Simulation: Level of detail

John Apostolakis (CERN)

Outline

- Simulation of interactions with matter
  - tools and toolkits
- Level of detail and adaptability
  - Geometry
  - Physics modelling
  - Hits and Signal generation
- Note: perspective and examples from Geant4
- Optical photons
- Highlights of Geant4

What can a simulation tool do?

- A radiation transport tool(kit) provides 'general' capabilities to undertake most/all of the key tasks:
  - tracking, and geometrical propagation
  - modelling of physics interactions,
  - visualization, persistency
- and enable a user to describe a setup's
  - geometry,
  - radiation source,
  - details of 'sensitive' regions

Why focus on level of detail?

- The process of developing a transport simulation is typically iterative
  – Starting with a simple description, needing a quick first answer – use as ‘Engineering tool’.
  – Developing incrementally the setup description and the precision needed
  – Eventually need prediction that takes into account all potential effects, interactions.
- Thus handling low, intermediate and high levels of detail, with corresponding precision and computing requirements is important in many use cases.

Geometry description

- Different types of descriptions possible:
  - Solid modeling (describing each volume)
  - Boolean operations between surfaces
  - Regular ‘voxel’ structures
- Geometries can have nesting or not
  - Flat geometry has one level. All volumes are in the world super-volume
  - Hierarchy enables each volume to contain others.

Geometry choices

Overall Structure:

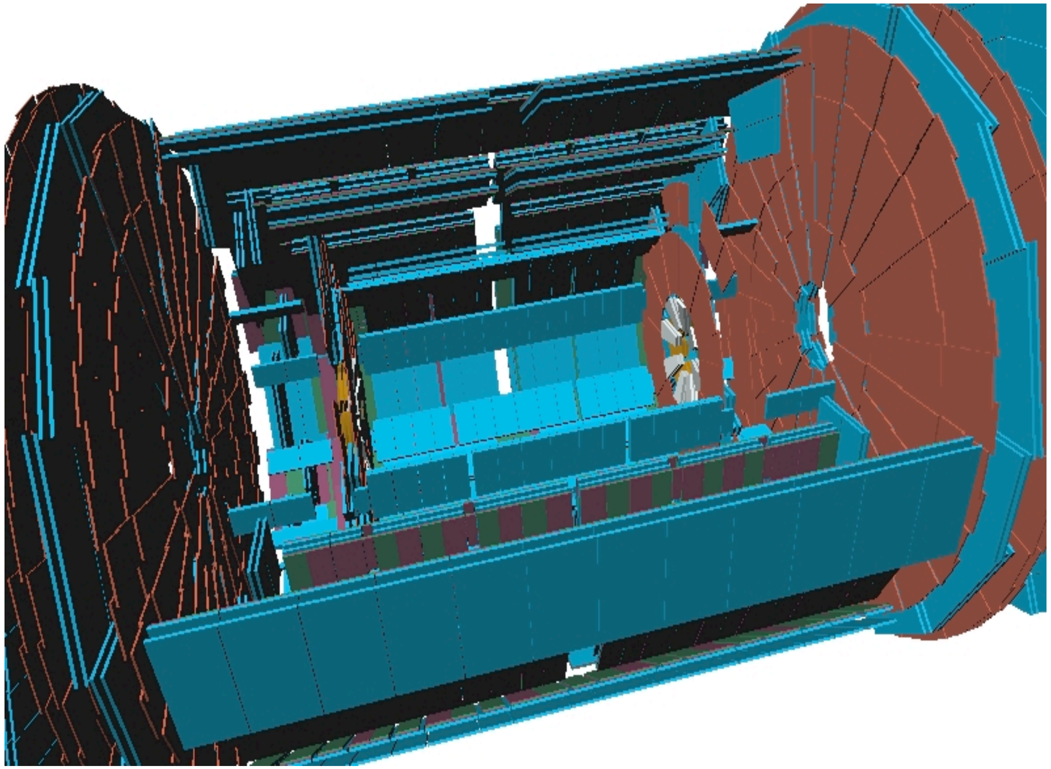
- Hierarchy: supports larger number of irregular volumes
  - Choice supported by Geant4, enabling sub-structures to be created (eg for parts of instruments)
- Flat: simpler description, handling
  - Easy for simple setups
  - Typically limits the number of sub-volumes
    - Although navigation optimisation can alleviate partially

Level of detail: geometry

- Detail of single volume
  – Simple ‘solid’ or complex product of boolean operations
- Description of setup
  – From detail of each screw or ‘element’ on a chip
  – Wires individually, as approximate bundle or simplified structure
  – Realistic description of passive and active volumes
  – Simplified description of elements (all or some)

Example: Geant4 Geometry

- Extremely versatile
- Large number of volume shapes (CSG + BREP)
- Hierarchical combination of volumes
- Materials
  - isotopes, elements, compounds, phase, temp
  - user-created or use NIST database



Spanning simple to complex setups

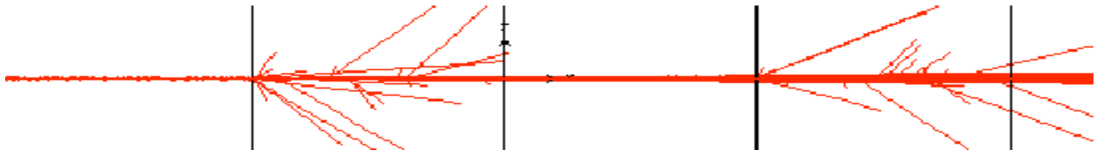
- In the Geant family of codes (including Geant4) it is possible to create simple or complex geometries
  - Incrementally refining a geometry using a hierarchy:
    - One 'logical' volume can be placed in several places
    - Adding detail to 'logical' volume makes it appear in all locations
    - Repetitions can be done by placing many volumes or creating repeated volume (eg parameterised volumes.)
  - Input from external sources: XML, CT, some CAD sources.
- Cost of complexity
  - CPU cost is typically proportional to average # of boundaries in a track;
  - Very complex shapes can cost extra (~20% in one experiment.)

Material composition

- Rough: average Z, A
- Medium: 'all' elements
  - Basically covering the significant constituents
- High detail
  - Trace elements
  - Isotope composition for important elements
  - Chemical composition (for low energy EM, neutrons)
- Potential avenues
  - Definition of 'standard' materials (eg NIST)
  - Materials created by users from elements, isotopes

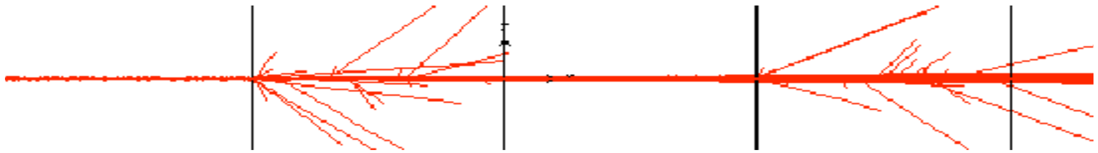
Production thresholds – or 'cuts'

- Many EM processes produce infinite or 'just' many low energy secondaries
  - Their contribution to observables is limited, and the time for their simulation is large
- The mechanism for deciding which secondaries to ignore and/or which tracks to abandon is a defining feature of a simulation tool(kit)
  - Electrons/gammas below a critical energy (or range) are not generated
  - Typically a different threshold can be chosen for γ and e^-.



