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Geant4 Introduction and Applications Workshop

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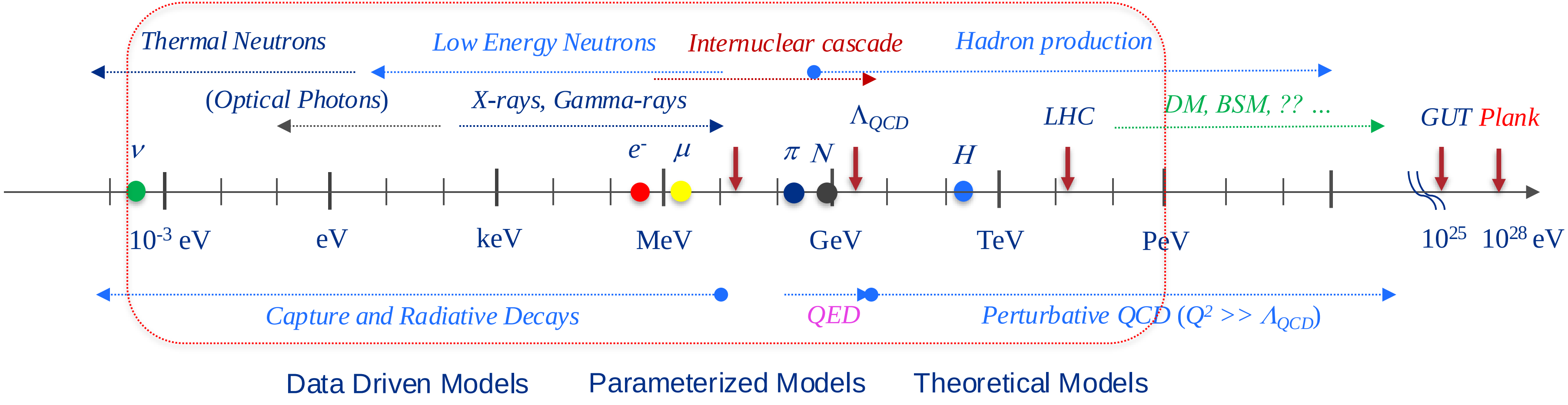
This talk

- Introduction to Geant4 simulation toolkit – Part-B
  - Physics coverage
  - Connecting to external physics engines such as Penelope and FLUKA
  - Prospect toward heterogeneous computing with GPUs
- Objectives
  - Brief overview of Geant4 physics processes and models, and interfaces to other MC packages
  - Geant4 strategies and R&D activities for future computing ecosystems
- References
  - Physics Reference Manual, https://geant4-userdoc.web.cern.ch/UsersGuides/PhysicsReferenceManual/html/index.html
  - Physics List Guide, https://geant4-userdoc.web.cern.ch/UsersGuides/PhysicsListGuide/html/index.html
  - Geant4 Tutorials, https://geant4.web.cern.ch/collaboration/events?past

Geant4 Physics Coverage

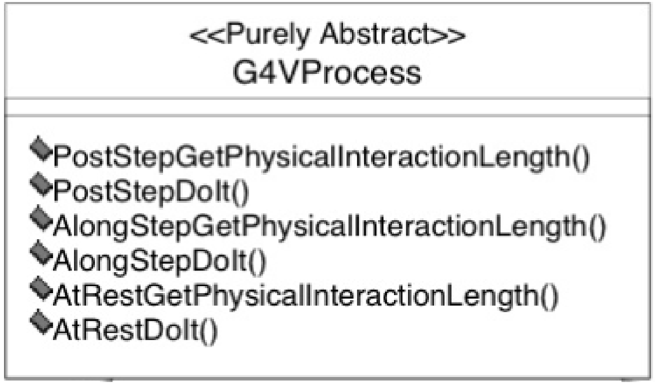
- Geant4 provides a variety of physics components per particle type in a wide range of the particle's energy (up to the PeV scale).



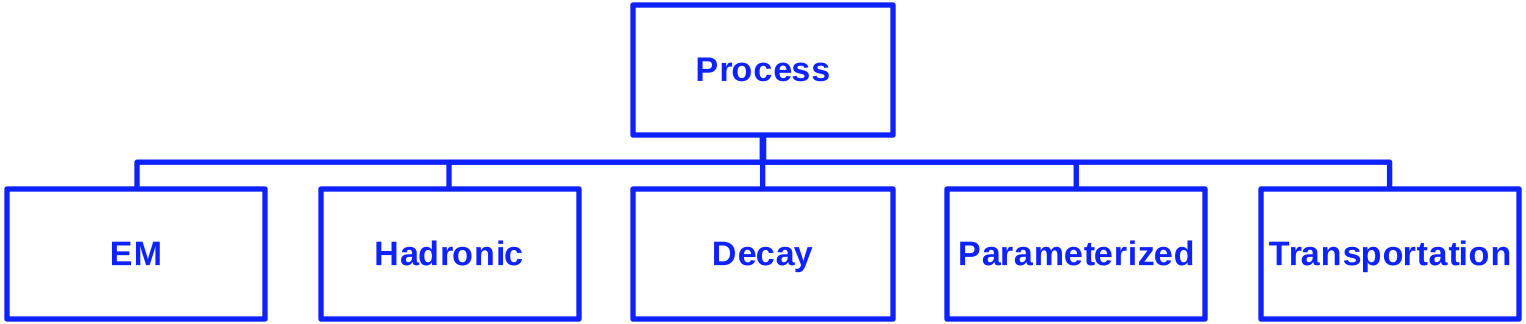
- Geant4 physics, especially hadronic models are largely driven by combinations of data, pure theoretical models and parameterizations.
- As a toolkit, Geant4 supports flexible interfaces to construct a set of physics processes (physics list) and configure physics needed for applications (accuracy vs. performance).

Geant4 Processes

- Processes describe how particles interact with a material, and all are derived from the interface *G4VProcess* (common software design).
  - 3 flavors (can be combined)
    - Discrete (PostStep)
    - Continuous (AlongStep)
    - At rest (AtRest)
  - 2 key methods
    - GPIL (Get Physics Interaction Length)
    - DoIt (Sampling the final state)

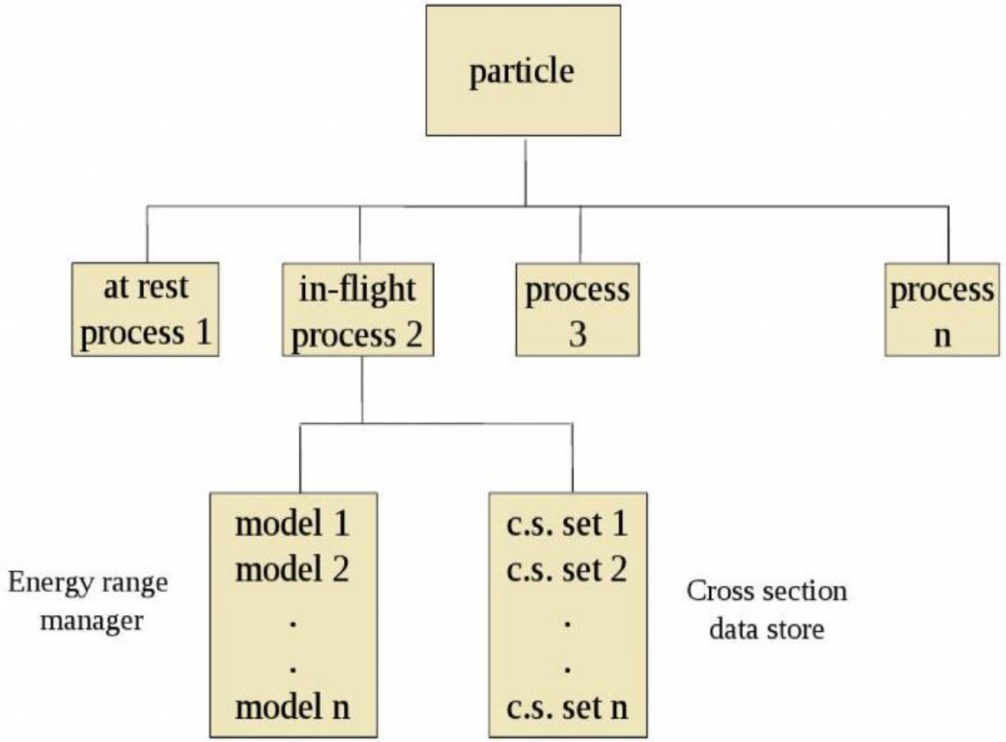


- Major categories of the Geant4 process



Geant4 Processes and Models

- Physics List defines particles and associated processes of an application.
- Processes determines the location and the final state of interactions between a particle and material.
- Each process may be implemented directly or with an associated model linked to the process.
- Geant4 often provides multiple models for a given (especially hadronic) process.
- A process must have a (multiple) cross section(s) assigned.



Geant4 Physics List

- *G4VUserPhysicsList* is an object responsible for specifying:
  - Particles to be used in a simulation application
  - Processes and assigning them to each particle type
- It provides a very flexible way to set up the physics environment:
  - *G4VPhysicsConstructor* allows particles and their associated processes to be grouped together according to a physics domain and can be viewed as a subset of a complete physics list.
  - *G4VModularPhysicsList* provides the use of "physics constructor" which handles a well-defined category of physics, e.g., EM, hadronic, etc.
- Geant4 also provides packaged physics lists which are:
  - Ready-to-use, developed by experts in specific application domains
  - Extensively validated by developers and the user communities
- Alternatively, users can use *G4PhysicsListFactory* which knows about all the available reference physics lists.

Packaged Physics Lists: Examples

- FTFP_BERT
  - Recommended for HEP applications
  - Includes G4EmStandardPhysics (EM0 constructor)
  - FTF – FRITIOF string model (> ~ 4 GeV)
  - BERT - Bertini cascade model (< ~12 GeV)
  - P – G4Precompound deexcitation model
- QGSP_BIC_HP
  - Recommended for medical applications
  - Includes G4EmStandardPhysics_option4 (EMZ)
  - QGS – quark gluon string model (> 12 GeV)
  - FTF – FRITIOF string model (9.5 - 25 GeV)
  - BIC – Binary cascade (200 MeV – 9.9 GeV)
  - P – G4Precompound deexcitation model
  - HP – High precision model for N, p, d, t, ^{3}He, α (< 20 MeV)
- Other physics lists and extensions in *G4PhysicsListFactory* →

- FTFP_BERT_HP
- FTFP_BERT_TRV
- FTFP_BERT_ATL
- FTFQGSP_BERT
- FTFP_INCLXX
- FTFP_INCLXX_HP
- FTF_BIC
- LBE
- QBBC
- QGSP_BERT
- QGSP_BERT_HP
- QGSP_BIC
- QGSP_BIC_AllHP
- QGSP_FTFP_BERT
- QGSP_INCLXX
- QGSP_INCLXX_HP
- QGS_BIC
- Shielding
- ShieldingLEND
- ShieldingM
- NuBeam
- FTFP_BERT_HPT
- FTFP_INCLXX_HPT
  QGSP_BERT_HPT
- QGSP_BIC_HPT
- QGSP_INCLXX_HPT
- Shielding_HPT
- ShieldingM_HPT

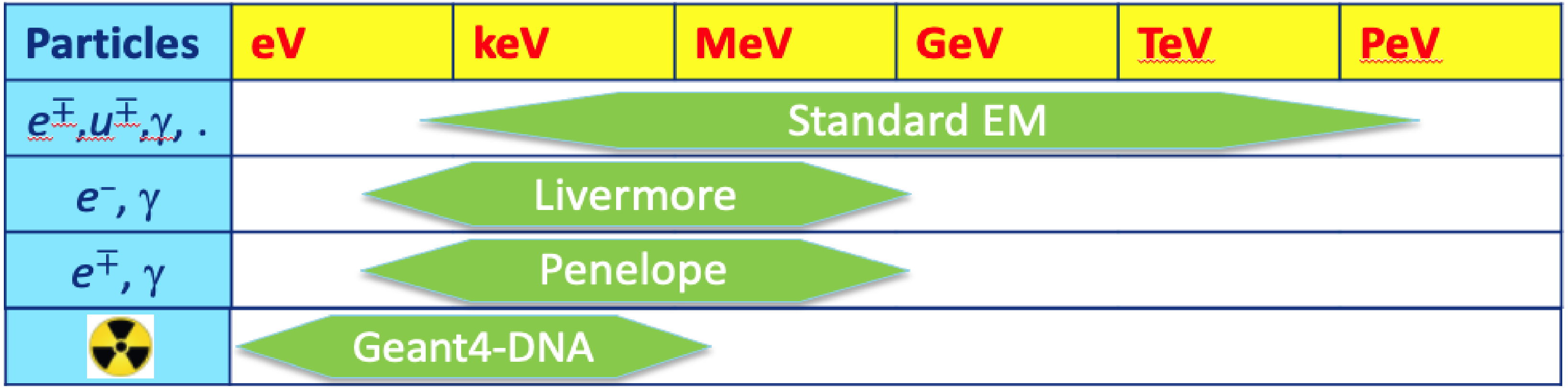
⊕

EM0
EMV
EMX
EMY
EMZ
LIV
PEN
GS
SS
WVI
LE
HPT

EM Processes and Models

Geant4 Electromagnetic and Optical Processes

- Electromagnetic (EM) processes
  - Standard EM – a complete set of processes covering charged leptons (mainly $e^{\mp}$ and $\mu^{\mp}$) and γ : energy range 1 keV to ~PeV (the default for HEP applications)
  - Low energy EM – specialized for $e^{\mp}$ and γ, charged hadrons with more atomic shell structure details. Some processes valid down to 250 eV or below. Others not valid above a few GeV.
  - Geant4-DNA (from a few eV to ~MeV) for micro-dosimetry studies



- Optical photon processes: λ >> atomic spacing (E_{γ} < 100 eV) photons (x-rays, UV, visible)

Standard EM Physics Processes and Models

- γ and $e^{\pm}$ models in the Standard EM physics (constructor)

