Geant4 in production: status and developments

John Apostolakis (CERN)

for the Geant4 LCG team
(includes joint work with
other G4 collaboration members)

Outline

1. EM Calorimeter Response
   - Cuts, stability of EM energy deposition: issue, improvements
2. Hadronics and shower shape
   - Shower evolution studies (together with Phys. Val. sub-project)
   - Thin-target comparisons extended
3. New capabilities
   - Extensions to geometry modeler, scoring, ..
4. Production use of Geant4
   - Robustness shown in large scale productions
   - Users create applications and extend the toolkit
5. New Collaboration Agreement, License

EM Calorimeter response

Cut/threshold dependence

Improvement in Multiple Scattering

Energy deposition and cuts: issues

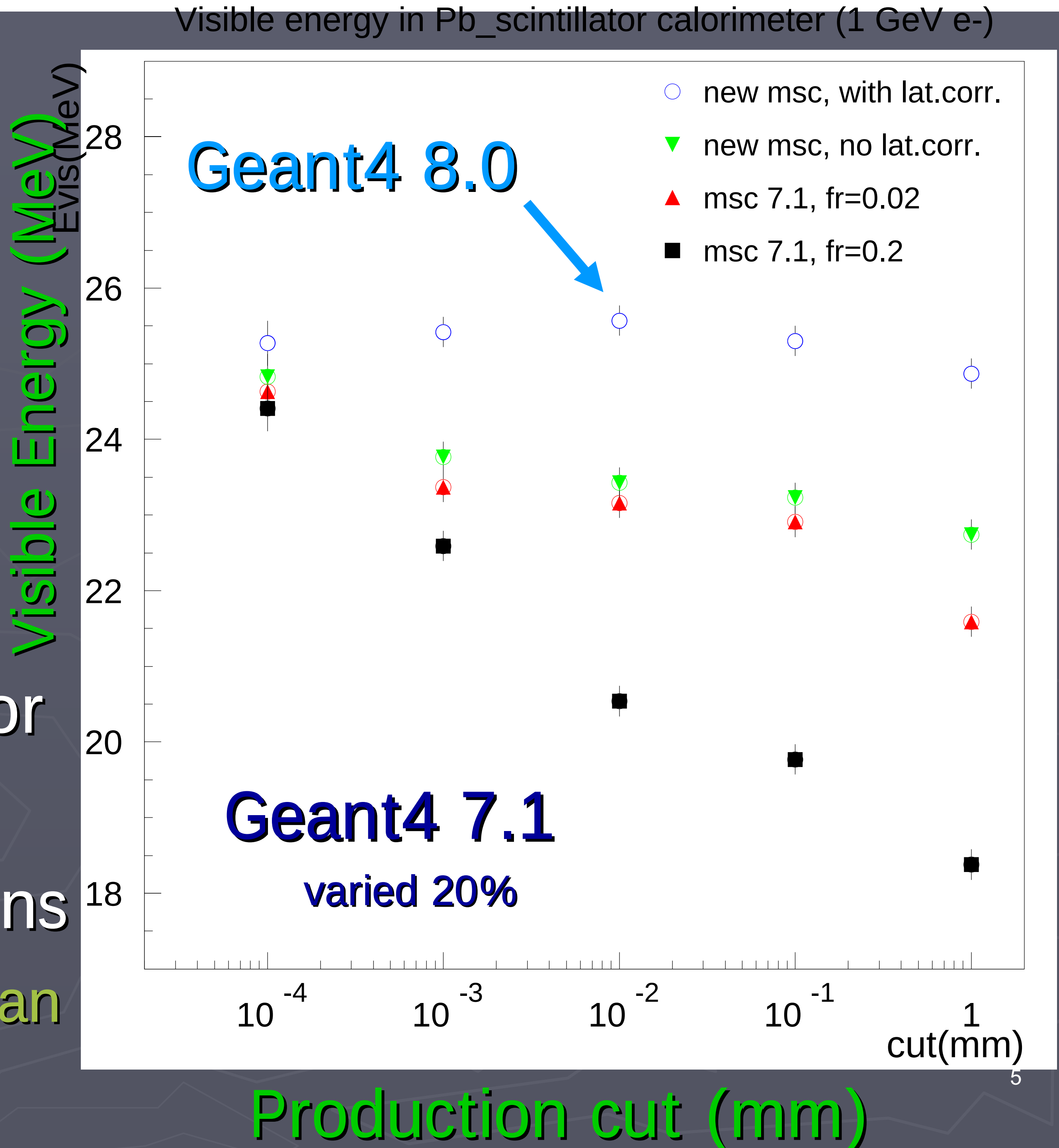
- Electron transport is key to accurate energy deposition, resolution
  - in setups with materials with very different Z
- Users reported results strongly dependent on cut value (or step limits)
  - Sampling calorimeters: Atlas (Cu–lAr), ILC (W-Si), LHCb (Pb-Sci)
  - In water phantoms with perturbing layer (Poon & Verhaegen)
- Cut dependence verified in HEP sampling calorimeters (eg Cu-lAr, Pb-Sci)
  - Energy deposited varied 10-30% for cuts changed from 1 μm to 1 mm
    - Effect existed in previous Geant4 releases (5.x, 6.x and 7.x)
- Investigation concluded G4MultipleScattering needed improvement
  - Revisions provided in Geant4 8.0 address this issue
    - Correlation between angular deflection and lateral displacement
    - Step size limitation, introduced also in initial volume/material