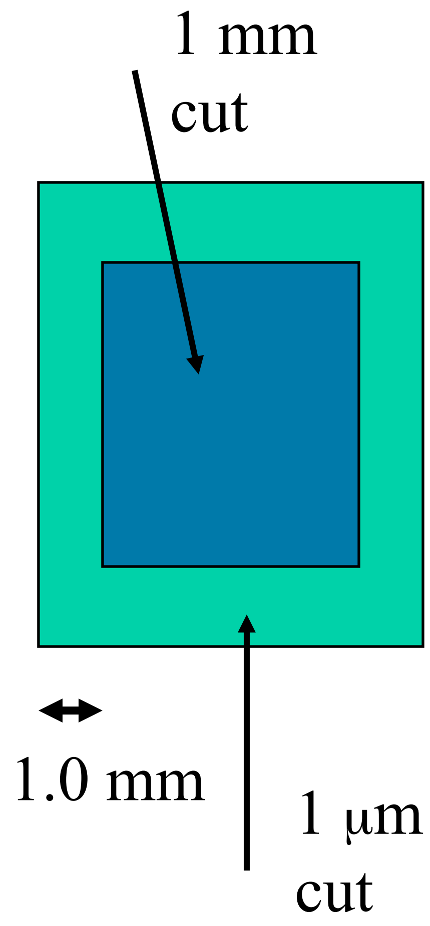
Cuts in Geant4 (the simple way)

- Geant4 starts with a unique production threshold ('cut') expressed in length (range of secondary).
  - For all volumes
  - Possibly different for each particle (gamma, electron).
- This attempts to promote
  - Clear criteria for locality of energy deposition
  - better use of CPU in dense materials vs the E cut for equal precision.
- With one cut/threshold value the part of the detector with the lowest need fixed the cut for all the simulation.
  - Eg a silicon sensor (50 μm) dictates to a veto counter (2.0 cm).



Refining cuts by 'region'

- Enable 'regional' choices between
  - Sacrificing accuracy of energy deposition
  - Accepting a performance penalty
- Lifting the uniqueness of cuts
  - Implemented by introducing geometrical 'regions'
    - A set of production threshold attach to a region
      - e.g. 10 microns for e-, 2.5 microns for gamma
  - Example: beam cleaning element



Why focus on adaptability?

- A transport simulation is not an isolated application
  - The geometry description is often created in other applications (e.g. CAD) or measured (e.g. CT)
    - Can be recreated at a cost in time and effort, or
    - Imported or translated for full or high detail.
  - Many times it is embedded in a larger application
  - Output/interface to additional tools
    - For computing the signal from the energy deposition or describing the effect on a semiconductor device.

Tool or Toolkit?

- Engineering tool
  – Ready-made to provide answer for specific problem(s)
- Research tool
  – Enables tayloring, adaptation, wider investigation of systematic effects
- Toolkit
  – May not come with a full set of ready-made tools
  – Enables users to created both types of tools

Some tools created using Geant4

- BDS, G4BEAMLINE
  – Simulate beam lines
- Geant4 Application for Tomographic Emission
  – Simulates PET and SPECT detectors
- MRED (Vanderbilt, proprietary)
  – Simulates detailed effect of radiation on semiconductor devices (coupled with commercial TCAD device simulation)
- ESA-funded engineering tools for satellites

Optical processes in Geant4

- Optical photons are produced by the following Geant4 processes:
  - **`Cerenkov`**
  - **`Scintillation`**
  - **`TransitionRadiation`**
  - Warning: optical photons are generated by these processes without energy conservation
    - their energy is not subtracted from 'energy deposition'

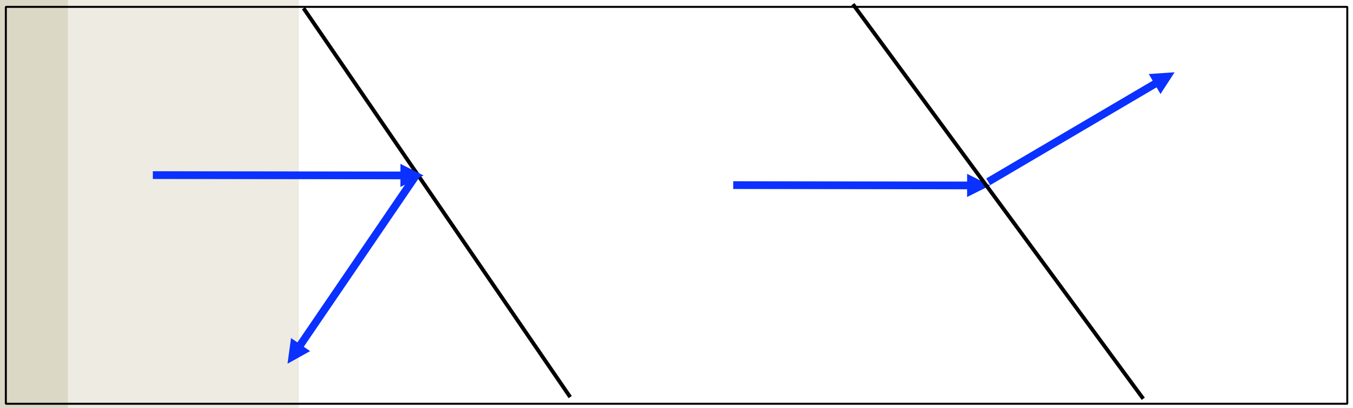
- Optical properties defined in material property tables
  - reflectivity, transmission efficiency, dielectric constants, surface properties
  - Photon spectrum properties also defined in Material
    - scintillation yield, time structure (fast, slow components)
  - Properties are expressed as a function of the photon's momentum

Processes undergone by optical photons

- Optical photons can undergo:
  - bulk absorption
  - Rayleigh scattering
  - wavelength shifting
  - refraction and reflection at medium boundaries
- Geant4 keeps track of polarization
  - but not overall phase → no interference