Primary	Process	Model	Default Energy Range
γ	Compton Scattering	KleinNishina	1 MeV - 100TeV
	Pair-Production	BetheHeitler	$2m_e$ - 100 TeV
	Photo-Electric Effect	Livermore	200 keV - 100 TeV
	Rayleigh Scattering	Livermore	100 keV - 100TeV
$e^{\mp}$	eIonization	MøllerBhabha	100 eV - 100 TeV
	eBremsstrahlung	SeltzerBerger	100 eV - 1 GeV
		Relativistic	1 GeV - 100 TeV
	eMultiple Scattering	UrbanMsc	100 eV - 100 MeV
		WentzelVI	100 MeV - 100 TeV
	eCoulomb Scattering	BetheWentzel	100 MeV - 100 TeV
e^{+}	eplusAnnihilation	EPlusGG	100 eV - 100 TeV

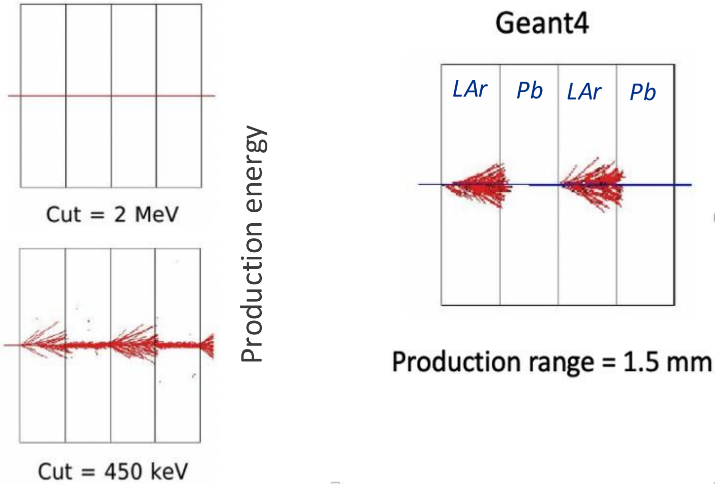
- $\mu^{\pm}$ processes (include pair-production and muon-nuclear interaction)
- EM-like processes for charged hadrons (for single and multiple scattering, energy loss, …)

Threshold for Secondary Production

- Physics processes usually produce secondary particles according to DCS of associated models, which sometimes follow a power law by the secondary particle energy (k),

$$\frac{d\sigma}{dk} = f(k, E_{inc}, Z, \ldots) \sim \frac{1}{k^n} \to \infty \quad \text{as} \quad k \to 0 \qquad n = \begin{cases} 1 & \text{for bremsstrahlung} \\ 2 & \text{for } \delta\text{-ray production} \end{cases}$$

- To avoid the infrared divergence, Geant4 imposes a production cut → a cutoff in length
  - Depositing the average energy at the creating point is equivalent to tracking them to zero energy if its absorption length is small
  - One length for all materials (different energies depending on the material and the particle type)
- Production cut: energy vs. length (example)
  - 500 MeV p in a *LAr-Pb* sampling calorimeter
  - The energy deposition in *LAr* is not well modeled with the production threshold in energy
- *G4ProductionCuts* can be set in different Regions



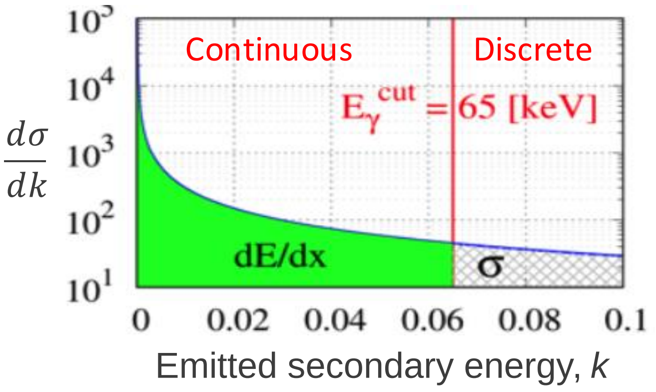
Continuous Energy Loss

- The production cut introduces two distinct mechanisms for handling physics processes: secondary photons (or δ-rays), with the initial energy
  - Above the cut ($k > E^{cut}$), are generated: Discrete

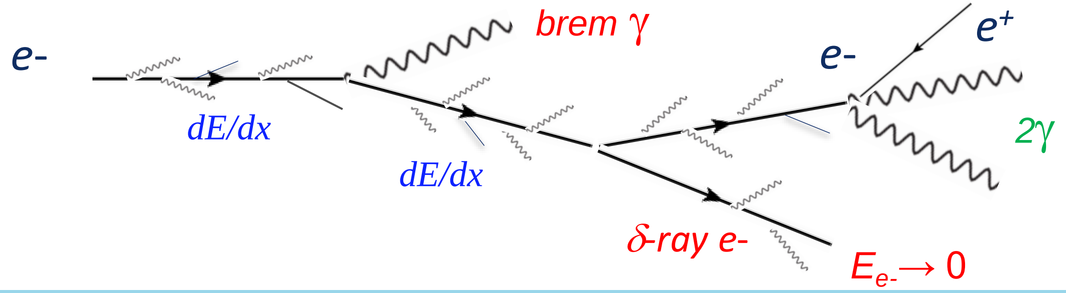
$$\sigma(E, k^{cut}, Z) = \int_{k^{cut}}^{k^{max}} \frac{d\sigma(E,k,Z)}{dk} dk$$

  - Below the cut ($k < E^{cut}$), are not generated: Continuous

$$E_{soft}(E, k^{cut}, Z) = \int_0^{k^{cut}} k \frac{d\sigma(E,k,Z)}{dk} dk \quad \rightarrow \quad -\frac{dE}{dx} = nE_{soft}$$

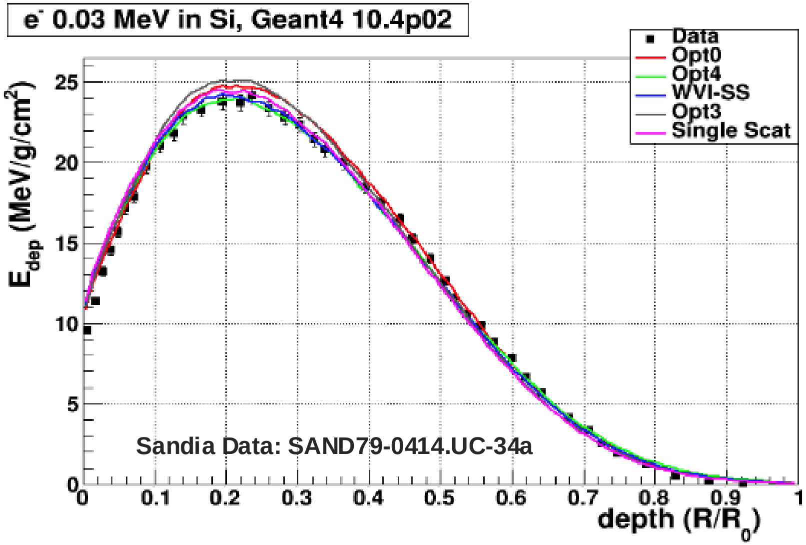


- The mean energy per unit length (dE/dx) due to the threshold is accounted as a continuous energy loss of the primary particle along its trajectory



Elastic and Multiple Scattering (MSC) Models

- Event-by-event modeling of elastic scattering (mostly based on the Wentzel theory)
  - Electron Coulomb scattering ($e^{\mp}$)
  - Single Coulomb scattering (SS) (any charged, focused on muons and hadrons)
  - Ion Coulomb scattering (Ion)
  - Screened Nuclear Recoil (*p*, ion for space)
- Multiple scattering models
  - Urban model (HEP default below 100 MeV)
  - WentzelVI (HEP default above 100 MeV)
  - Goudsmit-Saunderson (GS) ($e^{\mp}$)
  - LowEnergyWentzelVI
- Special features of Geant4 MSC models
  - Boundary crossing algorithms
  - True path length ←→ geometry path
  - Interleaving with other along step processes (energy loss, and transportation)
  - Many tunable options for different accuracy requirements (vs. computing performance)

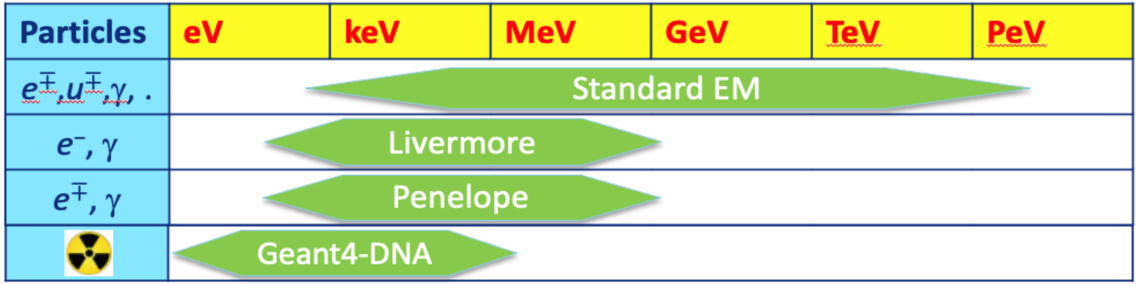


Standard EM Physics Constructors

Constructor	Components	Comments
G4EmStandardPhysics	Default: nothing or _EM0 (QGSP_BERT, FTFP_BERT,...)	For ATLAS and other HEP simulation applications
G4EmStandardPhysicsGS	standard EM physics and the GS e± MSC model for $e^{\pm}$ for HEP	Alternative to EM0 i.e., for HEP
G4EmStandardPhysicsSS	single scattering (SS) model description of the Coulomb scattering	Validation and verification of the MSC
G4EmStandardPhysicsWVI	WentzelVI + Single Scattering mixed model for Coulomb scattering	High and intermediate energy applications
G4EmStandardPhysics_option1 (EMV)	Fast: due to simpler MSC step limitation (FTFP_BERT_EMV)	Similar with one used by the CMS experiment
G4EmStandardPhysics_option2 (EMX)	updated photoelectric model but no-displacement in MSC	Similar with one used by the LHCb experiment
G4EmStandardPhysics_option3 (EMY)	**Urban** MSC model for all particles	Proton/ion therapy
G4EmStandardPhysics_option4 (EMZ)	GS MSC model with Mott correction and error-free stepping for $e^{\pm}$	Most accurate EM physics description

Low Energy EM Physics

- Extend the coverage of Geant4 EM interactions with matter
  - Down to very low energies (sub-keV scale). For photons, electrons, hadrons and ions (up to 1 GeV)
  - Precise treatment of EM showers and interactions at low-energy (keV scale)
- Possible domains of applications
  - Space science
  - Medical physics
  - Micro-dosimetry for radiobiology



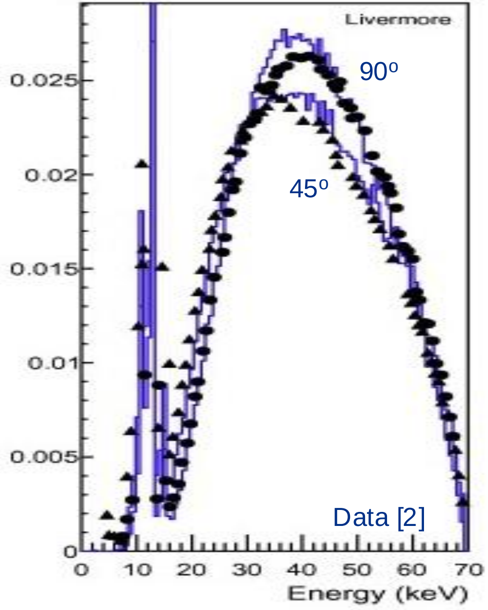
- Choices of models include
  - Livermore library: e^{-} and γ, based polarized processes [250 eV–1GeV]
  - Penelope MC: e^{-}, e^{+} and γ, (version 2008 as default) [250 eV – 1 GeV]
  - Micro-dosimetry models for radiobiology (Geant4-DNA project): [4 eV – ~100 MeV]
  - Atomic de-excitation (fluorescence, Auger *e*-, PIXE, etc)

Livermore Models

- Based on evaluated data tables from the Livermore data library (EADL, EEDL, EPDL97, binding energies (Scofield), mixture of experiments and theories). Available models are:

Physics Process	Process Class	Model Class	Low Energy Limit
		Gammas	
Compton	G4ComptonScattering	G4LivermoreComptonModel	eV
Polarized Compton	G4ComptonScattering	G4LivermorePolarizedComptonModel	eV
Rayleigh	G4RayleighScattering	G4LivermoreRayleighModel	eV
Polarized Rayleigh	G4RayleighScattering	G4LivermorePolarizedRayleighModel	250 eV (kill)
Conversion	G4GammaConversion	G4LivermoreGammaConversionModel	1.022 MeV
Polarized Conversion	G4GammaConversion	G4LivermorePolarizedGammaConversion Model	1.022 MeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	eV
Polarized Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	eV
		Electrons	
Ionization	G4eIonisation	G4LivermoreIonisationModel	eV
Bremsstrahlung	G4eBremsstrahlung	G4LivermoreBremsstrahlungModel	10 eV

Bremsstrahlung γ spectrum from 70 keV e- on Pb (45º and 90º) [1]



- Physics constructors: G4EmLivermorePhysics and G4EmLivermorePolarizedPhysics

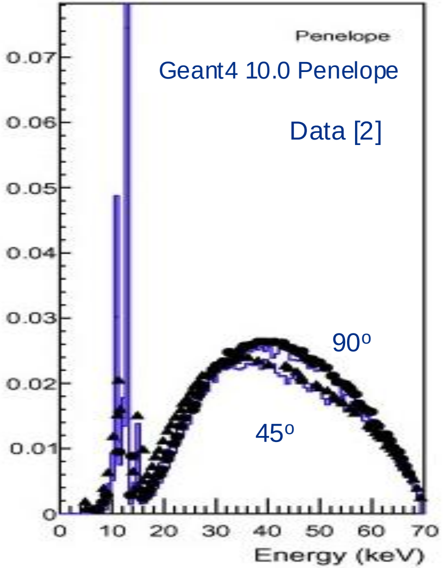
[1] L. Pandolar, et. al., Nucl. Instr. Meth. B 350, (2015) p 41-48, [2] Data: R. Ambrose, et. al., Nucl. Instr. Meth. B, 56 (57) (1991), p 327-329

