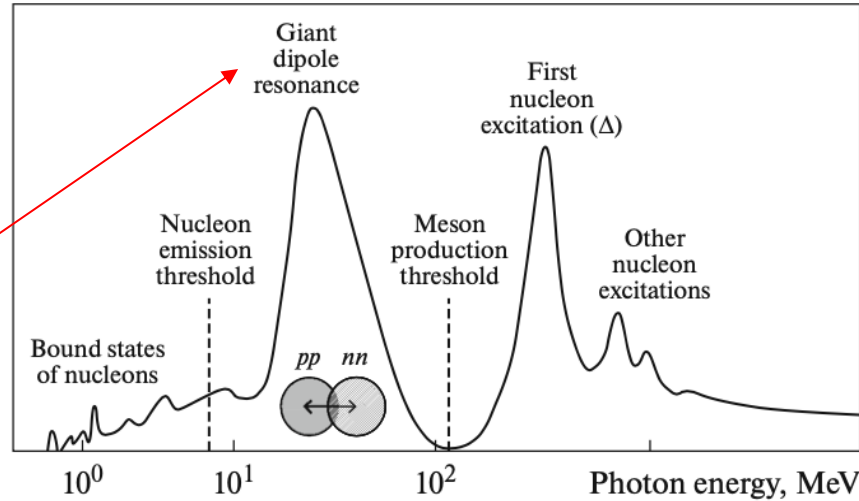
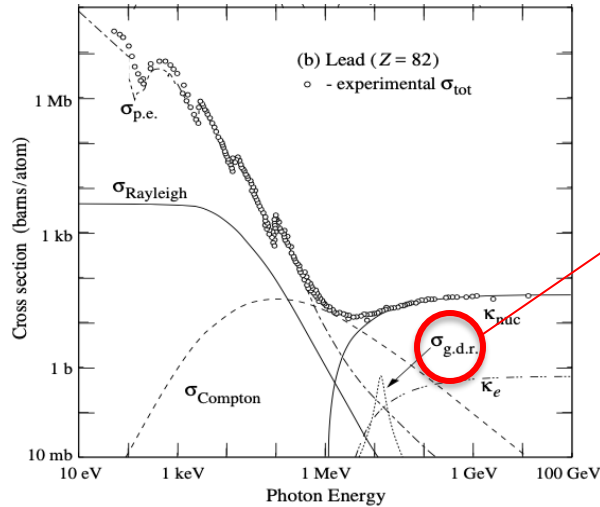
- Geant4 supports direct interactions of photons, electrons and muons with nucleus above the hadron production threshold:  $\gamma$  ( $e^\pm$ ,  $\mu^\pm$ ) + nucleus  $\rightarrow$  X



- These processes are in [G4EmExtraPhysics](#) (physics constructor) which is a part of the default physics list `FTFP_BERT`
  - [G4HadronInelasticProcess](#)("photonNuclear", G4Gamma::Gamma()) : QGS, Bertini, (LEND) models
  - [G4ElectronNuclearProcess](#): electro-nuclear model ([G4ElectroVDNuclearModel](#))
  - [G4PositronNuclearProcess](#): electro-nuclear model ([G4ElectroVDNuclearModel](#))
  - [G4MuonNuclearProcess](#): muon-nuclear models ([G4MuonVDNuclearModel](#))

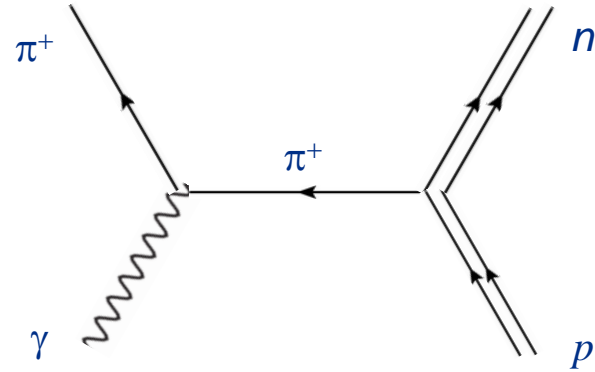
- At low energies they are absorbed and excite the nucleus as a whole
- Giant dipole resonance (GDR) region (10 - 30 MeV)
- $\Delta$  region between pion threshold to 450 MeV
- At high energies, they act like hadrons ( $\pi$ ,  $\square$ ) and form resonances with protons and neutrons