M. Maire, L. Urban

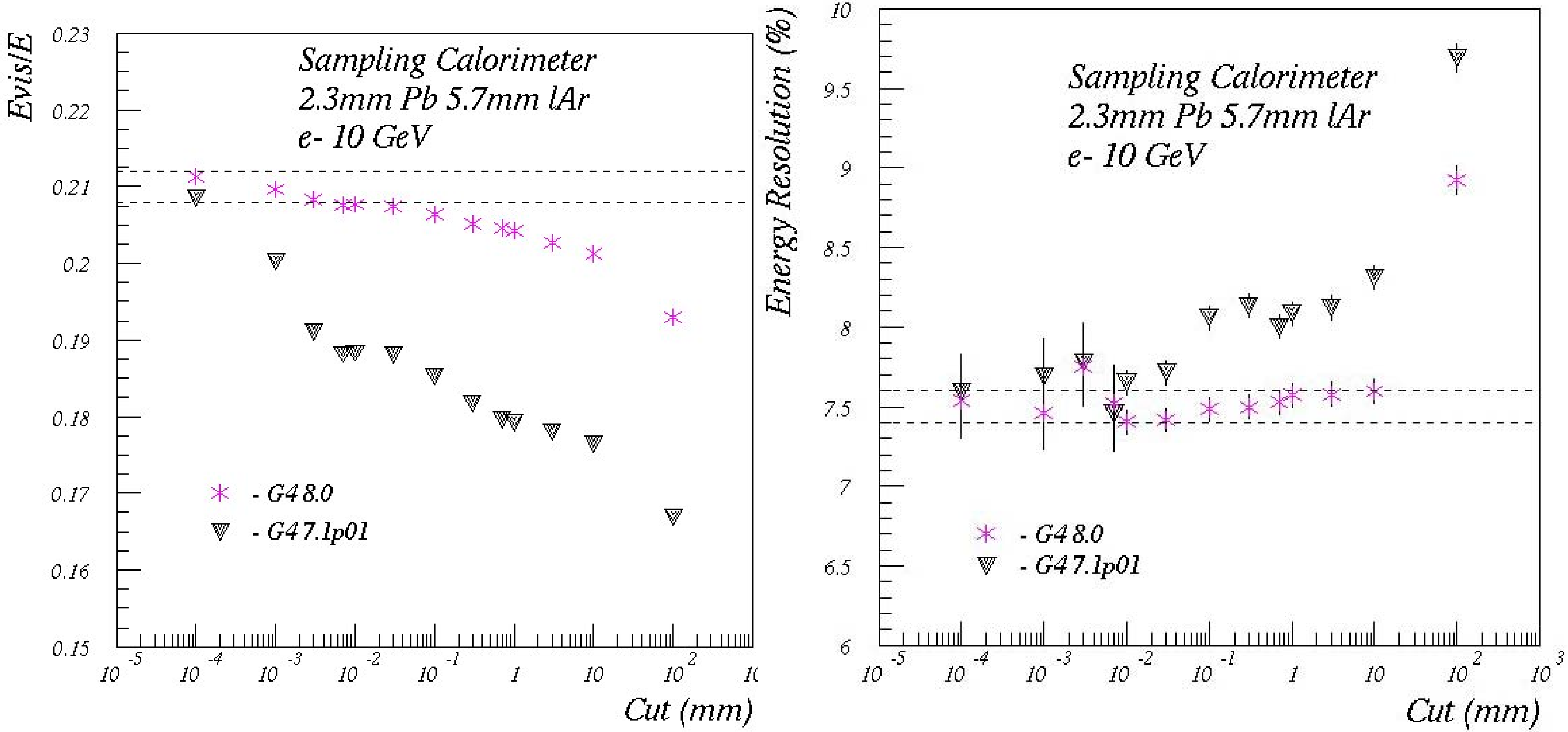
First results

Visible Energy
In Pb scintilator
Calorimeter
1 GeV electrons

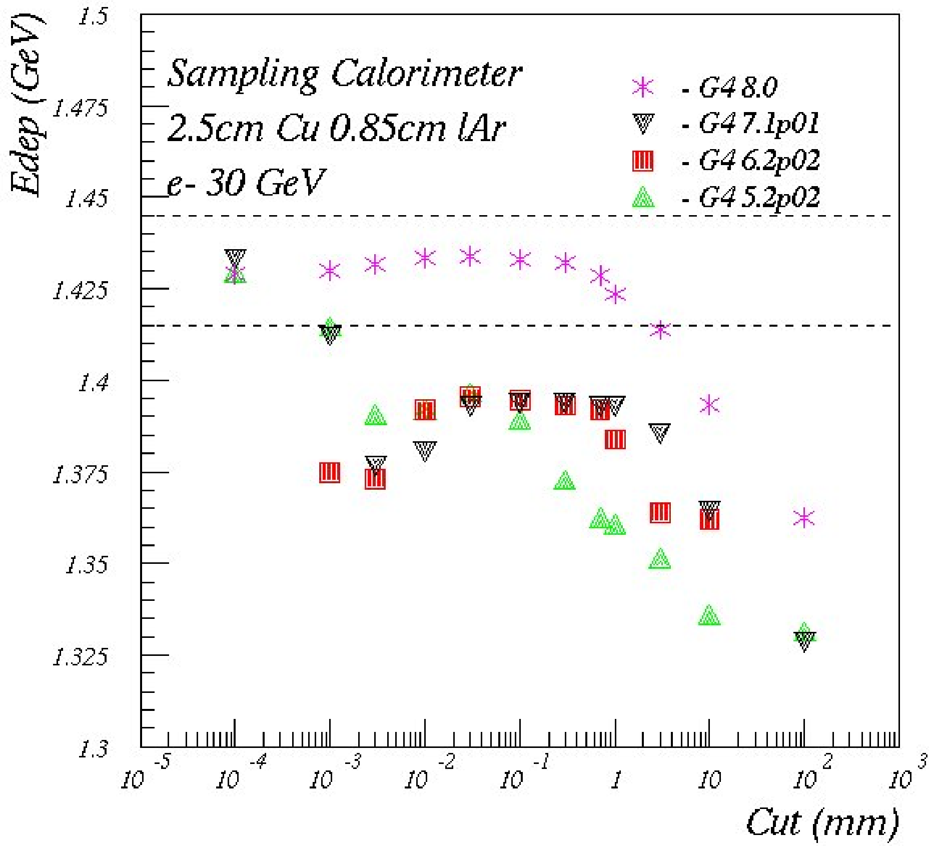
M. Maire, L. Urban

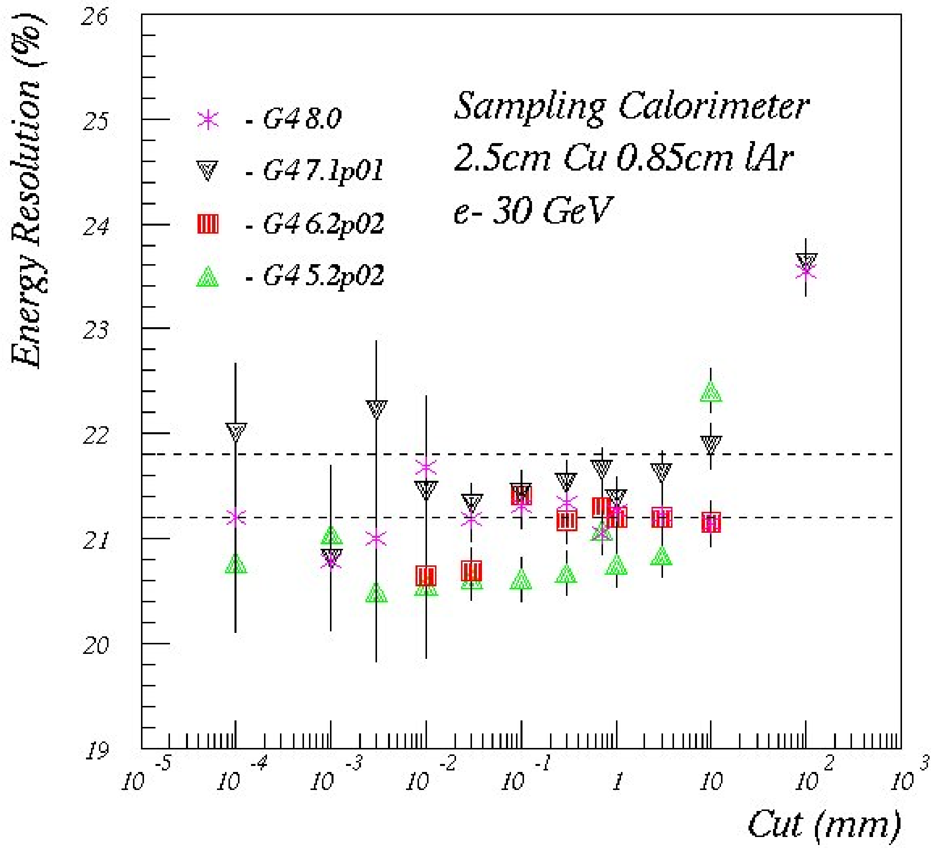