Penelope Models

- Geant4 includes the low-energy models for $e^{\pm}$ and γ from the Monte Carlo code PENELOPE (v2008), specifically developed by the Barcelona group (F. Salvat et al.)
- Great care was dedicated to the low-energy description of atomic (shell) effects, fluorescence, Doppler broadening, etc.
- Physics constructor: *G4EmPenelopePhysics*

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

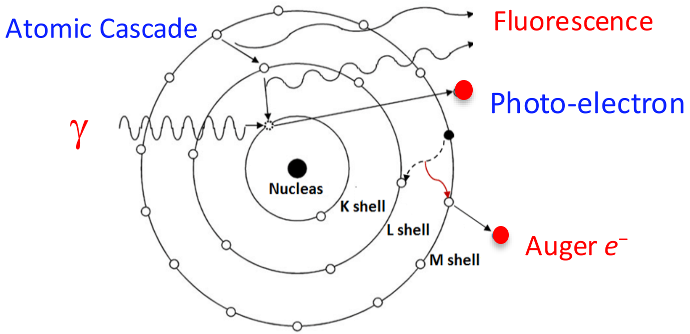
Bremsstrahlung γ spectrum from 70 keV e- on Pb (45º and 90º) [1]



[1] L. Pandolar, et. al., Nucl. Instr. Meth. B 350, (2015) p 41-48, [2] Data: R. Ambrose, et. al., Nucl. Instr. Meth. B, 56 (57) (1991), p 327-329

Atomic De-excitation

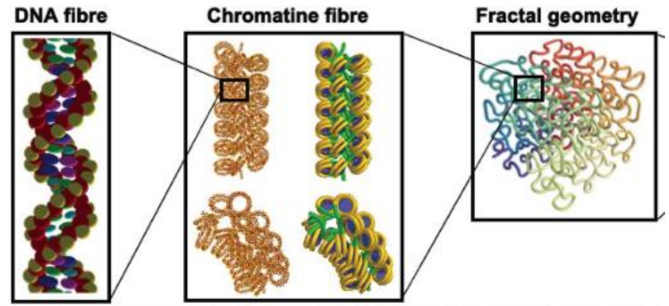
- Atomic de-excitation is initiated by other EM physics interactions
  - E.g., Photo-electric, ionization, Compton scattering by e^- and ions
  - These interactions leave the target atom in an excited state
- EADL (Evaluated Atomic Data Library) contains transition probabilities
  - Fluorescence: radiative transition characteristic X-ray emission
  - Auger e^- emission: initial and final vacancies are in different shells
  - Coster-Kronig e^- emission: initial and final holes are in the same shell

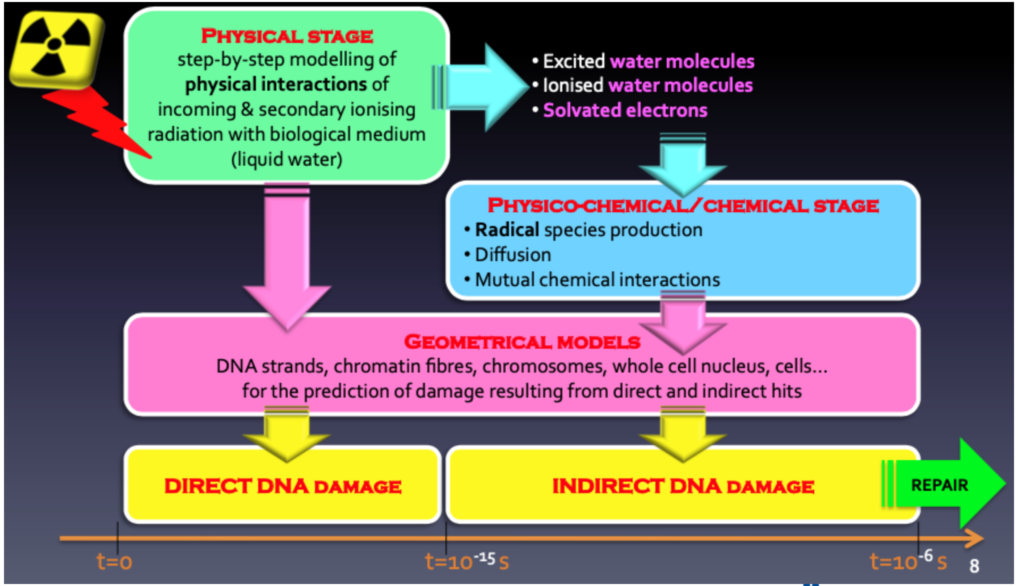


- The atomic de-excitation is compatible with both the standard and the low-energy EM physics categories (configurable by the user interface in G4RadioactiveDecay)

Geant4-DNA

- Extend the simulation of interactions of radiation with biological systems at the cellular and DNA level (micro dosimetry) to predict early and late damage in the context of manned space exploration missions (initiated in 2001, ESA)
- Include elastic scattering, excitation (electronic + vibrations), ionization, charged exchange and molecular attachment → still very actively developing area
- Offer DNA geometry libraries (e.g.)





- Applications:
  - Radiobiology and hadron therapy
  - Radioprotection for space missions
  - Not limited to biological materials

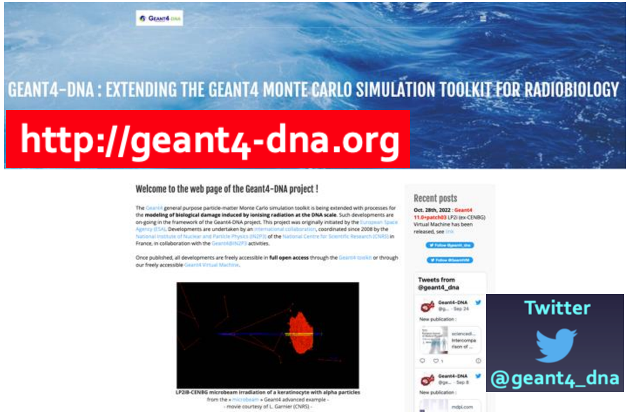
Geant4-DNA Physics Constructors

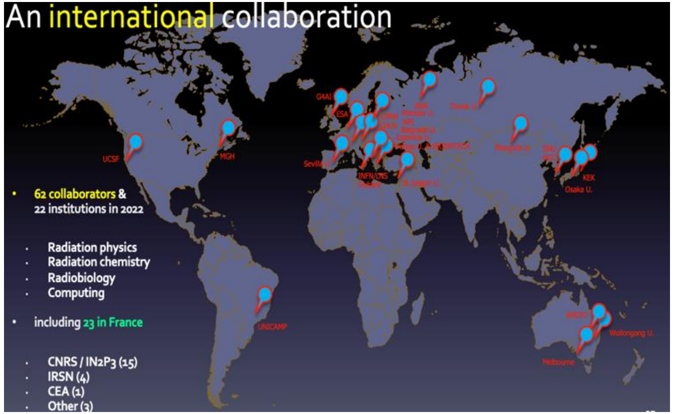
- Available DNA physics constructors and three recommended G4DNA physics constructors for liquid water

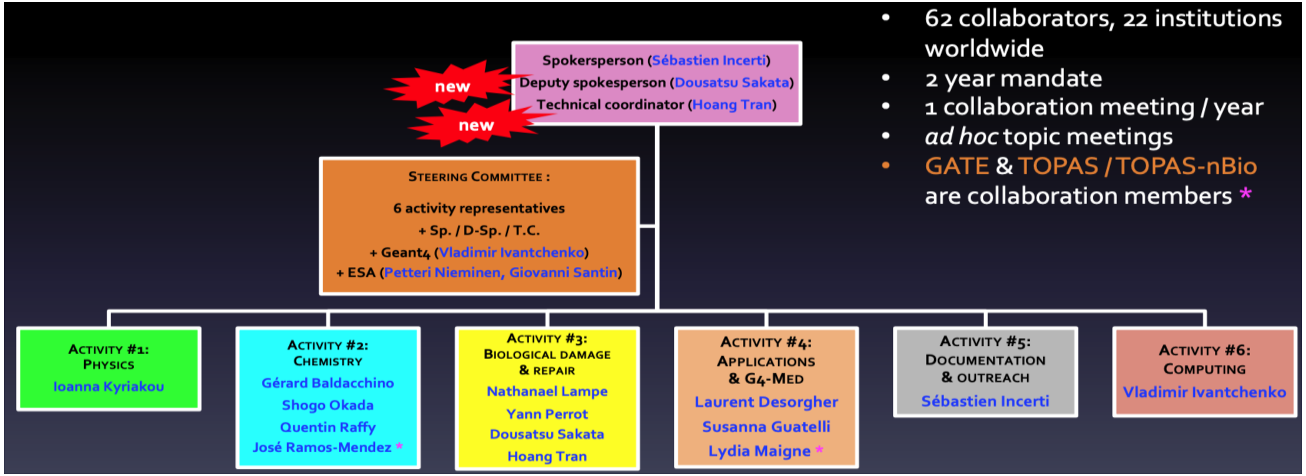
Constructor name	Content
G4EmDNAPhysics	Default models
G4EmDNAPhysics_option1 (beta)	Same as G4EmDNAPhysics but uses New multiple scattering model G4LowEWentzelVIModel
G4EmDNAPhysics_option2	Same as G4EmDNAPhysics but faster (usage of CDCS for ionisation processes)
G4EmDNAPhysics_option3	Same as G4EmDNAPhysics (historical)
G4EmDNAPhysics_option4	Electron ionisation and excitation models by Ioannina team
G4EmDNAPhysics_option5 (beta)	Same but faster (usage of CDCS)
G4EmDNAPhysics_option6	CPA100 models
G4EmDNAPhyics_option7	EmfietzoglouExcitationModel + BornExcitationModel
G4EmDNAPhyics_option8	Elastic scattering using CPA100 model

- Also provides *G4EmDNAChemistry* constructors for liquid water and their applications

Geant4-DNA Website and Collaboration







Optical Physics in Geant4

- Optical photons: wavelength >> atomic spacing (~10 nm) or $E\gamma$ < 100 eV (Visible, UV, x-rays)
  - Treat as waves (G4OpticalPhoton ≠ G4Gamma) and polarization plays a role
  - Boundary processes are significant → detail treatments are complicated (G4REALSURFACEDATA Dataset)
  - Skin surface can be shared between volumes (cf. boarded surface)
- Geant4 provides interfaces for material (optical) properties (refraction index, scintillation yield, surface property, etc.)
- Optical photon processes
  - Generation: Scintillation, Cerenkov, Transition Radiation
  - Transport: Absorption, Rayleigh, Wavelength shift, boundary (reflection and refraction)
- Surface/boundary models: Gliser and Unified ← RealSurface2.2 data
- For a typical optical simulation (especially scintillation), CPU load can become quite heavy (>10000 photons/MeV of the energy loss) and can be offloaded to accelerators (GPUs)

Hadronic Processes and Models

Hadronic Processes and Cross Sections

- Hadronic physics processes include
  - G4HadronElasticProcess
  - G4HadronInelasticProcess
  - G4NeutronCaptureProcess
  - G4NeutronFissionProcess
  - G4RadioactiveDecay
  - EM-like Processes (of charged hadrons)
    - Coulomb, multiple scattering
    - Ionization, Bremsstrahlung
  - Photo- and lepto-nuclear processes
- Geant4 separates hadronic process cross sections from hadronic final states models.

- Depend on the particle type and energy
  - Example for pion- from FTFP_BERT

```
-----------------------------------------------------------------------
                              Hadronic Processes for pi-
 Process: hadElastic
       Model:             hElasticGlauber: 0 eV  ---> 100 TeV
    Cr_sctns:  BarashenkovGlauberGribov: 0 eV  ---> 100 TeV
 Process: pi-Inelastic
       Model:                        FTFP: 3 GeV ---> 100 TeV
       Model:              BertiniCascade: 0 eV  ---> 6 GeV
    Cr_sctns:  BarashenkovGlauberGribov: 0 eV  ---> 100 TeV
 Process: hBertiniCaptureAtRest
-----------------------------------------------------------------------
G4ProcessManager: particle[pi-]
[0]=== process[Transportation :Transportation] Active
[1]=== process[msc :Electromagnetic] Active
[2]=== process[hIoni :Electromagnetic] Active
[3]=== process[hBrems :Electromagnetic] Active
[4]=== process[hPairProd :Electromagnetic] Active
[5]=== process[CoulombScat :Electromagnetic] Active
[6]=== process[Decay :Decay] Active
[7]=== process[hadElastic :Hadronic] Active
[8]=== process[pi-Inelastic :Hadronic] Active
[9]=== process[hBertiniCaptureAtRest :Hadronic] Active
[10]=== process[StepLimiter :General] Active
[11]=== process[UserSpecialCut :General] Active
```