I. M. Kapitonov DOI: 10.3103/S0027134923030116



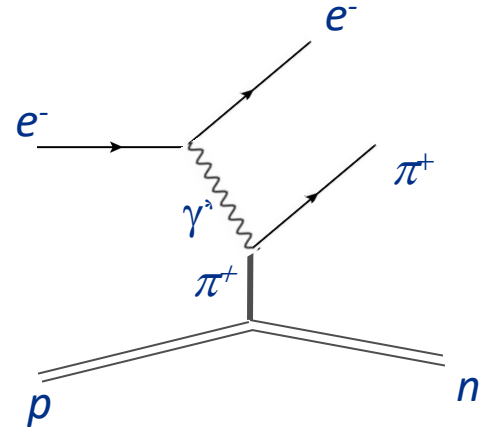
# Gamma-nuclear interactions

- Cross section
  - Parameterization of experimental data from M. Kossov
  - Photonuclear data by IAEA below 140MeV
  - (Optionally) LEND gamma cross section below 20 MeV
- Final state models (two models)
  - Bertini (200 MeV – 3 GeV)
  - QGSP (3 GeV – 100 TeV)
  - Optional
    - Precompound/de-excitation (below 200 MeV)
    - LEND (20MeV)



# Lepto-nuclear interactions

- Electrons and muons interact hadronically through **virtual photons**
  - Electron or muon passes by a nucleus and exchanges virtual photon
  - Virtual photon then interacts directly with nucleus (or nucleons)
- Cross sections
  - $e^\pm$  parameterization of experimental data from M. Kossov
  - $\mu^\pm$  by theoretical computation from Kokoulin
- Final state models (two models)
  - *G4ElectroVDNuclearModel* and *G4MuonVDNuclearModel*
    - $e^\pm$  cross section and  $\mu^\pm$  cross section, respectively
    - Weizsacker-Williams conversion of virtual to real gamma
    - For  $E_\gamma < 10$  GeV, direct interaction with nucleus using the Bertini cascade
    - For  $E_\gamma > 10$  GeV, conversion of  $\gamma$  to pions, then interaction with nucleus using the FTFP model



# Special Topics

- FLUKA
  - A general purposed tool for calculations of particle transport and interactions with matter
  - Covering an extended range of applications spanning from proton and electron accelerator shielding to target design, calorimetry, activation, dosimetry, detector design, neutrino physics, radiotherapy etc.
  - Comparison with Geant4 has not been trivial, mostly due to having to re-write geometry, materials, fields
- Geant4-FLUKA.CERN interface since Geant4 11.2
  - Provide the new interface to get inelastic cross sections and final-states from Fluka-Cern
  - Use a custom FTFP\_BERT Physics List that replaces the [G4HadronPhysicsFTFP\\_BERT](#) constructor with [FLUKAHadronInelasticPhysicsConstructor](#)

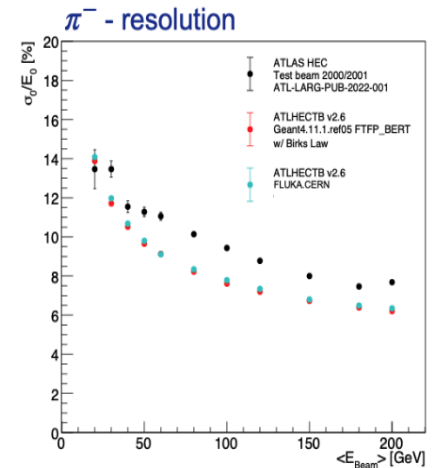
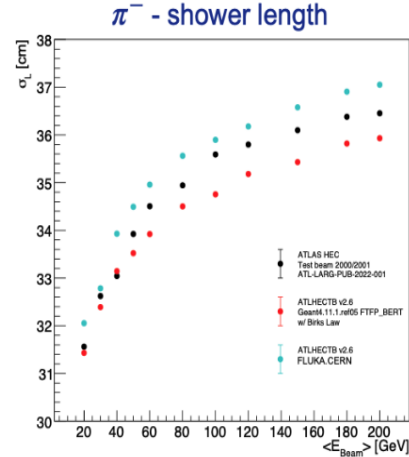
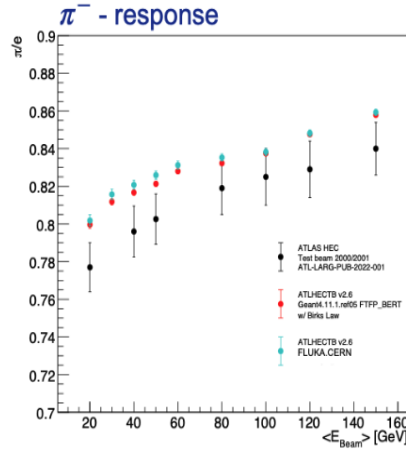
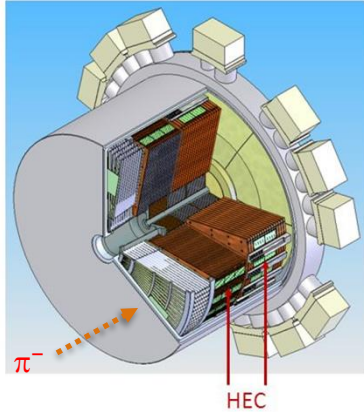
```
const auto neutronInelasticProcess = new G4HadronInelasticProcess("neutronInelastic", neutron);
G4PhysicsListHelper::GetPhysicsListHelper()->RegisterProcess(neutronInelasticProcess, neutron);

neutronInelasticProcess->AddDataSet(new FLUKAInelasticScatteringXS()); // fluka cross section
neutronInelasticProcess->RegisterMe(new FLUKANuclearInelasticModel()); // fluka model
```