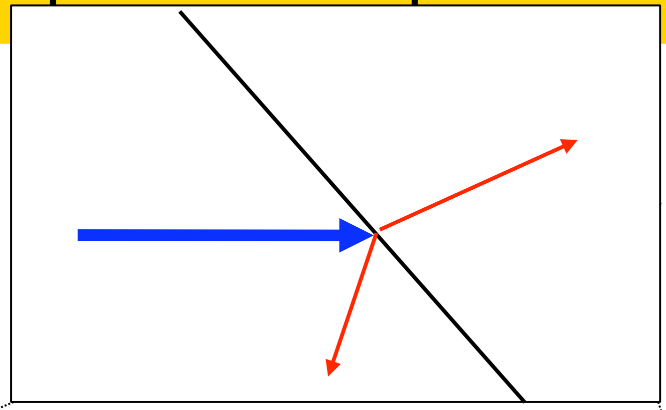
Photon ‘interactions’ at boundaries

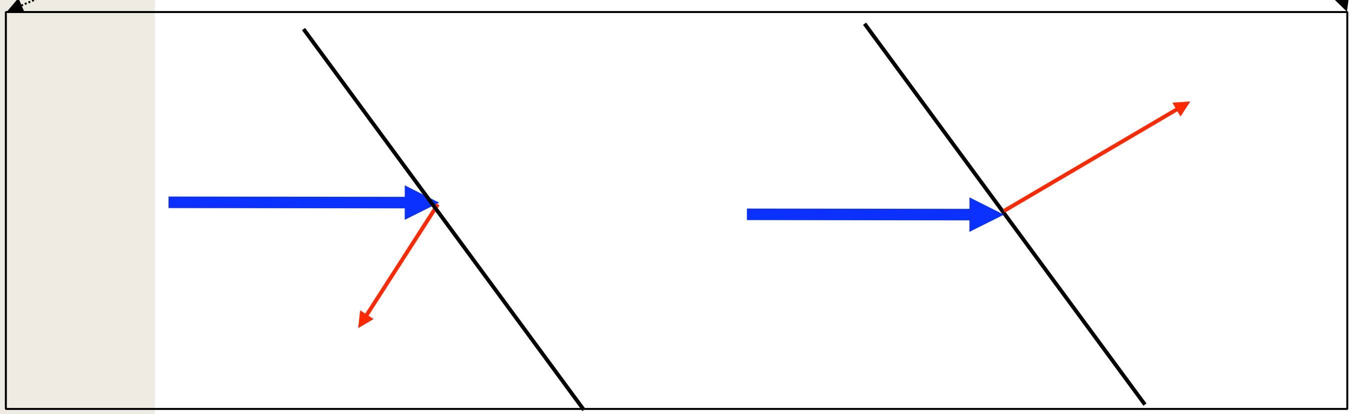
- Handled by G4OpBoundaryProcess
  - refraction
  - Reflection
- User must supply surface properties using G4OpticalSurface models
- Boundary properties
  - dielectric-dielectric
  - dielectric-metal
- Surface properties:
  - polished
  - ground
  - front- or back-painted, ...



Boundary interactions
Optical photons as particles

- Geant4 demands particle-like behavior for tracking:
- thus, no “splitting”
- event with both refraction and reflection must be simulated by at least two events





Geant4 General Notes

- Geant4 is an object-oriented C++ toolkit
  - the goal is to provide all that is needed to build a wide variety of physics simulation applications
    - range of physics models,
    - tracking, geometry hit collection and scoring
    - and auxiliary components
  - code is open, modular – available for all to download
    - Anyone can inspect, understand, tailor, revise, … improve.
  - extensive documentation and tutorials provided
- Principal references:
  - NIM A506, 250 (2003) and IEEE Trans. Nucl. Sci. 53, 270 (2006)

Further capabilities

- External EM fields affect charged particles
- Tracks 'hit' via user-written detectors
  - 'New' scoring of radiation observables via commands
- Event biasing

- Auxiliary capabilities
  - Visualisation via several systems
  - Input/Output ('persistency') for geometry, events

Physics Choices and 'Physics Lists'

- Application developer (expert developer, intermediary or user) has the final say on the physics chosen for the simulation. He/she must:
  - select the relevant particles and physics processes from those provided, for each particle type
  - validate the selection for the application area (or ensure it has been done.)
- 'Physics Lists' represent this collection
- Deciding or creating the physics list is the user's responsibility
  - reference physics lists are provided by Geant4
    - are continuously-tested and widely used configurations (eg QGSP)
  - other 'educated-guess' configurations for use as starting points.