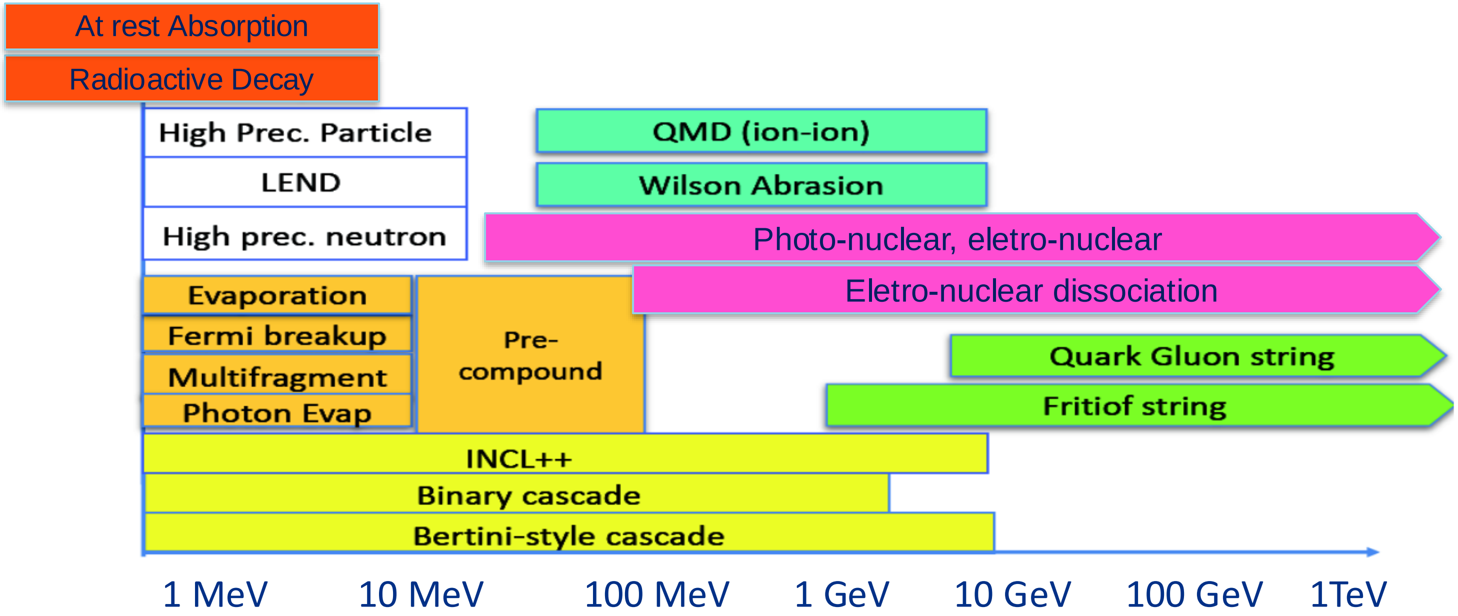
Geant4 Datasets

- Datasets from the latest Geant4 11.2 release

Dataset (env)	Data File	Related Process or model
G4ABLADATA	G4ABLA3.3	Data for the ABLA de-excitation model (INCLXX)
G4LEDATA	G4EMLOW8.5	Low-energy electromagnetic data
G4ENSDFSTATEDATA	G4ENSDFSTATE2.3	Nuclear properties from ENSDF
G4INCLDATA	G4INCL1.2	Data for the intranuclear cascade INCLXX model
G4NEUTRONHPDATA	G4NDL4.7.1	Neutron data of cross sections and final state dist.
G4PARTICLEXSDATA	G4PARTICLEXS4.0	Average cross sections derived from G4NDL
G4PIIDATA	G4PII1.3	Proton/alpha ionization (PIXE) cross section library
G4SAIDXSDATA	G4SAIDDATA2.0	SAID database for nucleon and π cross sections
G4LEVELGAMMADATA	PhotonEvaporation5.7	Photon evaporation (deexcitation) data from ENSDF
G4RADIOACTIVEDATA	RadioactiveDecay5.6	Radioactive decay data from ENSDF
G4REALSURFACEDATA	RealSurface2.2	Optical surface reflectance look-up tables

Hadronic Physics and Models

- Many models for pure hadronic processes (elastic, inelastic, capture, fission) (0 to ~TeV)
- Radioactive decay: at rest and in-flight
- High precision neutron models (thermal energies to ~20 MeV)
- γ and $e^{\pm}$ ($\mu^{\pm}$) induced nuclear reactions (~10 MeV - ~TeV)

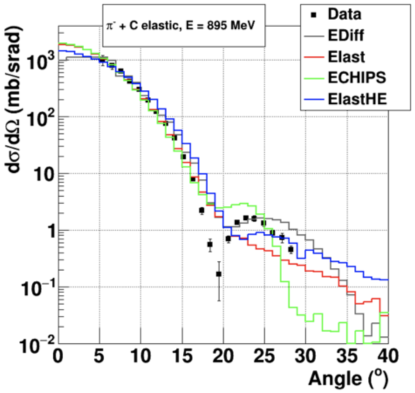


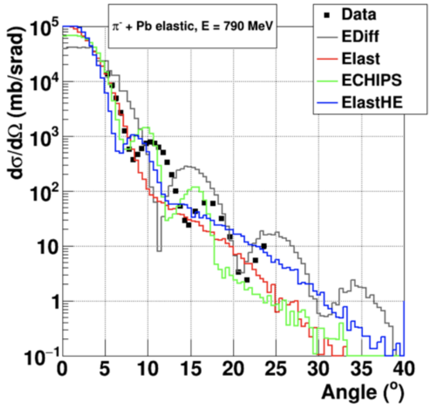
Hadron Elastic Models at Medium and High Energy

- Coherent elastic models

	Model	Differential Cross Section	Energy Range
proton	G4ChipsElasticModel (CHIPS)	BarashenkovGlauberGribov	0-100 TeV
neutron	G4ChipsElasticModel (CHIPS)	G4NeutronElasticXS (CHIPS)	0-100 TeV
pion	G4ElasticHadrNucleusHE (Glauber)	BarashenkovGlauberGribov	0-100 TeV
Kaon, Hyperons	G4HadronElastic (LHEP)	Glauber-Gribov	0-100 TeV
Anti-particles	LHEP/G4AntiNuclElastic	AntiAGlauber	0/100 MeV/100TeV
Nuclear-nuclear	G4NuclNuclDiffuseElastic	Glauber-Gribov	0-100 TeV

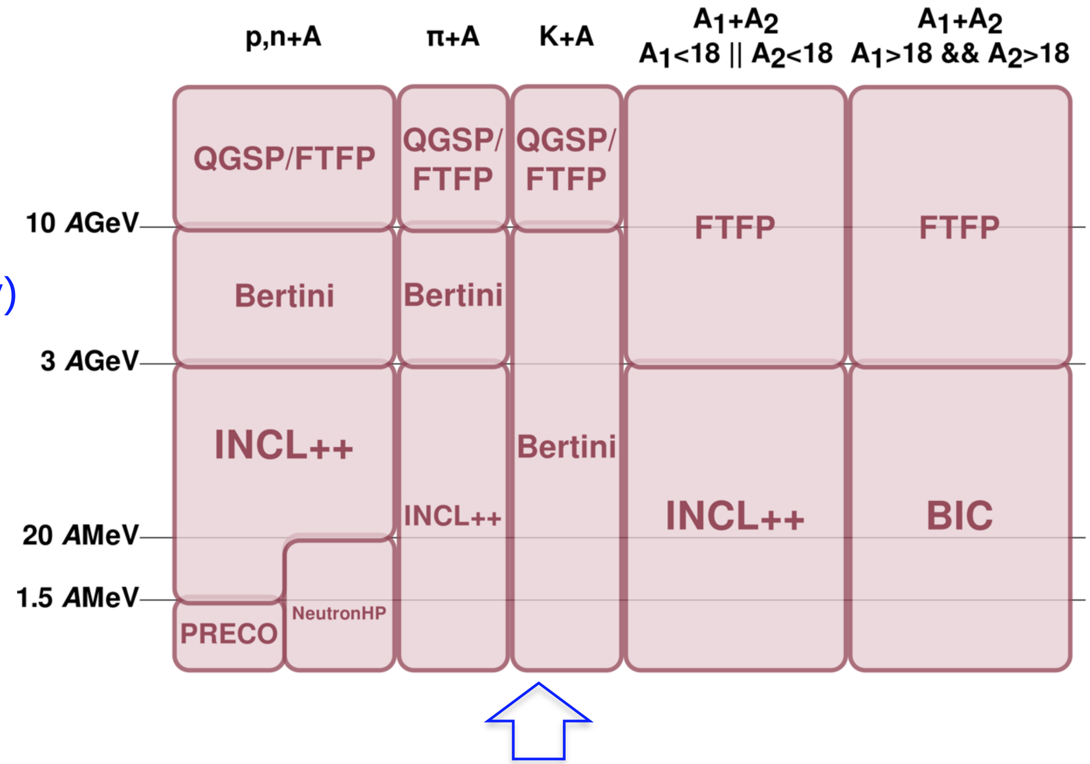
- Comparison to experimental data
  - Data: $\pi^{\pm}$ elastic from EXFOR database
  - Elast: Default elastic model
  - ECHIPS: CHIPS model
  - ElastHE: Glauber-Gribov
  - EDiff: Diffuse model





Hadronic Inelastic models at Medium and High Energy

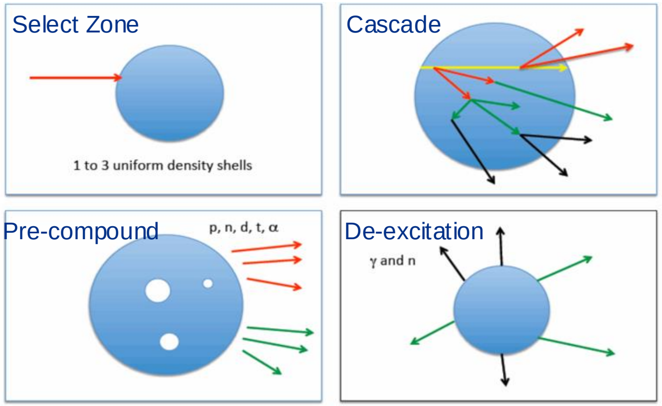
- Intra-nucleus cascade models
  - Bertini (BERT)
  - Binary (BIC)
  - INCL++ (Liege, INCLXX)
- Parton String models (high energy)
  - Quark-gluon string (QGS)
  - Fritiof (FTF)
- Other associated models
  - Pre-compound (P)
  - de-excitation (evaporation)
  - Fermi-breakup, fission



- Physics lists: FTFP_BERT, QGSP_BERT, QGSP_BIC, FTFP_INCLXX, QGSP_INCL++, etc.

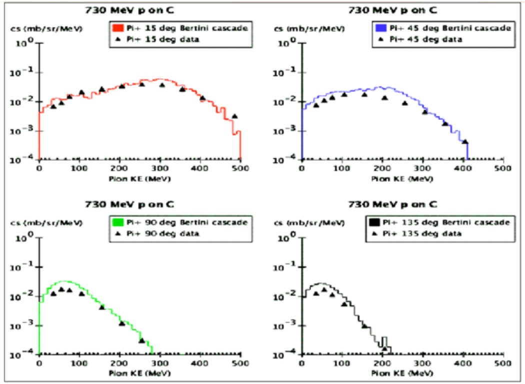
Bertini Intranuclear Cascade and Validation

- Intranuclear treatment (average solution of Boltzmann eq.) of stable hadrons (p, n, π, K, Λ, Σ, Ξ, Ω), γs in [0,10] GeV
  - Valid in de Broglie wavelength < intranuclear distance
  - Fast (10^{-23} – 10^{-22}): excitation, pre-equilibrium, fission
  - Slow (10^{-18} – 10^{-16}): evaporation

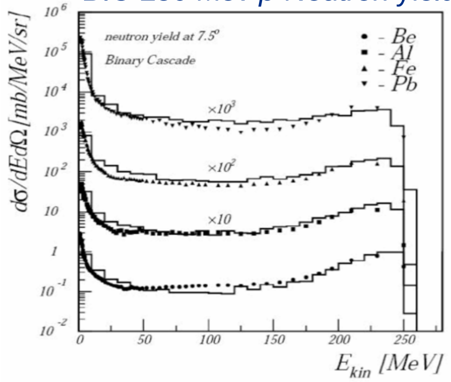


- Physics validation of cascade models: examples

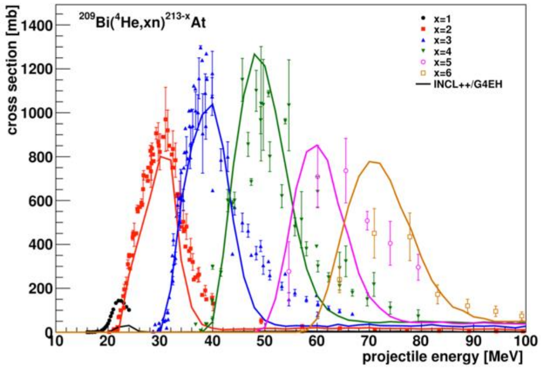
Bertini Cascade 730 MeV p + C → π +X



BIC 250 Mev p Neutron yield

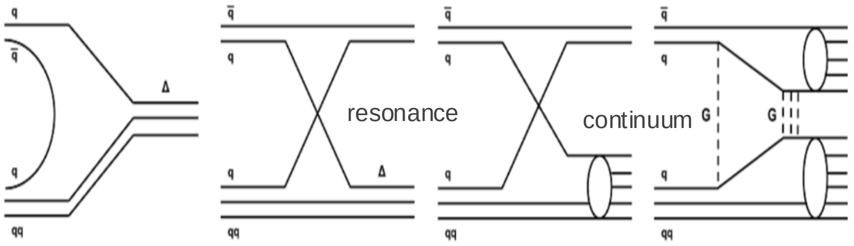


INCL++ Excitation for $\sigma(\alpha, xn)$ on ^{209}Bi

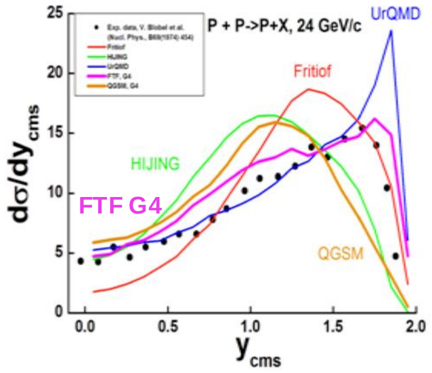


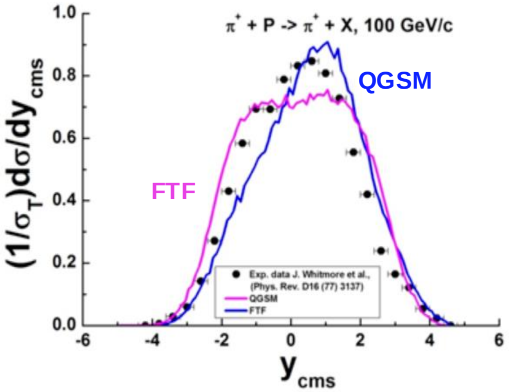
Fritiof (FTF) Model and Validation of Cross Sections