- Construct processes for other particle ( $\pi^\pm$ , Kaons, Hyperons, etc.) in the similar way

# Geant4-Fluka Comparison and Examples

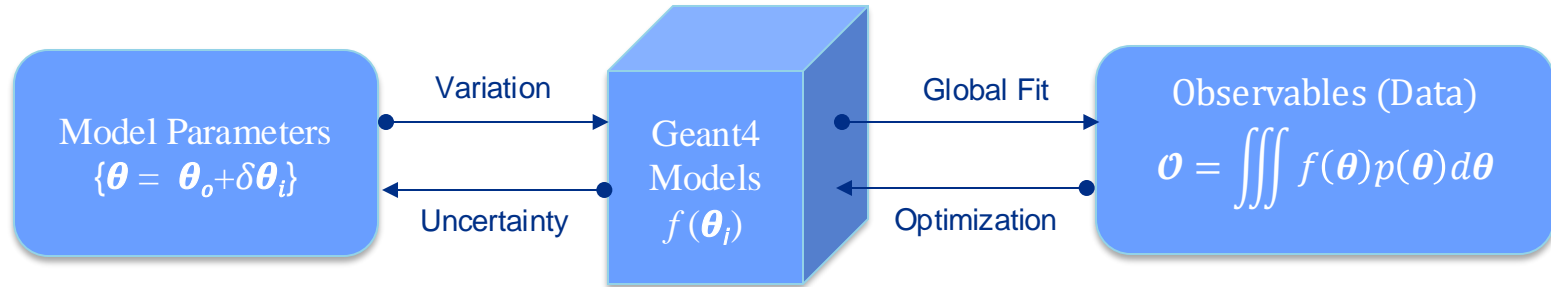
- Comparison with the ATLAS HEC (hadronic end-cap calorimeter)



- How to make use of the interface to `FLUKA` hadron inelastic physics in a G4 application
  - See the Geant4 example: examples/extended/hadronic/FlukaCern
  - ProcessLevel and PhysicsListLevel