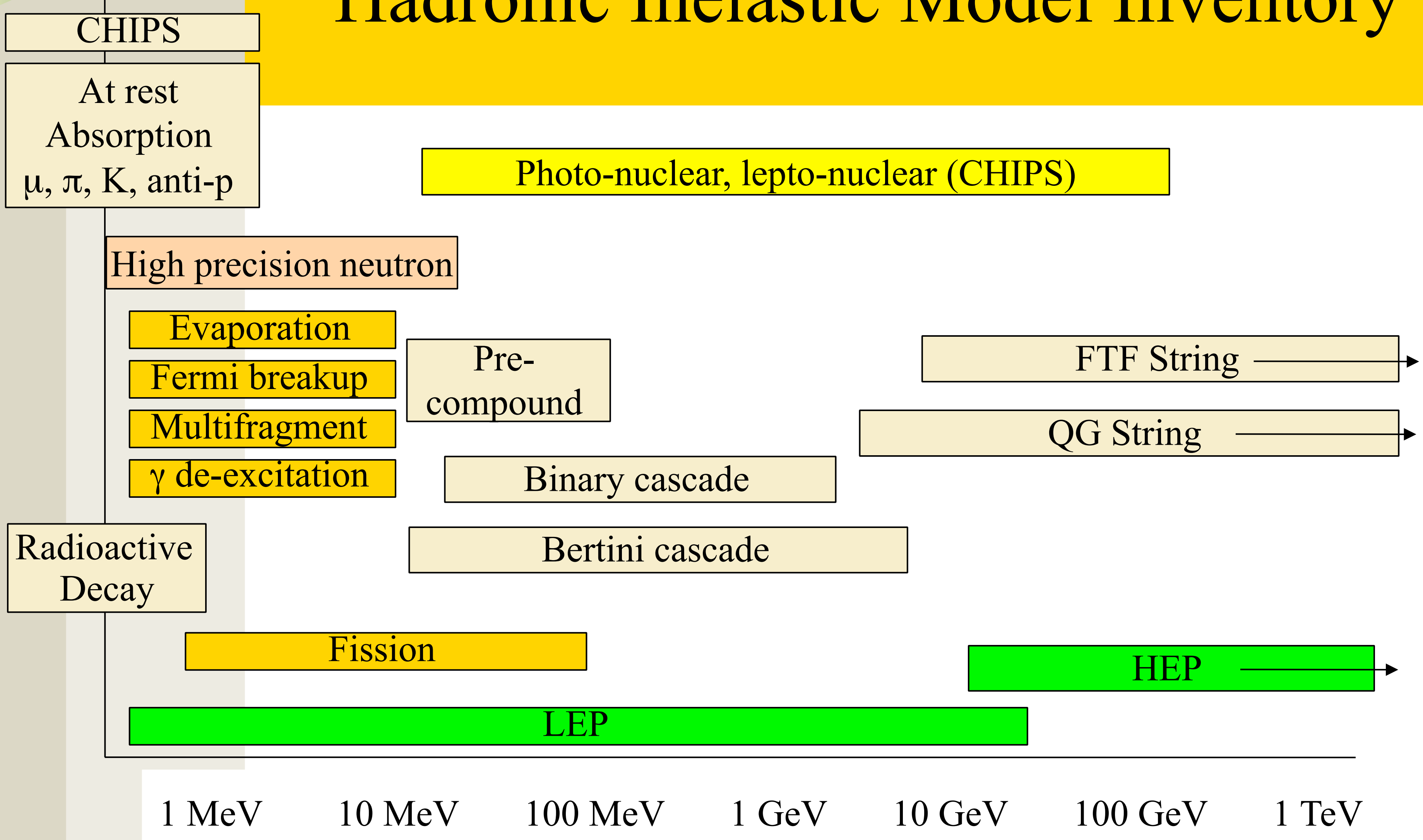
Electromagnetic Physics in Geant4

- “standard” package (1 keV and up)
  - multiple scattering, ionization, bremsstrahlung
  - Compton, pair production, photo-electric, annihilation
  - synchrotron, Cerenkov, transition radiation, high energy muon processes
- “low energy” package
  - uses database information to extend interactions below 1 keV
  - Atomic de-excitation, specialised processes water down to eV
    - And many of the same processes in “standard”
- optical photons
  - reflection/refraction, absorption, Rayleigh, wavelength shifting

Geant4 Hadronics Philosophy

- Offer choice of processes, models, and cross sections
- Separate total and reaction cross sections from final state generators
  - allows easy update, multiple implementations of cross sections
  - final state generators maintain ‘internal’ cross sections specific to model
- Develop on a modular framework
  - Allows experts (incl. users) to substitute specialized physics
  - easier to add new models, cross sections as they become available

Hadronic Inelastic Model Inventory



‘Theoretical’ models

- Evaporation and pre-compound models
- Cascade and CHIPS
  - Bertini-like
  - Binary Cascade
  - Chiral Invariant Phase Space
- Quark-Gluon String (QGS) model
  - And ‘variant’ FTF model, using Fritiof approach

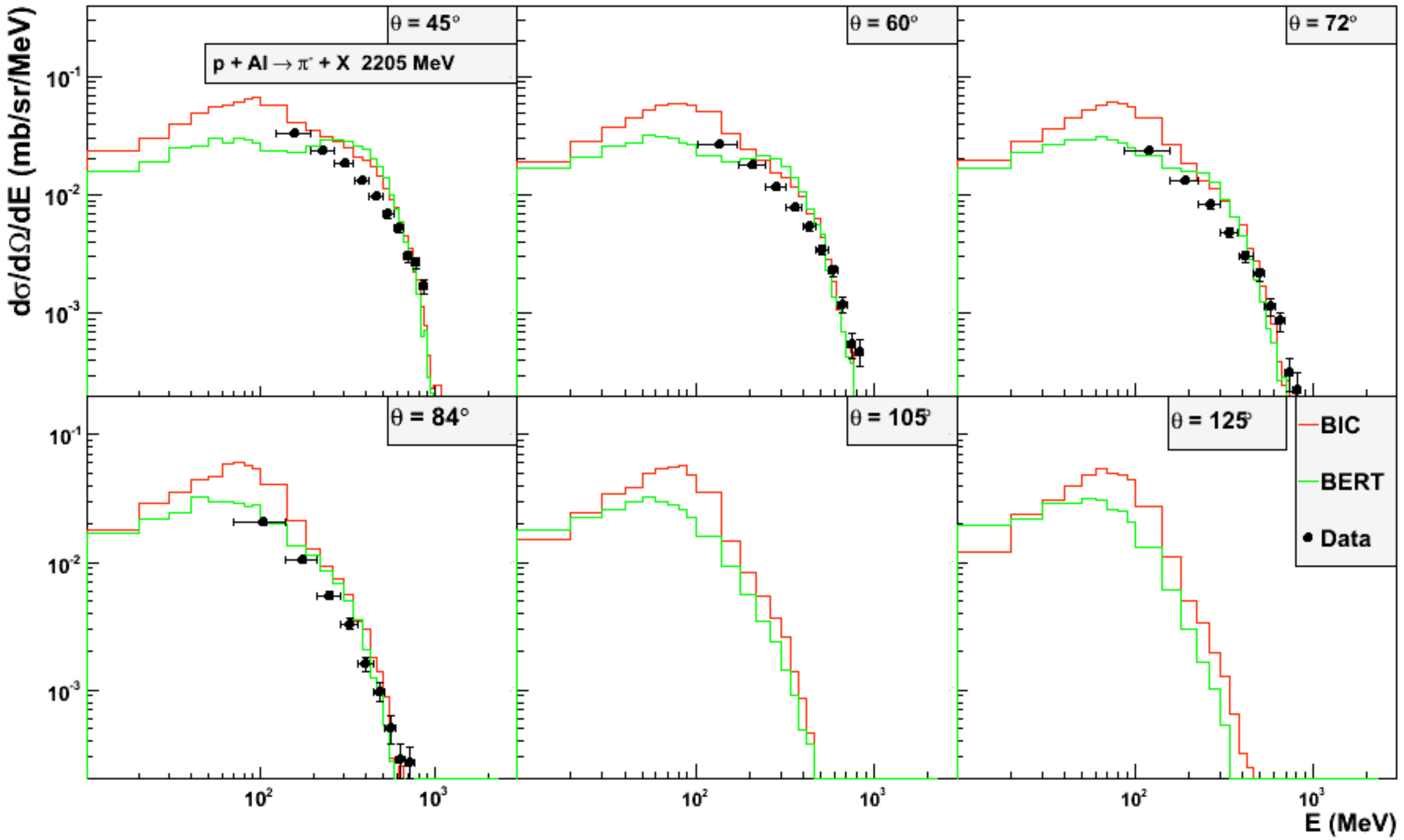
Binary Cascade

- Hybrid between classical cascade and full QMD model
- Detailed 3-D model of nucleus
  - nucleons placed in space according to nuclear density
  - nucleon momentum according to Fermi gas model
- Collective effect of nucleus on participant nucleons described by optical potential
  - numerically integrate equation of motion
- Particle interaction by resonance formation and decay

Bertini Cascade

- The Bertini model is a classical cascade:
  - it is a solution to the Boltzmann equation on average
  - no scattering matrix calculated
- Core code:
  - elementary particle collider: uses free-space cross sections to generate secondaries
  - cascade in nuclear medium
  - pre-equilibrium and equilibrium decay of residual nucleus
  - Nucleus modelled as shells of different densities