- Hadron-nucleus, nucleus-nucleus, antinucleus-nucleus ($p \gtrsim 3$ GeV per hadron or nucleon) and their interactions are binary reactions ($h_1 + h_2 \rightarrow h_1' + h_2'$) of quark-gluon strings
  - π^-p and π^+p interactions
  - pp and $p\bar{p}$ interactions
  - K^-p and K^+p interactions
  - …

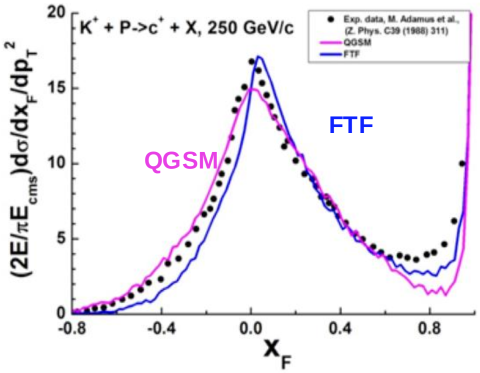


- Example of FTF spectra compared to other model predictions





x_F spectrum of positive charged particles

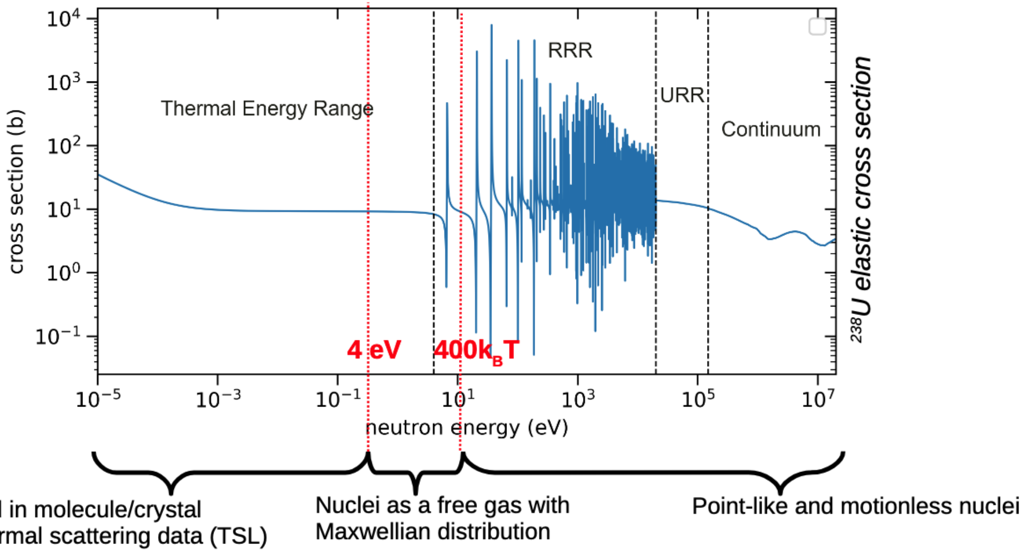


Low Energy Hadronic Models

- 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 captured by a nucleus, n + X(A, Z) → X(A+1, Z) + γ's
- Low energy models for elastic, inelastic, capture and fission (mostly depends on ENDF/B-VII)
  - NeutronHP: High precision neutron
  - LEND: (Livermore) Low energy neutron data
  - ParticleHP: Low energy charged particles

NeutronHP: High Precision Neutron

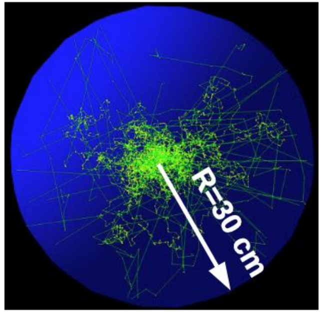
- Data (G4NDL) driven model which includes both cross sections and final states
  - Isotope dependent data for elastic, inelastic, capture and fission with the G4NDL format
  - G4NDL4.7 (mix of JEFF-3.3 and ENDF/B-VIII-0) includes thermal neutron scattering data (~30 materials)
  - Geant4 description is based on the Thermal Scattering Law (TSL) and relies both on experimental measurements and molecular dynamics calculations
- Recent updates and validations
  - Doppler Broadening Rejection correction
  - Updated G4NDL4.7.1 (~20 more materials and temperatures)
  - New URRPT1.1 dataset (URR description with probability table)
  - Available for Geant4 11.3 (Dec. 2024)

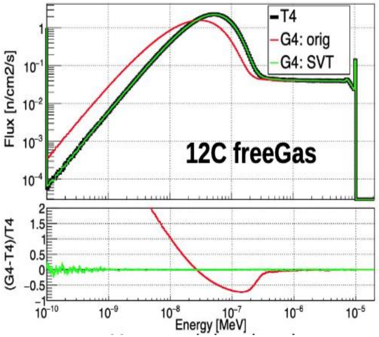


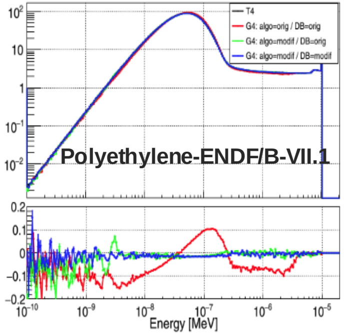
Geant4 NeutronHP Verification to Tripoli-4® [1] and MCNP6.2 [2]

- Implementation of the two tests in geant-val with reference dataset from Tripoli-4 and MCNP6.2 (work based on L. Thulliez, *et. al*., arXiv2109.05967, M. Zmeskal, *et. al*., arXiv2303.07300, arXiv2404.16389)

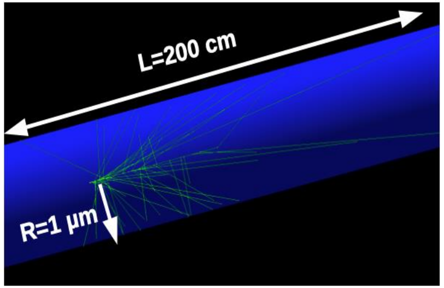
- Macroscopic benchmark
  - Neutron thermalization
  - Neutron Flux
  - TSL data
  - Unresolved Resonance

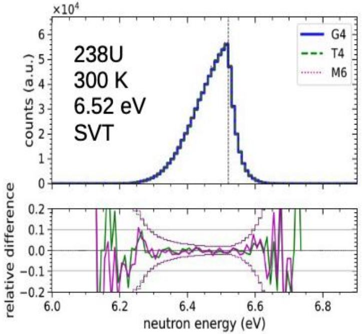


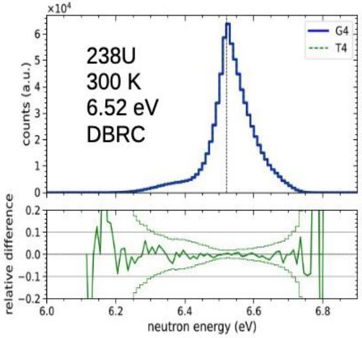




- Microscopic benchmark
  - Neutron energy and angle
  - TSL data
  - DBRC
  - Velocity of the Target (SVT)







- Agreement between Geant4 NeutronHP and Tripoli-4 and MCNP6.2 to better than 2%

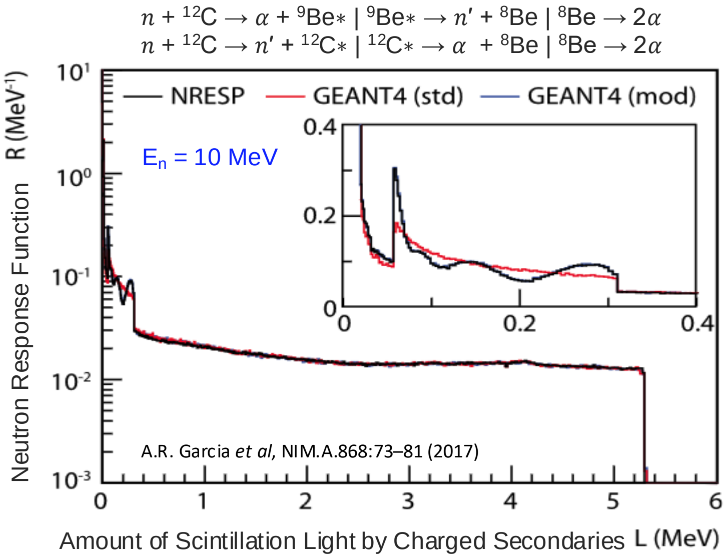
[1] E. Brun et al., TRIPOLI-4 ® , CEA, EDF and AREVA reference Monte Carlo code. Ann. Nucl. Energy 82, 2015, 151–160.
[2] C.J. Werner et al., MCNP Version 6.2, Technical Report, LANL, 2018, http://dx.doi.org/10.2172/1419730.

Livermore LEND Models and G4ParticleHP

- LEND models as an alternative to the NeutronHP models (e.g., in *G4HadronPhysicsShielding*)
  - Use Generalized Nuclear Data (GND) which is a modern format for storing nuclear data (faster), G4LENDDATA dataset (for neutrons and γs) ← LEND_GND1.3_ENDF.BVII.1

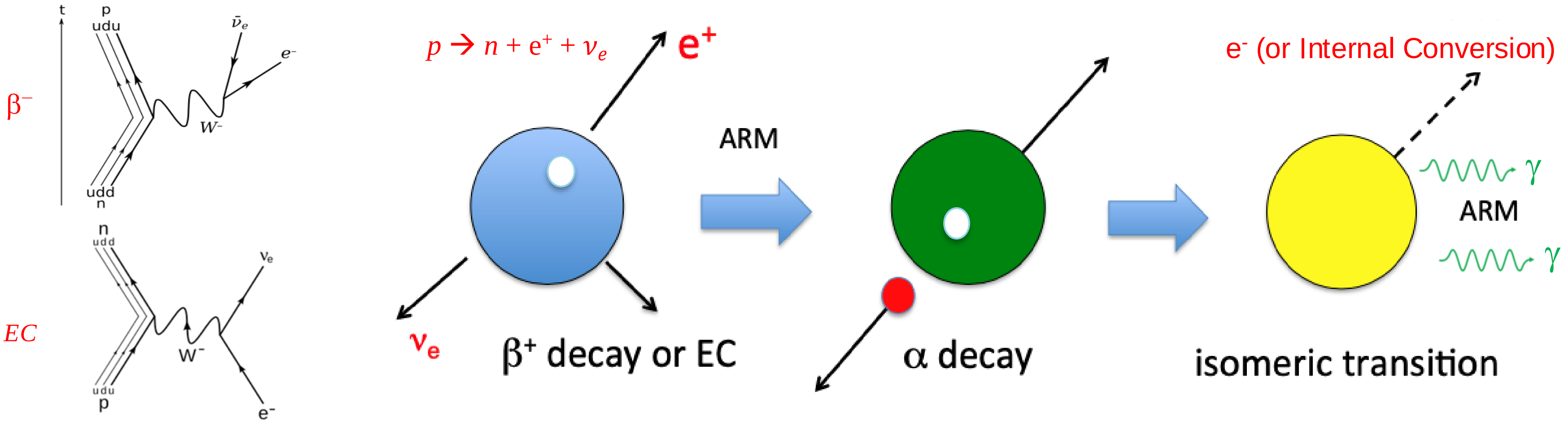
Process	Model Name	Cross Section
Capture	G4LENDCapture	G4LENDCaptureCrossSection
Elastic	G4LENDElastic	G4LENDElasticCrossSection
Inelastic	G4LENDInelastic	G4LENDInelasticCrossSection
Fission	G4LENDFission	G4LENDFissionCrossSection

- G4ParticleHP models simulate the interactions of proton, *d, t, ^{3}He,* α as well as neutrons
  - Mostly below 20 MeV for *n*
  - 0 < E < 200 MeV for charged particles
  - Use ENDF/B-VII (alternatively DBs: TENDL, IAEA, IBANDL)
  - Planned to consolidate with NeutronHP



Radioactive Decay and Chains

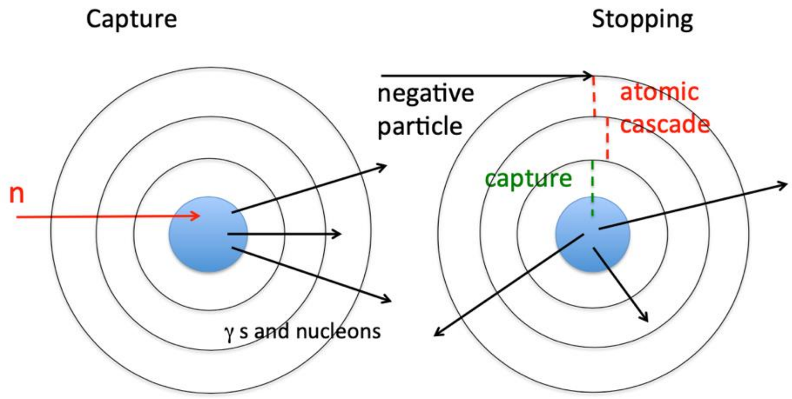
- *G4RadioactiveDecay* simulates radioactive nuclei decays by α, β± emission or electron capture (EC) based on ENSDF (Evaluation of Nuclear Structure Data File → G4RADIOACTIVEDATA)
- Nuclides with lifetime < 1ps decay immediately and trigger a chain of decays, for instance



- Atomic relaxation model (ARM) based on EADL (atomic cascade, Auger e^-, fluorescence)
- If daughter of nuclear decay is an isomer, deexcitation is done by using *G4PhotonEvaporation*
  - Uses ENSDF with all known gamma levels for 3110 nuclides (PhotonEvaporation5.7) with lifetime > 1ns

Capture and Stopping Models

- Neutrons, anti-neutrons never really stop, they just slow down from elastic scattering or are absorbed
- *G4NeutronCaptureProcess*
  - Models of in-flight capture for neutrons
    - *G4NeutronHPCapture* (below 20 MeV)
    - *G4NeutronRadCapture* (all energies)