# Optimizing Geant4 Physics Models

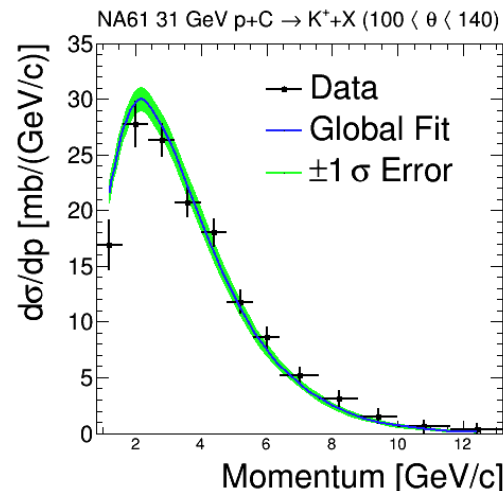
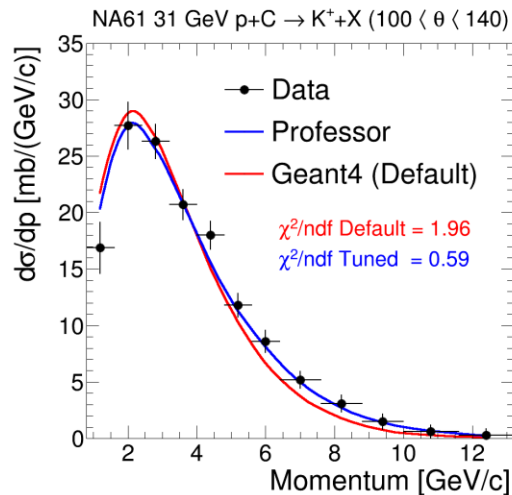
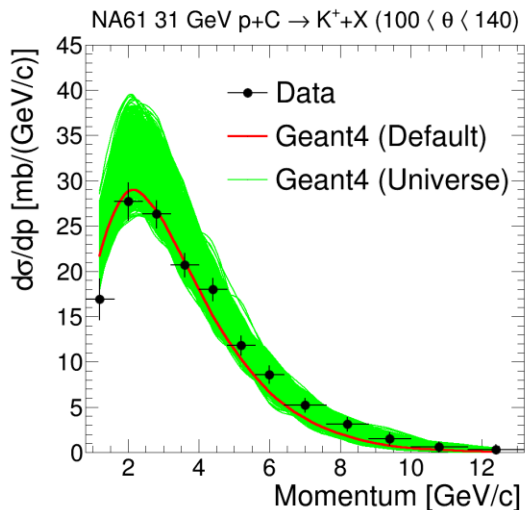
- Geant4 uses many underlying models to predict particle interaction kinematics, and uncertainty in these models (or model parameters) leads to uncertainty in physics measurements
- Since 10.4, Geant4 introduced configurable model parameters ( $\theta$ ) which opens a possibility to
  - Explore how much simulated observables ( $\mathcal{O}$ ) would change with variations of parameters (sensitivities)
  - Provide best sets of model parameters ( $\theta_o$ ) to match experimental data
  - Extract associated uncertainties ( $\delta\theta_i$ ) and estimate systematic errors on experimental observables ( $\mathcal{O}$ )



- G4HadronicDeveloperParameters is meant to be used by the Geant4 developers

# Variation of Geant4 Model Parameters

- Variation of 10 FTF parameters for NA61 31 GeV proton on C target as an example
  - Universe: simulation varying parameters within allowed limits - the spread (green lines) of 1000 samples
  - Example fitting with Professor (<https://professor.hepforge.org/>) on NA61 data
  - Propagating parameter uncertainty to observables,  $\vec{p}_i = \vec{p}_o + \sigma \mathcal{C} \vec{z}_i$  (C: Cholesky decomposition of  $\rho$ )



# Geant4 Physics Validation

- Geant4 provides a centralized validation portal site, geant-val (<https://geant-val.cern.ch/>) and runs various tests for public releases

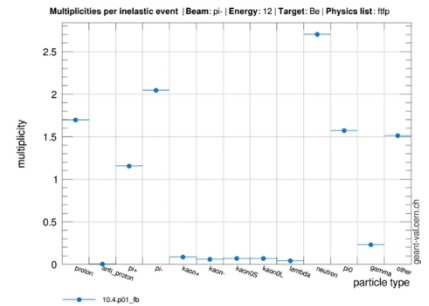
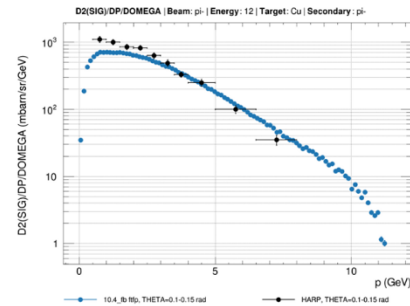
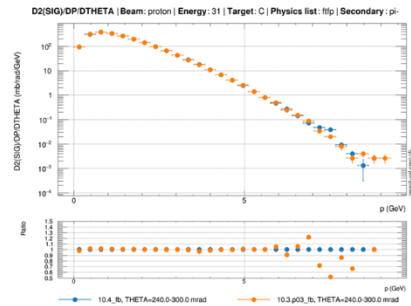
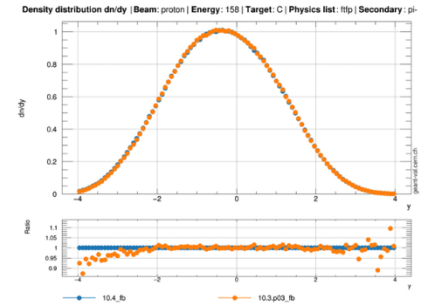
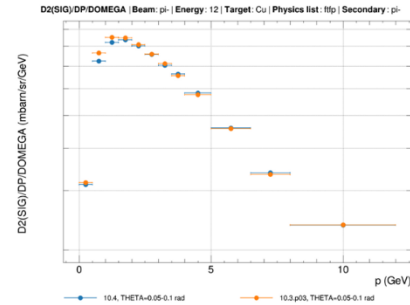
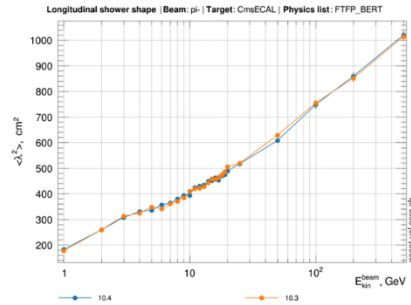
## Geant Validation Portal