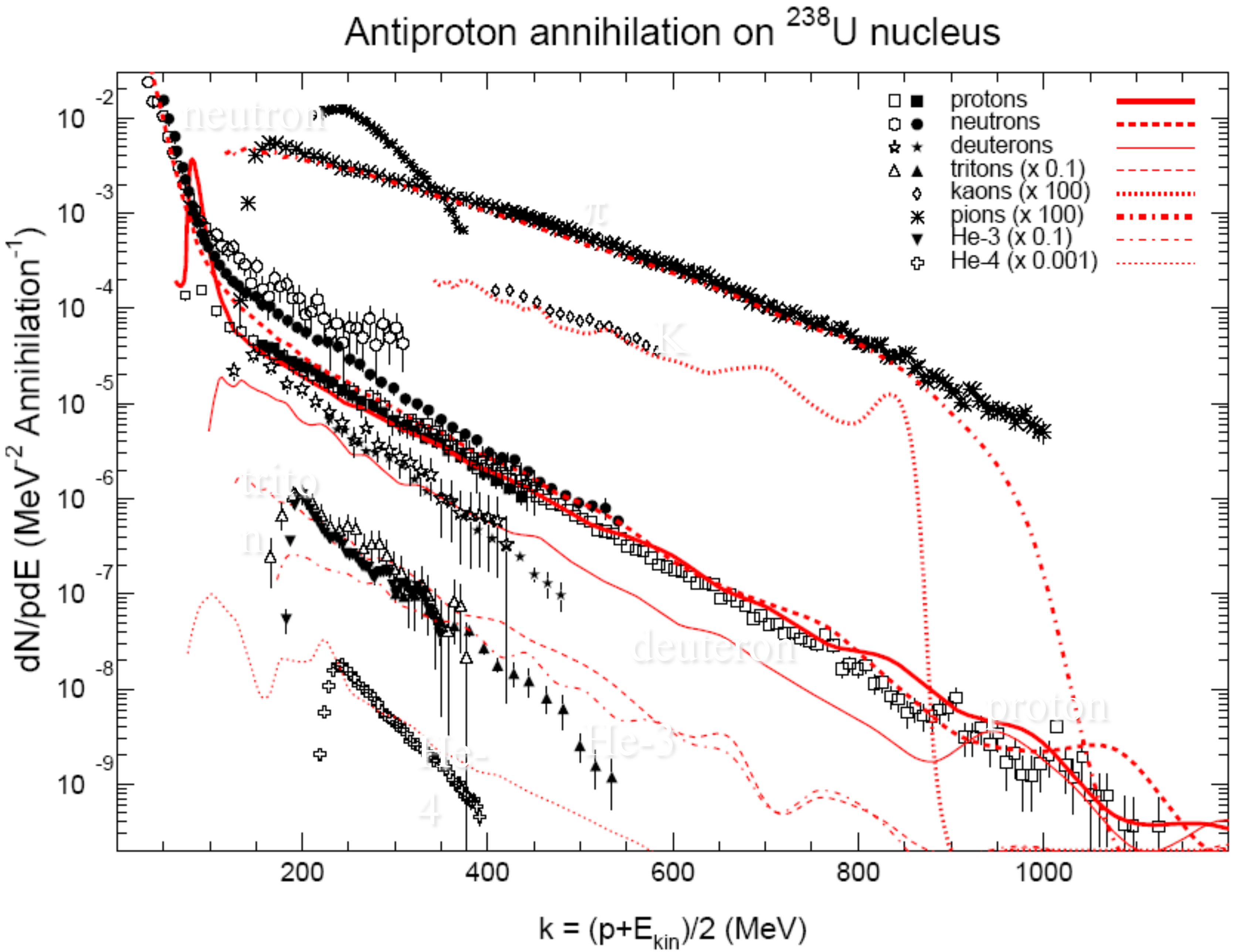
Pion production at 2205 MeV



Chiral Invariant Phase Space (CHIPS) Model

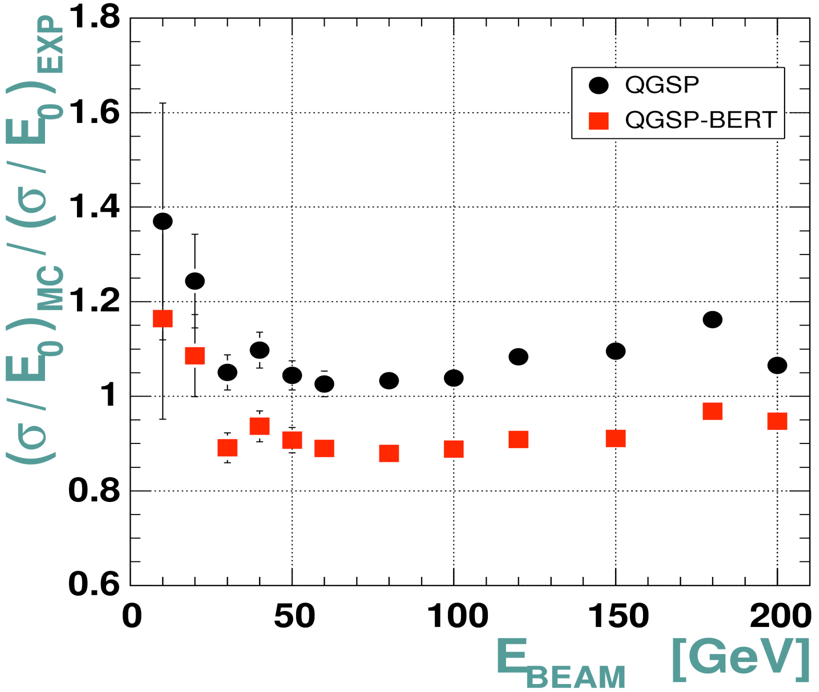
- Theory-driven model based on quasmons (an ensemble of massless partons uniformly distributed in invariant phase-space)
  - a quasmon can be any ground state hadron or excited system of hadrons
- Quasmon hadronizes by internal quark fusion and/or quark exchange with partons in neighbouring nucleon clusters
- Originally developed as a final state generator
  - now used for:
    - nuclear capture of negatively charged hadrons
    - gamma-nuclear reactions
    - lepto-nuclear reactions