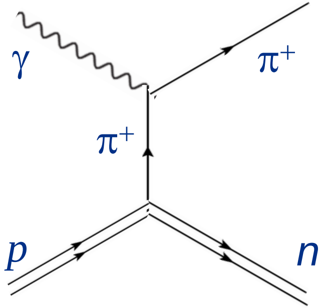
- Negatively charged particles can be captured by a nucleus
- *G4HadronStoppingProcess*
  - *G4HadronicAbsorptionBertini* (π^-, K^-, Σ^-, hadronic absorption at rest using the Bertini cascade)
  - *G4HadronicAbsorptionFritiof* ($\bar{p}$, $\bar{\Sigma}^+$, hadronic absorption at rest using FTF/Preco)
  - *G4MuonMinusCapture* (atomic cascade with decay in orbit, nuclear capture with the Bertini cascade)

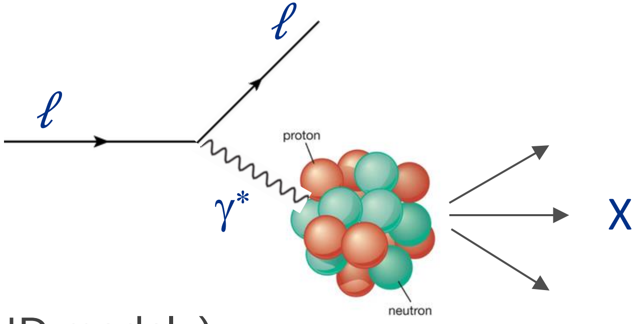
Fission Processes and Models

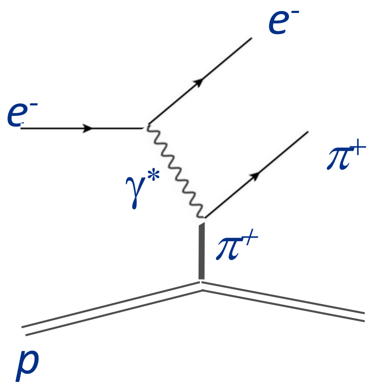
- Many hadronic inelastic models already include fission implicitly
  - Included de-excitation codes in BIC, INCL++, FTF, QGSP ($A \geq 65$) and the Bertini cascade ($A \geq 100$).
  - Considered as a competitor for evaporation process during the nucleus deexcitation transition.
  - In that case, don't add *G4HadronFissionProcess* to a physics list.
- *G4NeutronFissionProcess* handles neutron-induced fission of nuclei
  - *G4NeutronHPFission* (*G4ParticleHPFission*)
    - Specifically for neutrons below 20 MeV (G4NDL dataset)
    - 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*) using the GND format

Photo- and Lepto-nuclear Processes

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



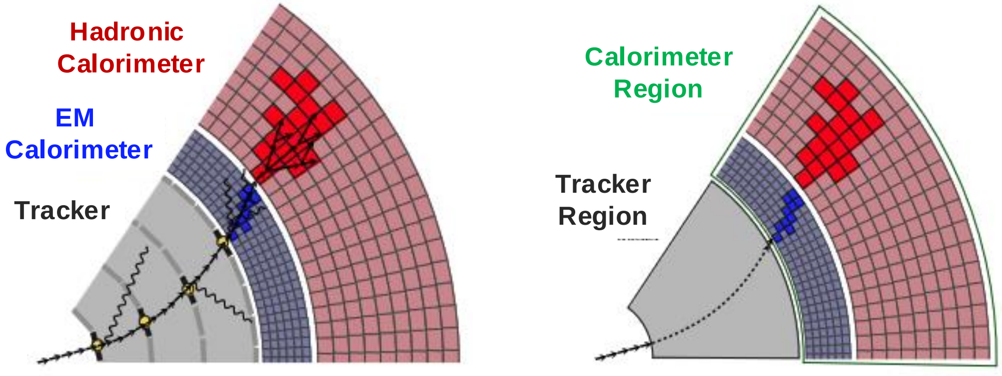




- Photo-nuclear (Bertini, LEND models)
  - At low energies (below nucleon emission threshold) they are absorbed and excite the nucleus as a whole
  - Giant dipole resonance (GDR) region (10 - 30 MeV) and Δ region between pion threshold to 450 MeV
  - At high energies, they act like hadrons (π, □) and form resonances with protons and neutrons
- Electrons and muons interact hadronically through virtual photons then interacts directly with nucleus (or nucleons) *G4ElectronNuclearProcess*, *G4MuonNuclearProcess*

Parameterized Processes

- Geant4 supports a fast simulation interface for a parametrized simulation
  - Replace Geant4 processes with external or user simulation codes
  - Allow a Geant4 process to be modified during simulation execution (e.g., Biasing)
- How does the interface work?
  - G4FastSimulationManager
    - Define G4Envelope (G4Region)
  - G4VFastSimulationModel
    - IsApplicable (particle definition)
    - ModelTrigger (dynamic conditions)
    - DoIt (model actions)
  - G4FastSimHitMaker

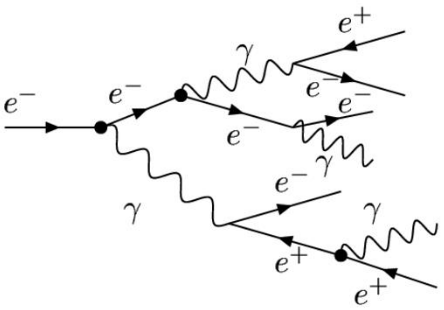


Charge Deposition in Track Region
Energy Deposition in Calorimeter Region

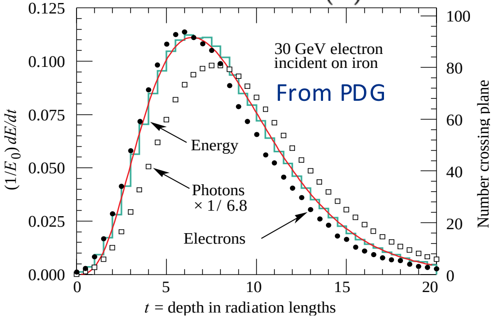
- Example: EM shower parameterization, Christal Channeling, Machine Leaning inference, etc.

Examples of Parameterized Physics

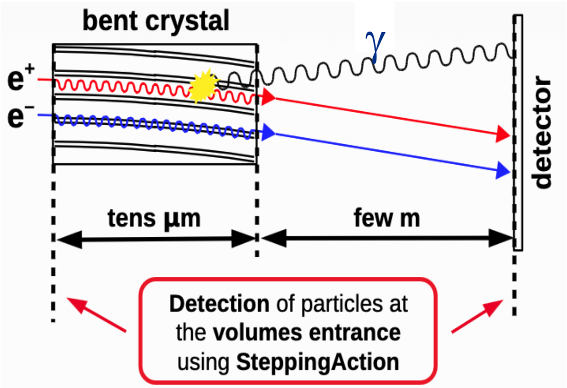
- EM cascade and shower parameterization (Gflash)
  - *GFlashShowerModel*
  - *GVFlashShowerParameterisation*
  - Energy deposition by shower profiles
    - Longitudinal distribution
    - Lateral (radial) distribution
  - Many examples

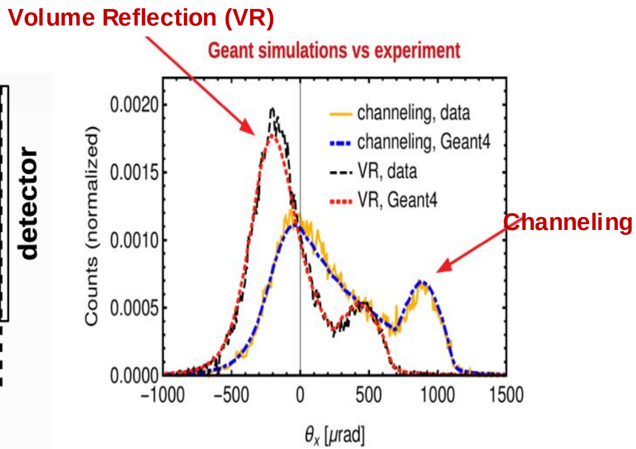


$$f(x;\alpha,\beta) = \frac{x^{\alpha-1} e^{-\beta x} \beta^{\alpha}}{\Gamma(\alpha)}$$



- Channeling in Crystal
  - *G4ChannelingFastSimModel*
  - *G4ChannelingPhysics* (example)
  - $e^{\pm}$ beam transport on ultra-short. crystal at Mainz Mikrotron [1][2]

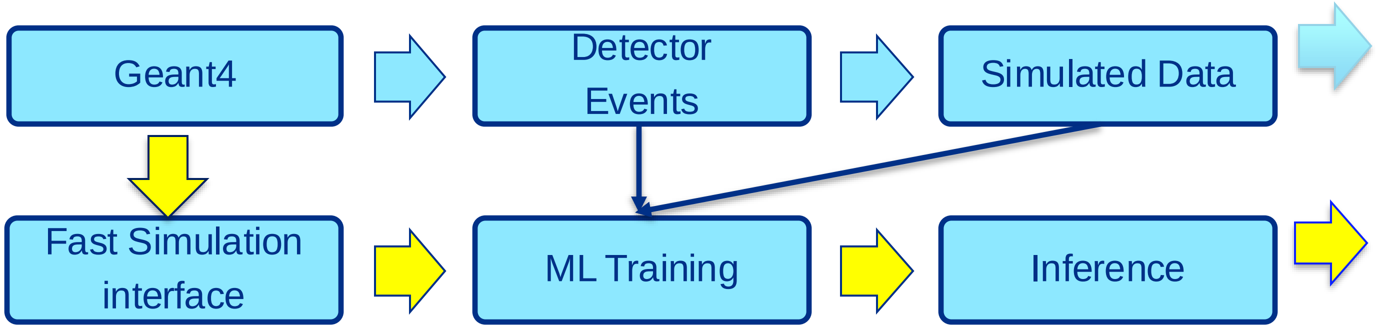


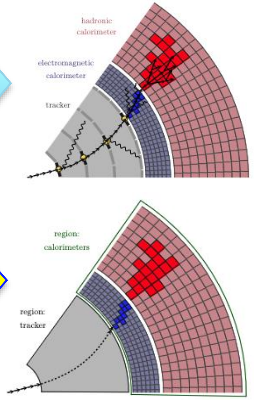


[1] 855MeV electron experiments at MAMI, A. Mazzolari et al. PRL. 112, 135503 (2014)
[2] A. Sytov et al. Eur. Phys. J. C 77, 901 (2017), JKPS 83, 132–139 (2023)

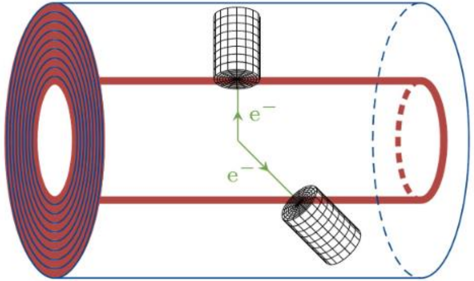
Fast Simulation Model for Machine Learning

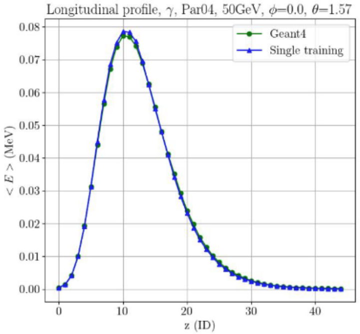
- The Geant4 fast simulation model provides a self-contained ML framework for training and inference: each experiment requires a specific ML designing model and target





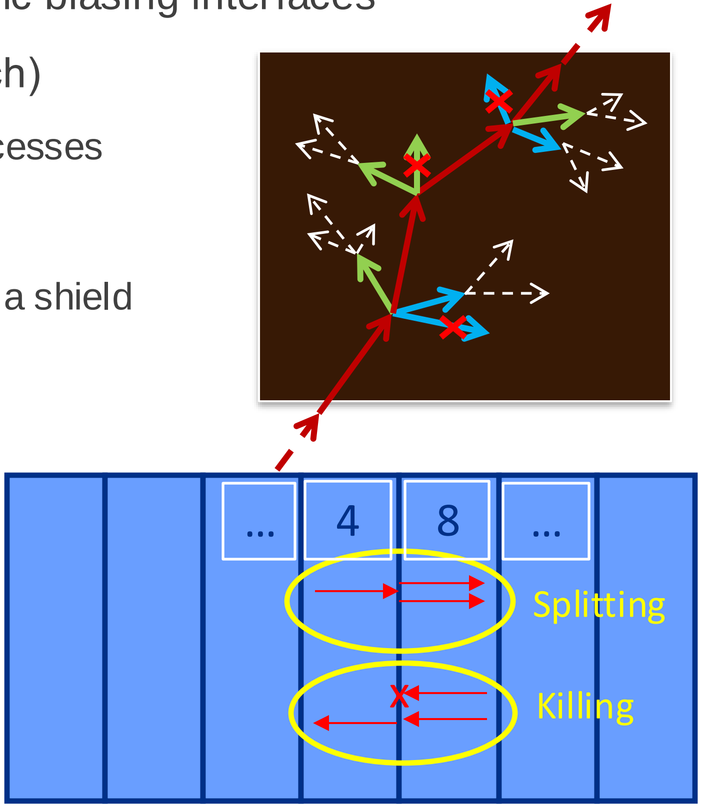
- Interface to upload neural network parameters for inference
  - Lightweight Trained Neural Network
  - Open Neural Network Exchange Libraries
  - Torch
- Calo Challenge





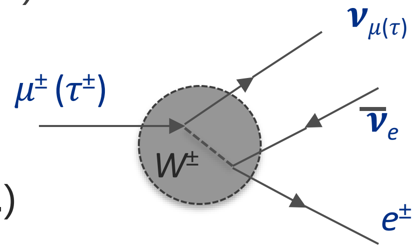
Event Biasing

- Geant4 provides various event biasing options and generic biasing interfaces
- Cross-section biasing (an “importance sampling” approach)
  - Available for photon inelastic, electron & positron nuclear processes
- Leading particle biasing (a killing-based biasing)
  - A technique used for estimating the penetration of particles in a shield
- Geometry-based importance biasing
  - Attach “importance” to cells in geometry
  - Change of probability density functions of interaction laws
- User Biasing
  - *G4WrapperProcess*
- Reverse Monte Carlo
- General Biasing Scheme: *G4GenericBiasingPhysics*

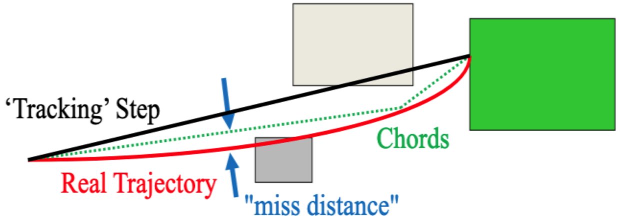


Decay Process and Transportion Process

- *G4Decay* process for all eligible (unstable and long-lived) particles using branching ratios and decay modes from the decay table stored in individual G4ParticleDefinition
  - For short-lived (e.g., heavy flavor) particles, user can pre-assign decay modes, or use *G4ExtDecayer* interface to invoke a decay handler from an external generator (e.g., PYTHIA)
  - Decay process can happen in flight (discreate) or at rest, and includes
    - Weak decay (leptonic, semi-leptonic decays, $\mu^{\pm}$, $\tau^{\pm}$, $K^{\pm}$, K^0_L, etc.)
    - EM and long-lived particle decay (Phase space, Dalitz, π^0, K_S, Λ, Σ^0, etc.)
  - *G4DecayWithSpin* (spin in a field) and *G4UnknownDecay (SUSY/BSM)*



- *G4Transportation* (process) is responsible for moving the particle through the geometry.
  - *G4PropagationInField* transports a charged particle in a field
    - Supports various field integration methods (steppers).
    - Supports both global and local fields
  - Interfaces for customizing field integration and tunable parameters to control accuracy and performance.