Calorimeter of ATLAS barrel type



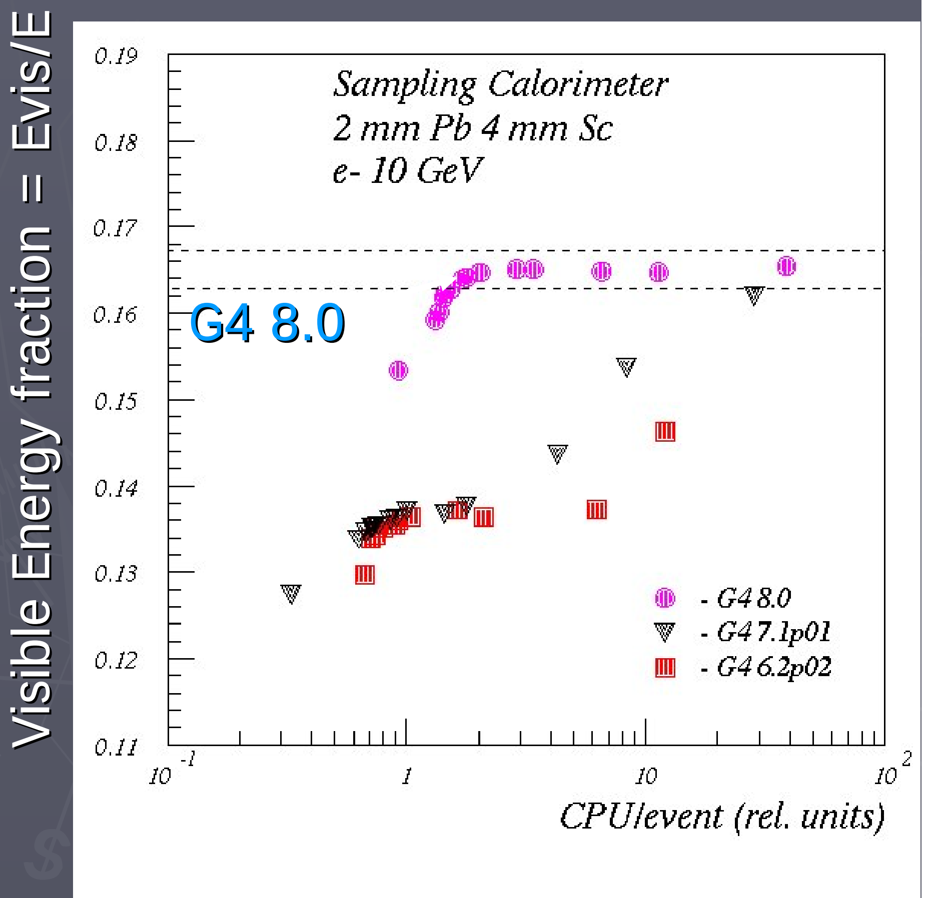
Simple Calorimeter like ATLAS HEC

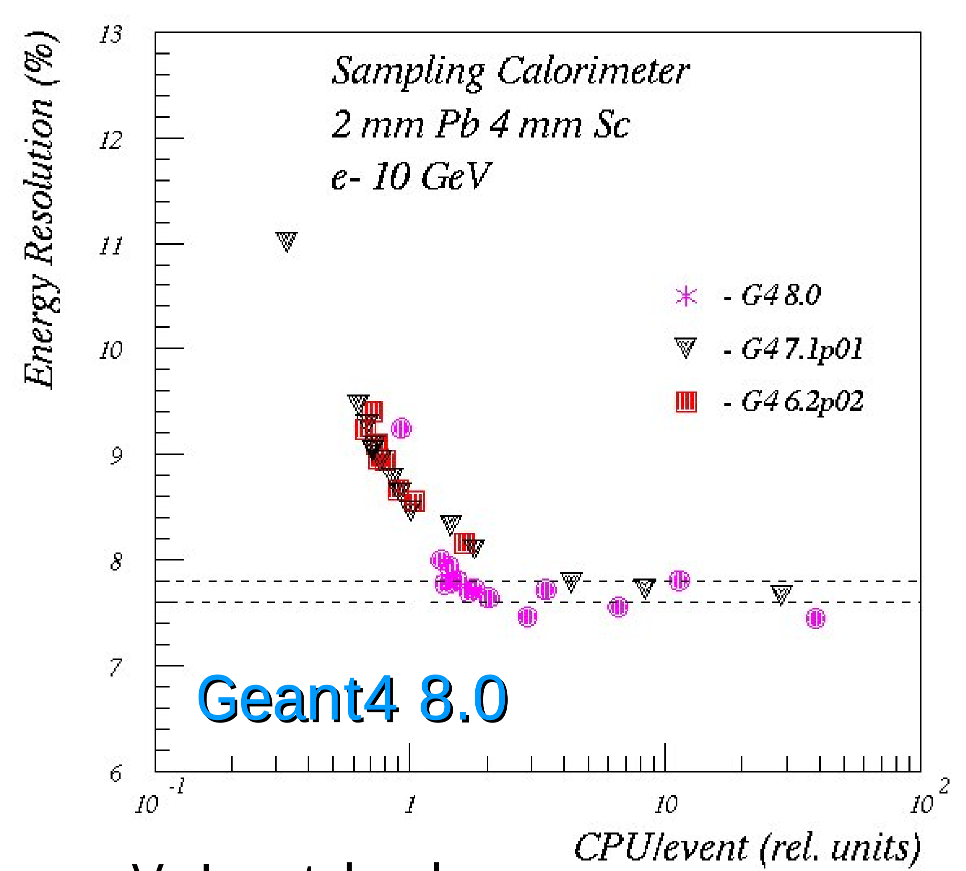




CPU versus physics performance

Simple calorimeter similar to LHCb setup





V. Ivantchenko

Stable $E_{visible}$, resolution for less CPU

Hadron/ion ionization

- User requirements trigger analysis of ionization models in the Standard packages
  - Review of corrections including shell correction term, high order corrections, Mott corrections, nuclear stopping power
  - PAI model evolution
  - Model of straggling
  - Angular distribution of secondary particles improved
- New process G4hhIonisation for heavy exotic particles
  - which may be produced at LHC
  - Suppresses all secondaries