Antiproton annihilation - CHIPS Model

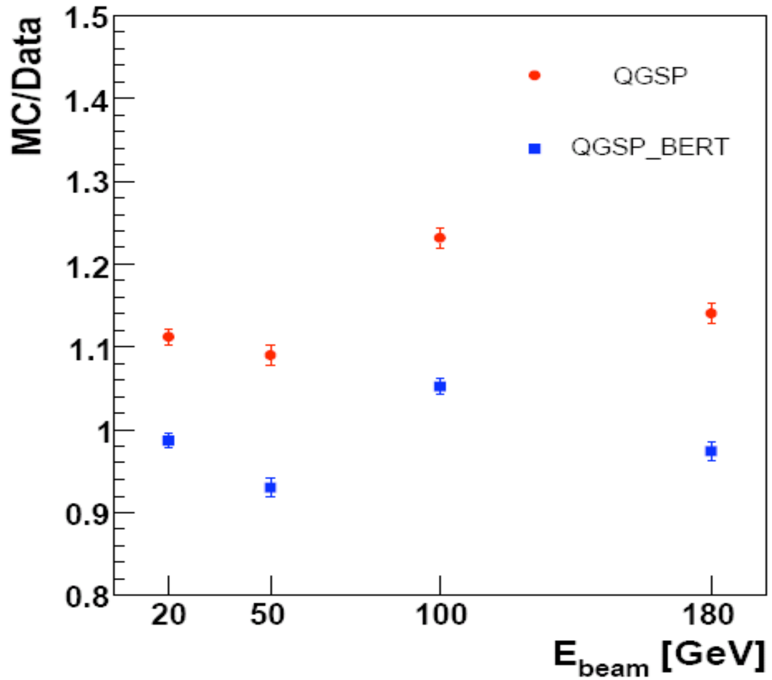


Pion resolution in ATLAS stand-alone test-beams

HEC



Tile

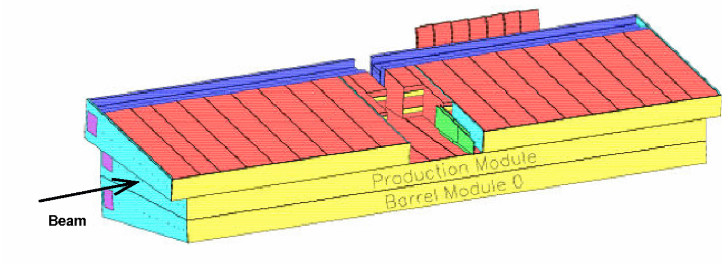


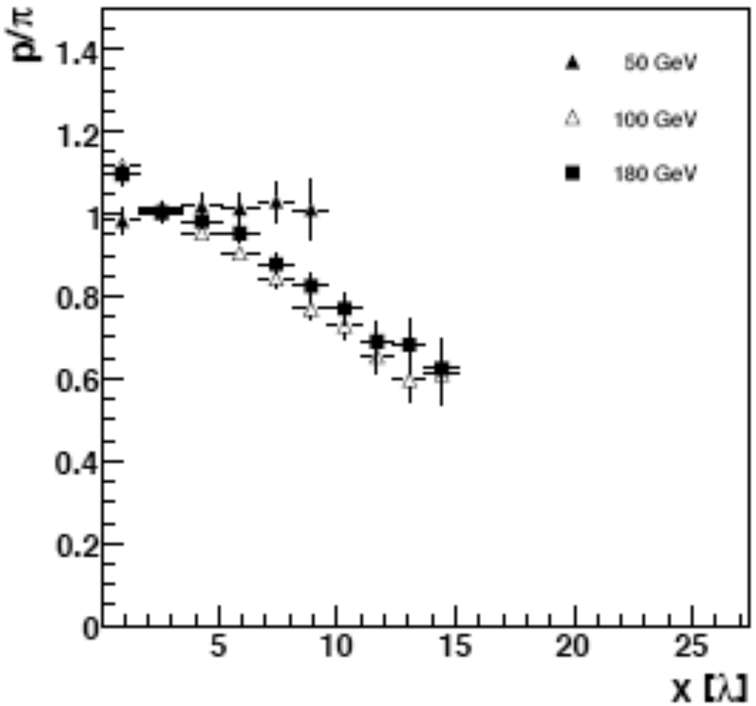
Bertini cascade makes resolution better:

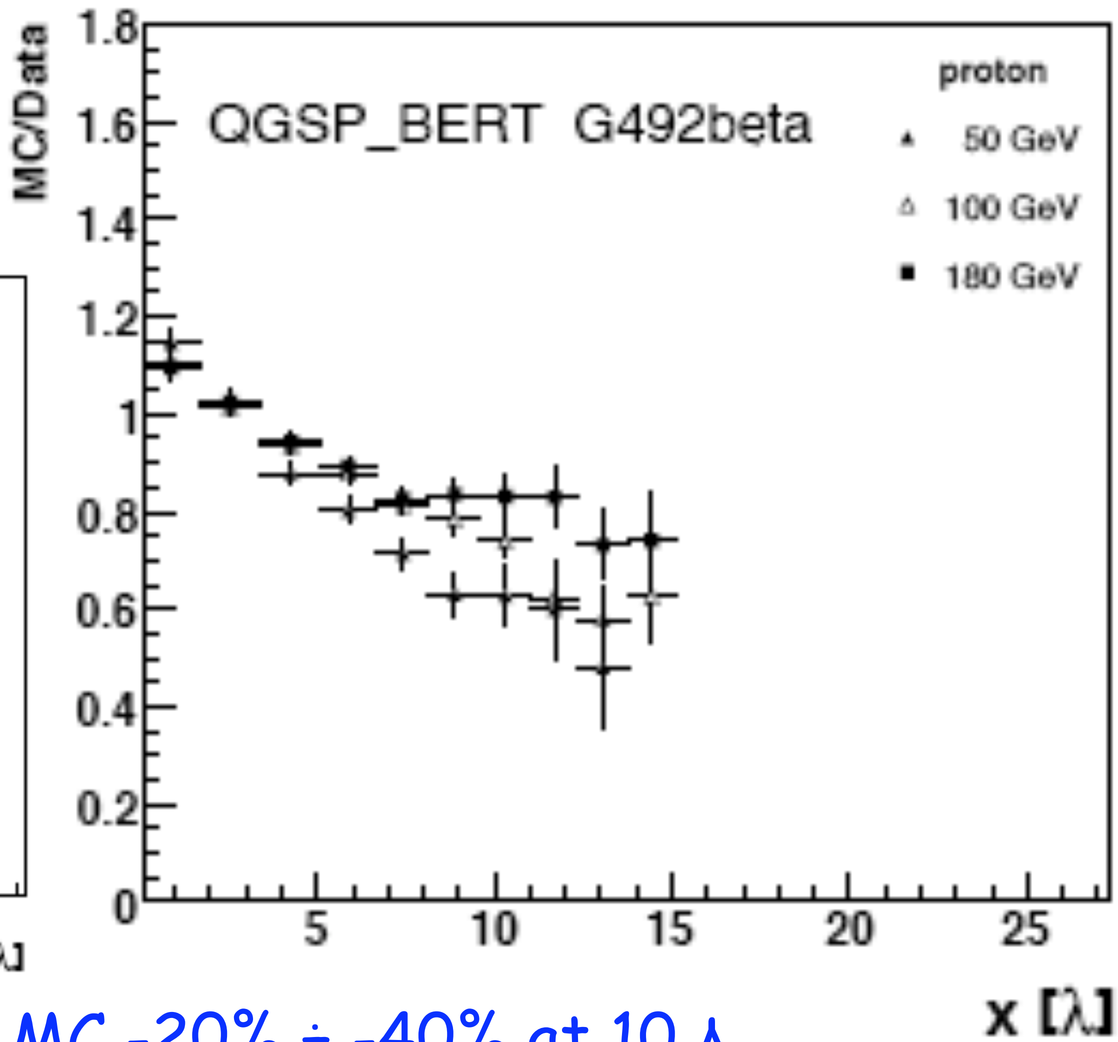
in Tile: better agreement with data (±10 %).

in HEC: MC resolution too good by -10%.