Connecting to external physics engines (Penelope and FLUKA as Examples)

Geant4-FLUKA.CERN Interface

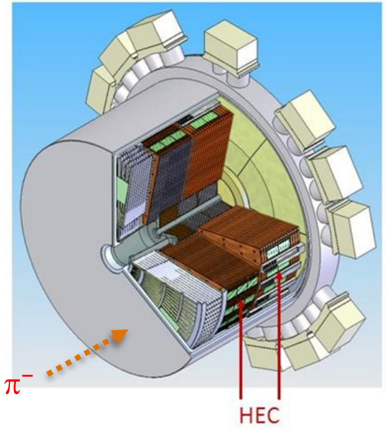
- FLUKA
  - A general purposed tool for calculations of particle transport and interactions with matter
  - Covering an extended range of applications spanning from proton and electron accelerator shielding to target design, calorimetry, activation, dosimetry, detector design, neutrino physics, radiotherapy etc.
  - Comparison with Geant4 has not been trivial, mostly due to having to re-write geometry, materials, fields
- Geant4-FLUKA.CERN (license required) interface since Geant4 11.2 (Dec. 2023)
  - Provides an 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*

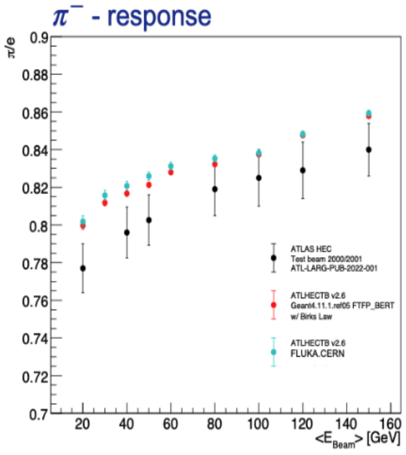
```
const auto neutronInelasticProcess = new G4HadronInelasticProcess("neutronInelastic", neutron);
G4PhysicsListHelper::GetPhysicsListHelper()->RegisterProcess(neutronInelasticProcess, neutron);

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

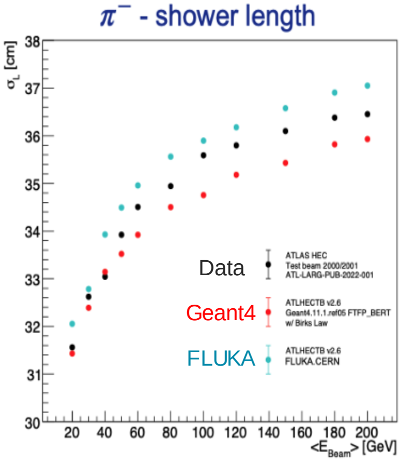
  - Construct processes for other particle ($\pi^{\pm}$, Kaons, Hyperons, etc.) in the similar way

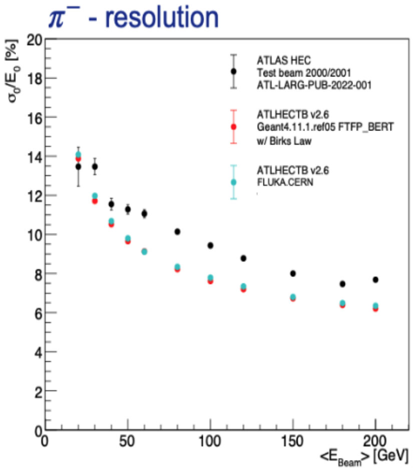
Geant4-FLUKA.CERN Comparison and Examples

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









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

Geant4-PENELOPE

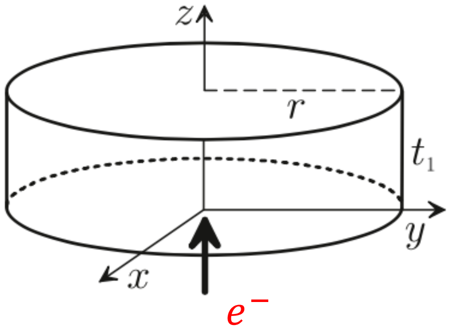
- PENELOPE
  - Monte Carlo simulation package that describes the transport of photons, electrons and positrons in complex geometries and materials of arbitrary composition.
- *G4EmPhenelopPhysics*
  - Geant4 C++ implementation for Penelope-2008 Fortran codes (without multiple and single scattering)
  - Use “FTFP_BERT_PEN” physics list from G4PhysicsListFactory
- PENELOPE (2018) and an interface to Geant4: PenG4 (https://gitlab.com/miancortes/PenG4)

M. Asai, M. A. Cortés-Giraldo, V. Giménez-Alventosa, V. Giménez Gómez, F. Salvat, "The PENELOPE Physics Models and Transport Mechanics. Implementation into Geant4", *Frontiers in Physics* 9: 738735 (2021). [doi: 10.3389/fphy.2021.738735]

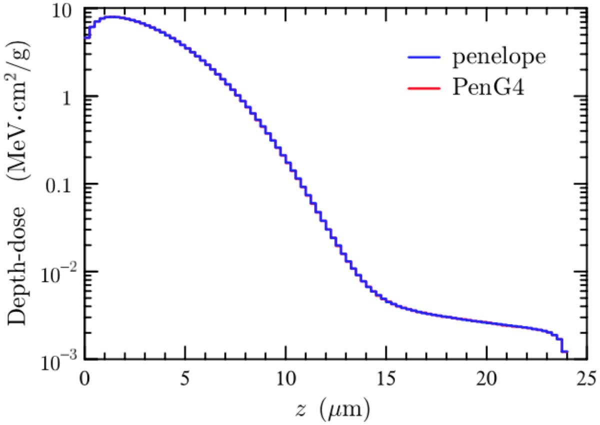
  - Literal translation of class II Penelope-2018 codes
  - Examples how to interface PENELOPE and Geant4 EM physics

PenG4 and PENELOPE Comparison

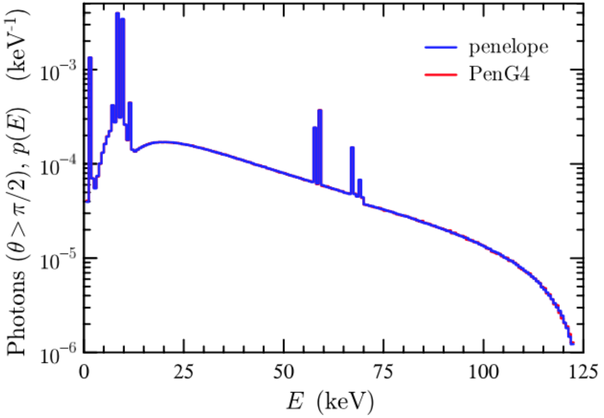
- Electron on a tungsten cylinder (r = 1cm, t_1 = 24μm) (from the PenG4 paper)



Depth-dose distribution



Energy distribution of photons

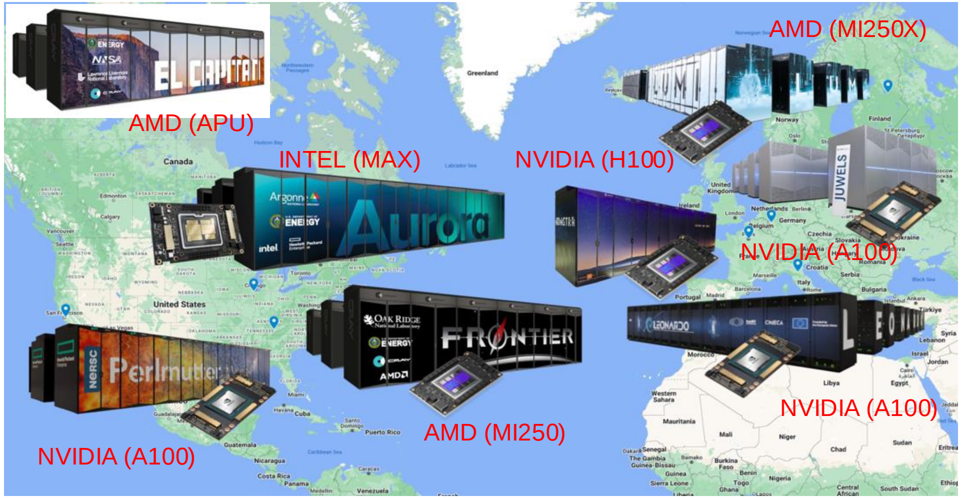


  - Consistent results between PenG4 and PENELOPE
  - Taking advantage of the multi-threading capabilities and advanced geometry and statistical tools of Geant4

Prospect toward heterogeneous computing with GPUs

Heterogeneous Computing

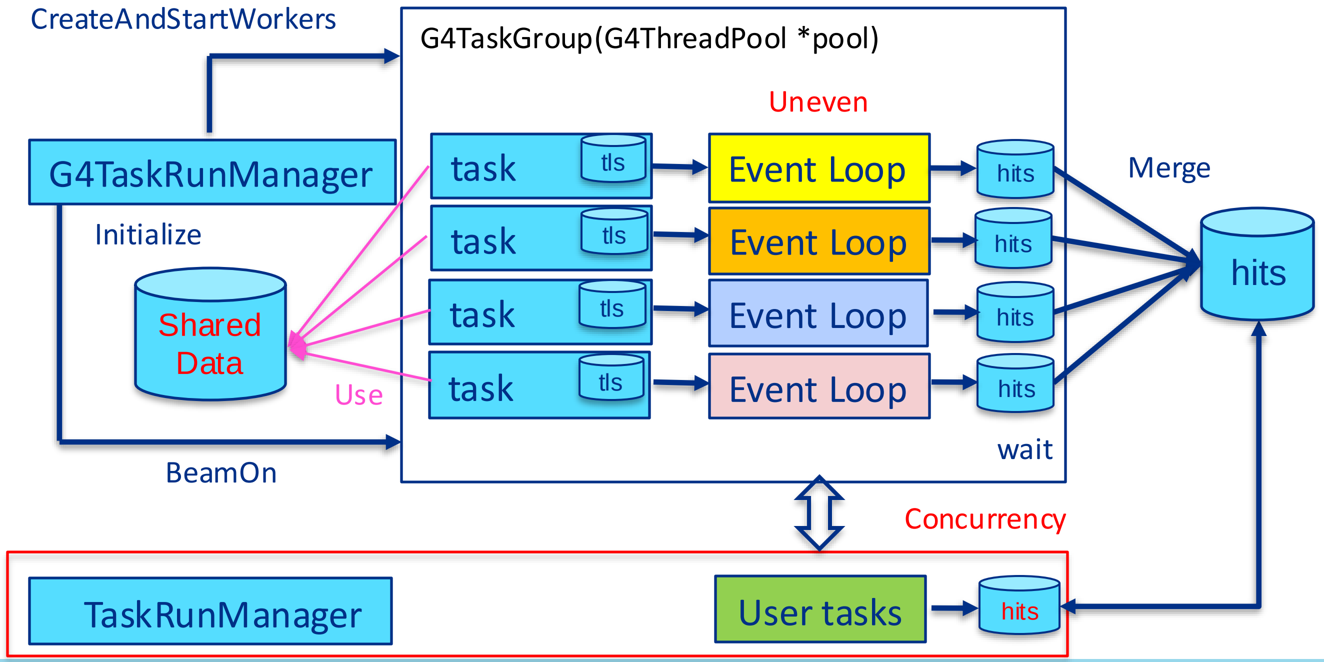
- Computing with more diverse processing elements other than CPU
  - Heavy CPU centric (HTC) → combination of CPU and Accelerators (GPUs, TPUs, NPUs, FPGA etc.)
  - Optimize for very specific domain applications for the triplet (power, performance, cost) and maximize workload by verticalization (hardware designs ←→ software stacks)
- Ever-changing hardware landscape
  - GPU is the current main HPC architecture
  - Equipped with different type of GPUs
  - Trend will be accelerated by AI/ML

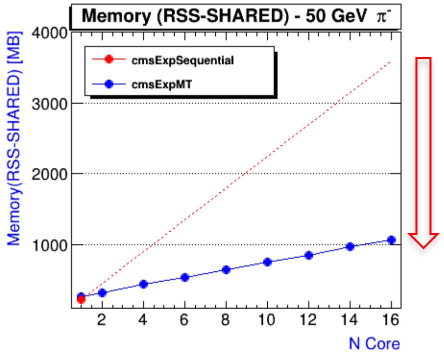


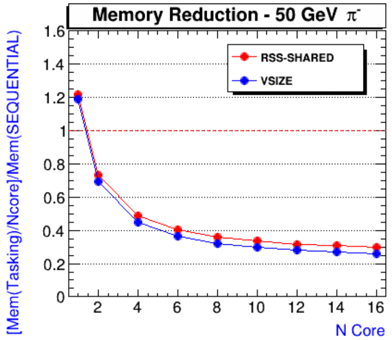
- Detector simulation needs to takes advantage of increasing heterogeneity in computing, especially Exa-scale computers under DOE flagship facilities with GPUs.

Geant4 Strategies

- Geant4 supports options for parallel workflows as events or tracks can be simulated independently
  – G4Multithreading (worker threads) for event level parallelism (Since 10.0)
  – G4Tasking (tasks) for sub-event (track) level parallelism (Since 11.0, 2021)







Toward Sub-event Parallelism in Geant4

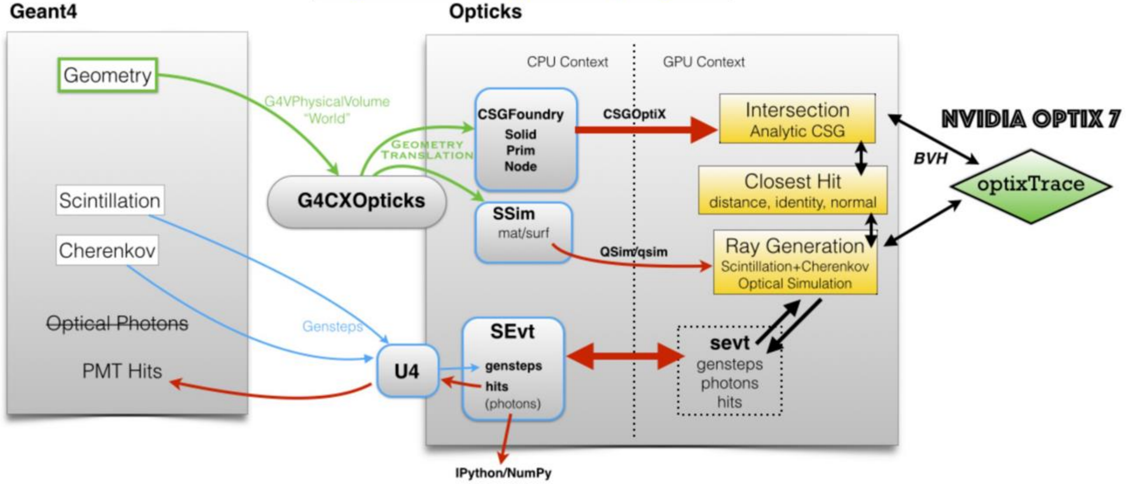
- Split an event into sub-events (sub-group of primary tracks) and task them separately