User Layouts

Stat comparison

Summary

Lookup tables

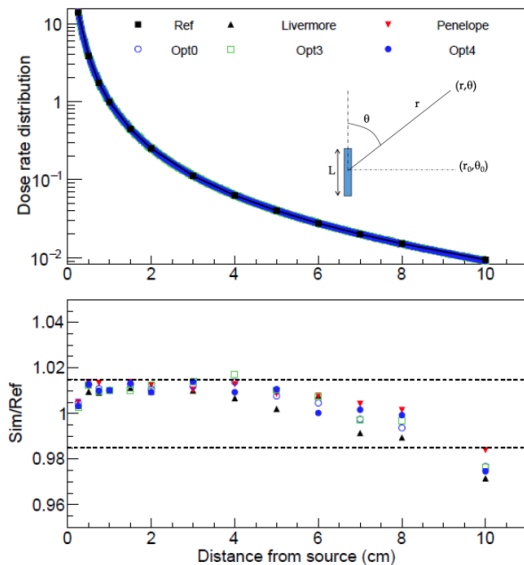


# Integrating Tests into geant-val

- **G4\_Med** (<https://twiki.cern.ch/twiki/bin/view/Geant4/G4MSBG>) is integrated in geant-val to execute regularly automatized regression tests on the CERN computing infrastructure: Just a few examples!

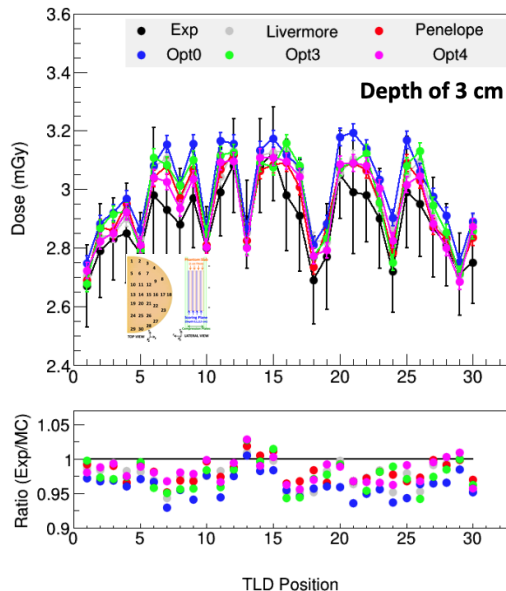
## Brachytherapy test

D. Cutajar, S. Guatelli, A. Le, A. Rosenfeld  
University of Wollongong

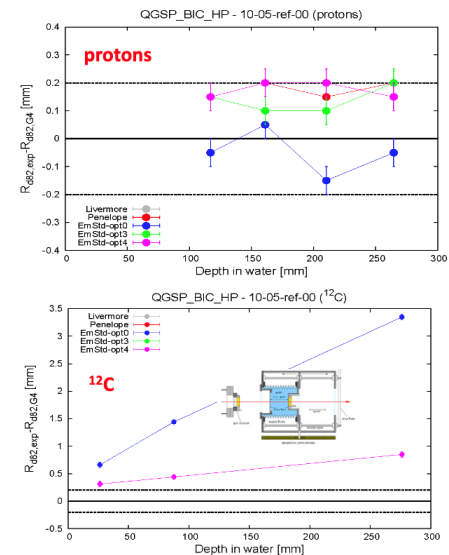


## Internal breast dosimetry

C. Fedon and I. Sechopoulos, Radboudumc (NL)



## Bragg Curves in Water for Proton & C-12 Beams



# Summary

- Geant4 provides several low energy hadronic models
  - NeutronHP, LEND, ParticleHP
  - Radioactive decay, capture and stopping, (neutron induced) fission models
- Gamma-nuclear and lepto-nuclear processes are also available
- There are many other hadronic physics processes and models
  - Please see Geant4 Physics Reference Manual for more details
- Geant4 hadronic physics is continually being improved and will be extended, and supports more physics coverages and user applications