Proton longitudinal shower profile in stand-alone ATLAS TileCal test-beam at 90°

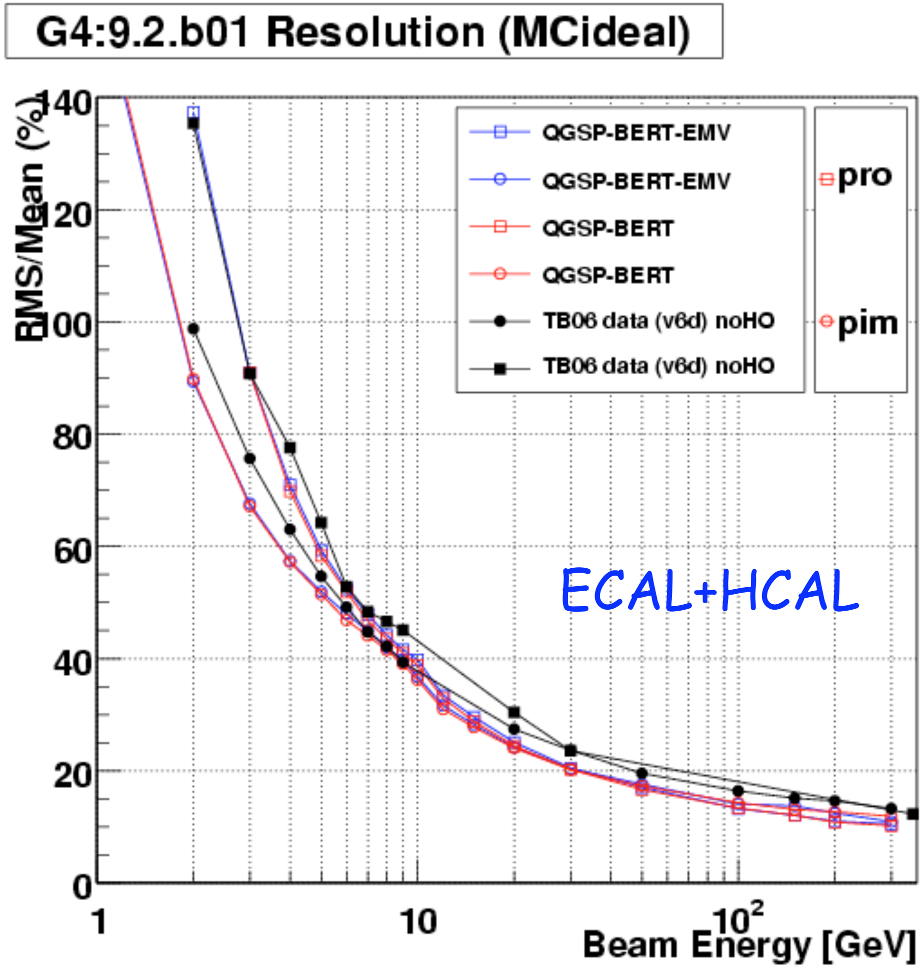


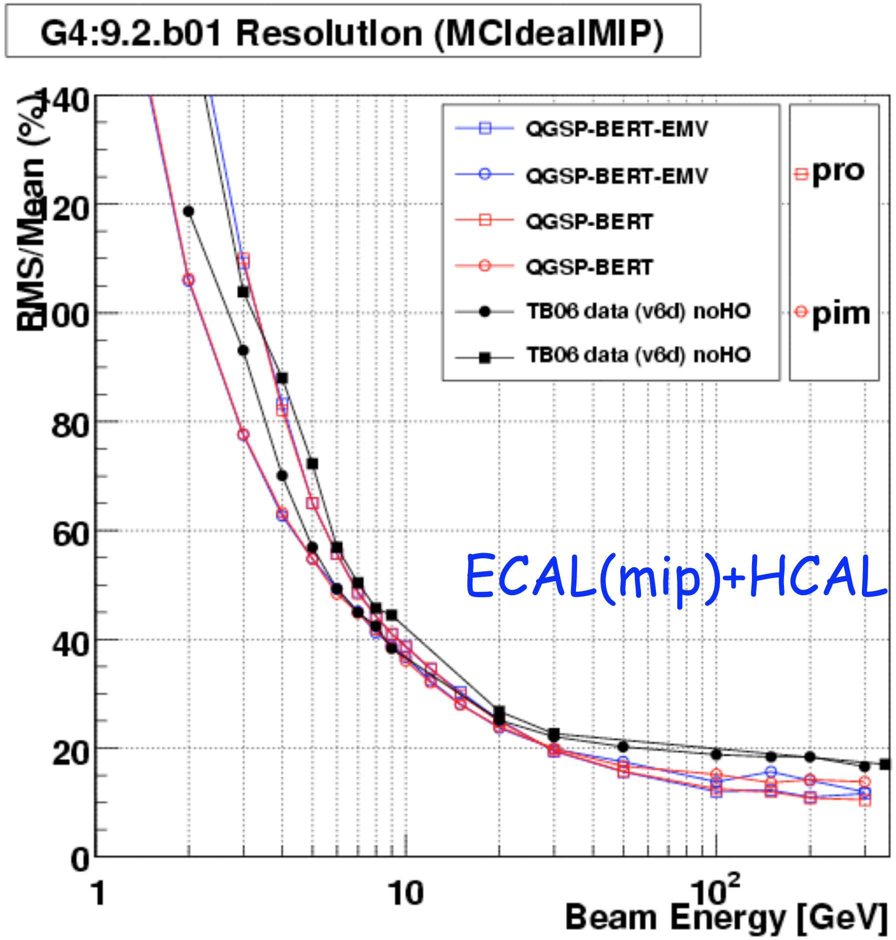




MC -20% ÷ -40% at 10 λ.

Pions and protons energy resolution in CMS combined test-beam





Resolution is too good in Monte Carlo

Backup slide(s)

Survey of Hadronic Models

- Three broad categories of processes/'models':
  - – tabulated: based on (large) databases
  - – theory-based: based on (theoretical) models
    - Parameters, if any, chosen by comparing with thin-target data
  - – parametrized: key aspects parameterised for speed
    - Parameters determined from fits to data

Geometry (cont)