- Supports offloading pipelines for scheduling specialized tasks with accelerators (GPUs), e.g.,
  - Optical photon transport in Cerenkov or Scintillation detectors
  - EM shower in calorimeter
  - Low energy neutron transport
- Phase-I: Geant4 Kernel extension (version 11.3)
  - Uses *G4SubEvtRunManager* and *G4WorkerSubEvtRunManager* for sub-event parallelism which takes a vector of tracks for a specific subevent type
  - Support parallel tasking for a single large problem (e.g., processing a big event)
- Phase-II: Extension for optimal use of sub-event parallelism
  - Support specialized physics lists and/or detector construction (geometry) dedicated to sub-tasks
  - Support trajectory and visualization for tracks inside sub-tasks

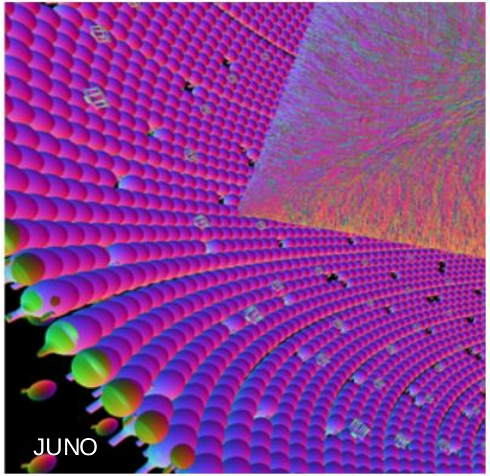
Example 1: Opticks/OptiX + CaTS

- Optical photons are copiously produced in optical materials (e.g., 45K/MeV energy loss in LAr). Optical photon simulation for a GeV-level charged particle requires significant computational resources (CPU and memory) → usually approximation by using lookup tables.

- Opticks[1] is a project that accelerates optical photon simulation by integrating NVIDIA GPU ray tracing (OptiX™). CaTS is an advance Geant4 example of interfacing with Opticks/OptiX™

https://bitbucket.org/simoncblyth/opticks



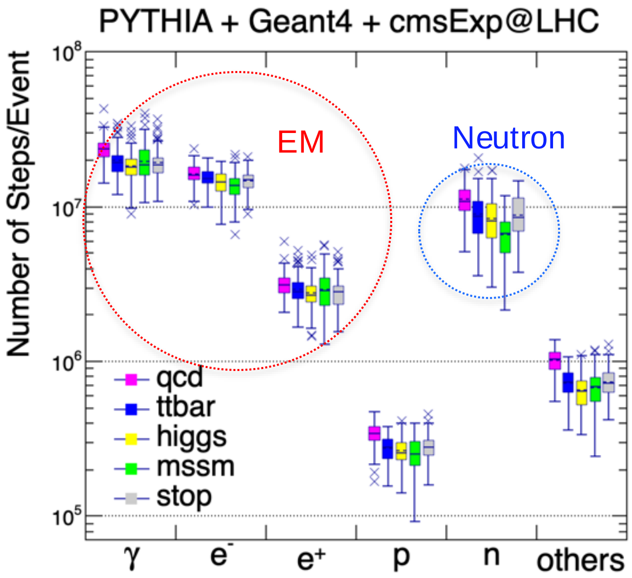


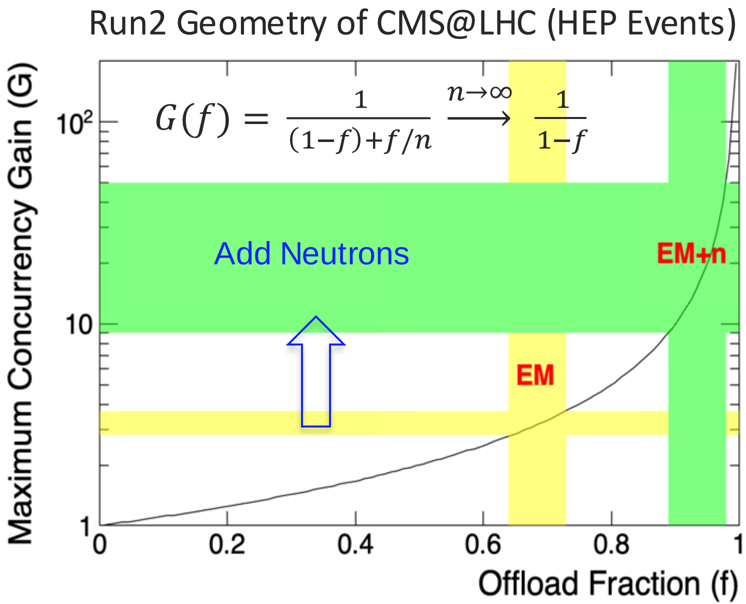
- Potential integration for HEP: DUNE (LAr-TPC), LZ (Liquid Xeon), Calvison, ePIC, etc.

[1] Opticks, S. Blyth, https://bitbucket.org/simoncblyth/opticks/).

Example 2: EM Particle Transport on GPUs

- Hybrid workflow simulation EM particles on GPUs while the rest of hadronic simulation on CPU

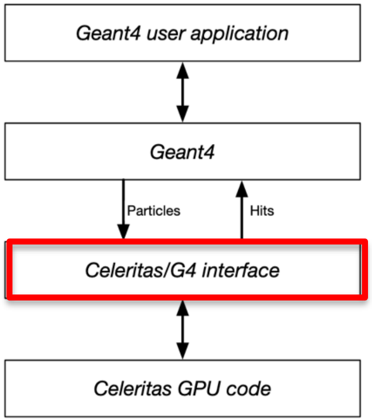


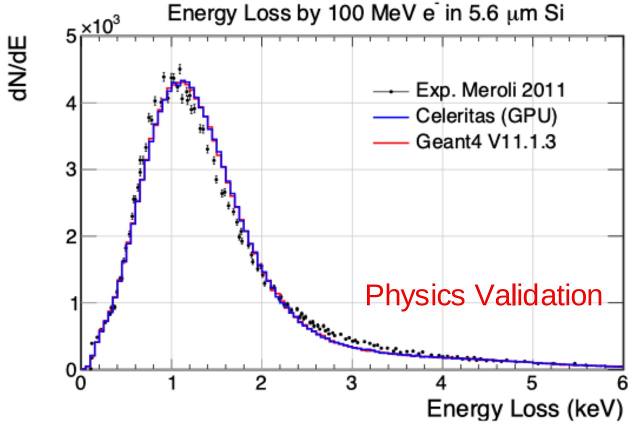


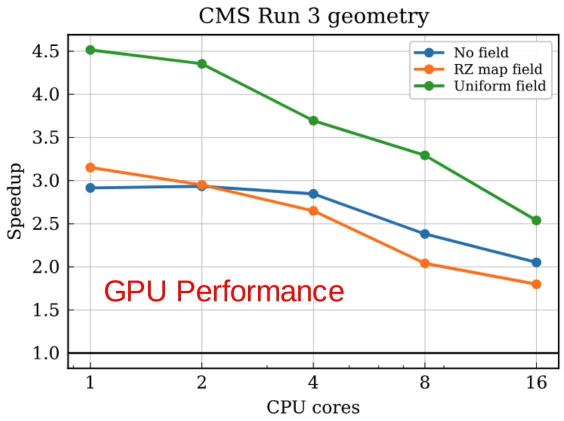
- The maximum gain (G) by the offloading fraction (f) when TimeGPU (f) ⩽ TimeCPU (1- f) with full concurrency (assuming no overhead).
  - EM particles: f = 67% → G = ~3 (EM + neutrons: f = 95% → G = 20)

Example 2: EM Particle Transport on GPUs

- Geant4 provides interfaces for GPU offloading
  - User (Tracking or Stepping) Actions
  - Fast Simulation interfaces
  - *G4VTrackingManager*: a custom tracking manager that is specialized for stepping selected particle types.
- R&D activities: Celeritas and Orange (US HEP-CCE) and AdePT and VecGeom2.0 (CERN)
  - Actively being integrated into experimental frameworks (CMS, ATLAS, etc.) and shows promising results



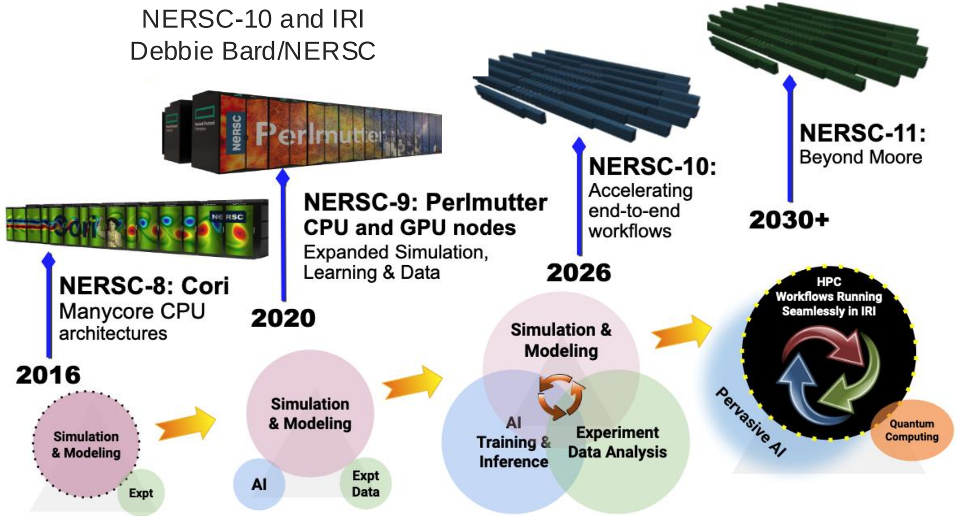




Future Ecosystem: Integrated Research Infrastructure (IRI)

- IRI is a new program encompassing all ASCR facilities and participating domain partners (ESnet6, NERSC-10, OLCF-6, HPDF and ALCF-4)
- e.g., NERSC-10 strategic planning: IRI of HPC systems accelerating end-to-end workflows
  - Simulation and modeling
  - AI Training & Inference
  - Experiment data analysis
- Beyond Moore
  - HPC workflow running seamlessly in IRI
- Innovation in software is a key

NERSC-10 and IRI
Debbie Bard/NERSC



- Geant4 is complying with the evolving HPC/heterogenous/IRI ecosystems
  - Efficient algorithms, data structure, interfaces for complex workflows → Sustainable and scalable toolkit

Summary

- Geant4 provides processes to cover nearly all particles over energies ranging in [0, ~PeV]
  - Major categories of processes are EM, hadronic, decay, parameterization and transportation
  - Geant4 packaged physics lists help to construct physics requirements for various user domains
- Geant4 provides flexible interfaces for external models and other MC libraries/packages
  - Fast simulation, parameterized physics
  - AI/ML training and inference
  - FLUKA.CERN, PENELOPE, PYTHIA, Opticks/OptiX, …
- Geant4 and its applications are continually evolving for modern computing ecosystems as well as improving physics models
  - Geant4 multithreading and tasking
  - Allow hybrid workflow for offloading specialized tasks to accelerators (GPUs)
- Geant4 provides many examples (basic, extended and advanced)