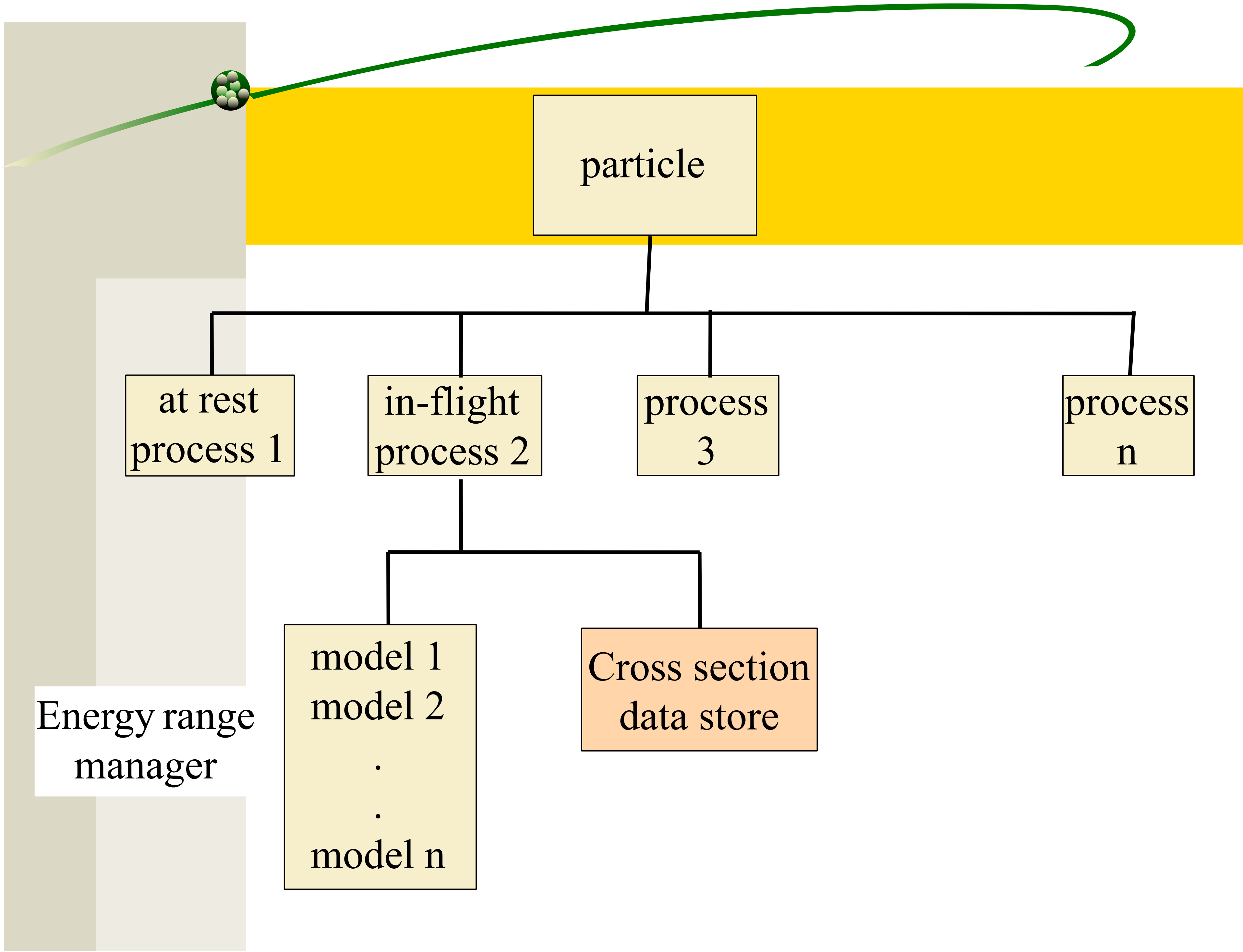
- Solid based geometry
  - – Easy for user to describe
- Built-in navigator
  - – Also tools to validate/check geometry model
- Multiple levels of hierarchy
  - – To describe complex structures
    - LHC detectors of few million of volumes

EM production threshold

- thresholds
  - Charged particles are tracked down to zero energy
  - Production threshold for delta electrons expressed in length
- Threshold in length chosen in order to optimise CPU use

Hadronic Processes

- At rest
  - stopped μ^-, π^-, K^-, anti-proton, Σ^-, anti-Σ^+
  - radioactive decay
- Elastic
  - models for π, K, p, n, hyperons
- Inelastic
  - different models for π, K, p, n, hyperons
  - ions
  - capture in flight
    - (n,γ), π^-
  - fission
    - neutron-induced
- Photo-nuclear, lepto-nuclear
  - (neutrino-nuclear not verified yet)


particle
at rest
process 1
in-flight
process 2
process
3
process
n
model 1
model 2
.
.
model n
Cross section
data store
Energy range
manager

Precompound and Nuclear De-excitation Models

- Precompound Model – used to take the nucleus from a highly excited state down to equilibrium
- May be used:
  - by itself for p, n below 170 MeV or
  - as a “back-end” for cascade or high energy models
- Model begins with nuclear excitation energy, a set of excitons, and a parametrized level density
- Excitons are decayed until equilibrium is reached, then control is transferred to competition of low energy models
  - evaporation, fission, Fermi breakup, multi-fragmentation, photon evaporation

High Precision Neutrons

- data-driven, based on G4NDL data library which consists of data from ENDF, JENDL, CENDL, BROND, JEF, MENDL
- covers
  - elastic
  - inelastic (n, p, d, t, ^{3}He, α in up to 4-body phase space final states)
  - radiative capture (discrete + continuous gamma spectra)
  - fission
- incident energies from thermal to 20 MeV
- modeling:
  - cross sections, angular distributions, final states all tabulated
  - sample from interpolated data tables

Absorption At Rest

- Processes available to handle all negative, long-lived hadrons
  - anti-proton and and anti-sigma+ included
- Also for μ^-, τ^-
- Above processes implemented by CHIPS model
- Alternative processes available for μ, π

Default Cross Sections

- Elastic, inelastic from GHEISHA with modifications
  - for p-A, $\pi-$A, use tabulated fits to data
  - interpolate in A where there is no data
  - for all others, make particle-specific corrections to p-A, $\pi-$A cross sections
- Capture
  - for neutrons only
  - $\sigma = 11.12\ \sigma(Z)$ / $KE^{0.577}$
- Fission
  - for neutrons only
  - direct table lookup for $^{233,235}U$, ^{239}Pu, KE < 10 MeV
  - all others: table lookup x (38.7 $Z^{4/3}$/A – 67) up to 1 TeV

Alternative Cross Sections

- Low energy neutrons
  - G4NDL available as Geant4 distribution data files
  - elastic, inelastic, capture, fission
  - Available with or without thermal cross sections
- “High energy” neutron and proton reaction σ
  - 14 MeV < E < 20 GeV
- Pion reaction cross sections
- Ion-nucleus reaction cross sections
  - Good for E/A < 10 GeV

Hadronics Summary

- *Hadronic processes require physics models and cross sections*
  - *user must choose (carefully)*
  - *more than one model and/or cross section allowed*
- *Many models offered – three main types:*
  - *tabulated*
  - *parameterized*
  - *theory-driven*
- *Most cross section sets provided by default*
  - *alternative cross sections are available*

Other Summary

- G4 provides full detector simulation capabilities & more
  - Flexible geometry modeler for many, complex volumes
  - Tracking, event biasing, scoring, hit creation
- Configurations of physics models provide physics options
  - Tailored for sets of application areas
  - Created, tested for key application areas
    - QGSP, LHEP, QGSC, with emerging cascade options (eg QGSP_BIC)
  - Starting points for further refinements, also by users
- Standard models of EM interactions (EM physics)
    - and extensions to low energies, specialised modeling