Hadronics

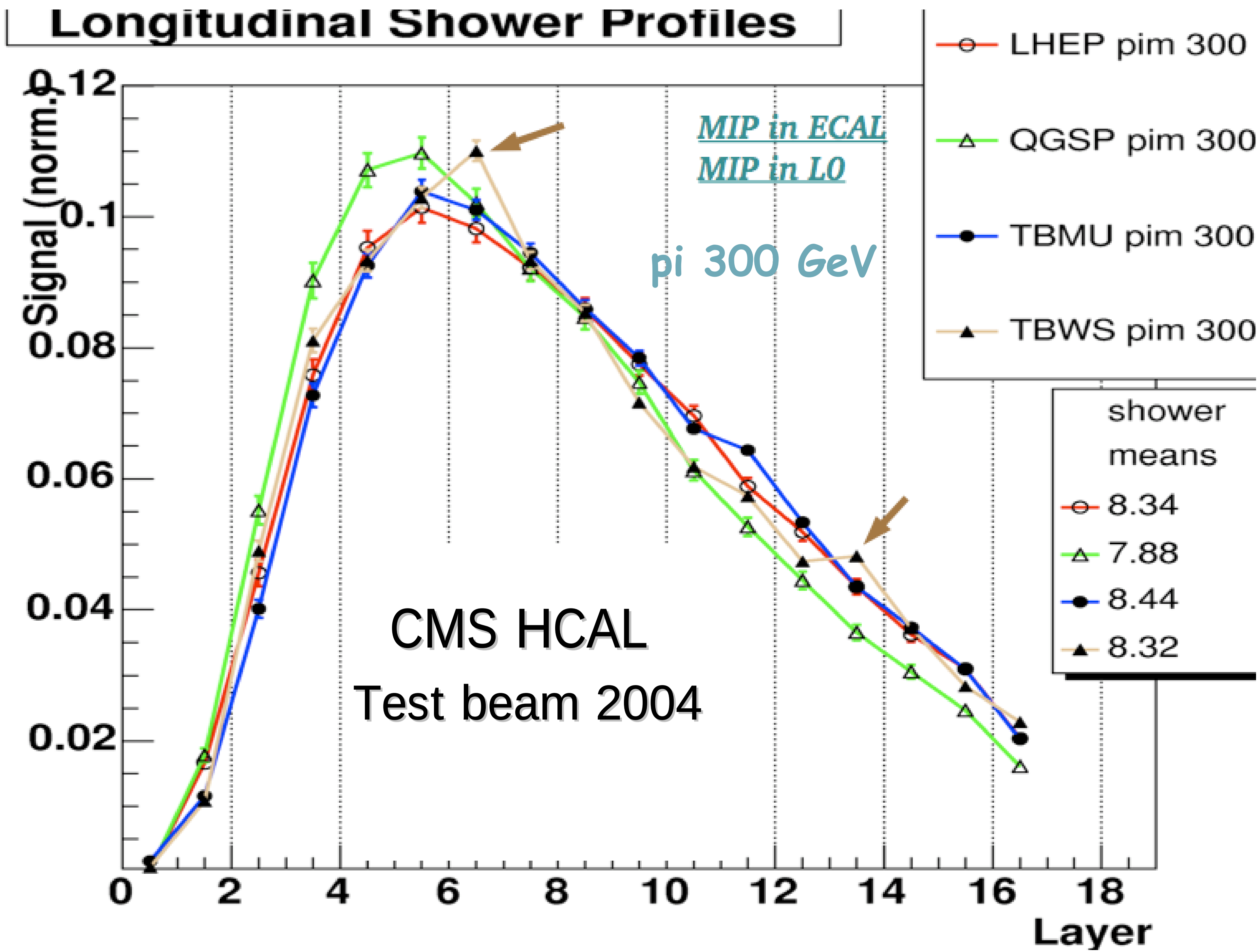
Detector observables

incl. Shower Shape

Thin-target

Hadronic showers

- Several test beams have compared Geant4 physics lists with data
  - ATLAS HEC, TileCal, …, CMS HCAL
- Conclusions generally agree
  - energy resolution and e/π well described
    - QGSP better, LHEP e/π not as good
  - Shower shape not well described
    - QGSP early and less deep
    - Energy ‘separation’, leakage problems



Longitudinal Shower Profiles
Signal (norm.)
0.12
0.1
0.08
0.06
0.04
0.02
0
2
4
6
8
10
12
14
16
18
Layer
MIP in ECAL
MIP in L0
pi 300 GeV
LHEP pim 300
QGSP pim 300
TBMU pim 300
TBWS pim 300
shower
means
8.34
7.88
8.44
8.32
CMS HCAL
Test beam 2004

Investigating shower shape

- Identifying key aspects of showers
  - That influence shape, especially depth
- Find what is responsible for differences between physics lists (esp QGSP) and data
  - For important processes check
    - Cross sections
    - Final state generators (ie models)
  - Analyze the composition of the shower

Aspects considered/investigated

- Cross section (pi, p, n)
- Forward leading particles from high energy interactions
- π^0 production
- neutron and proton production
- energy deposition due to elastic interactions

Some of the issues, steps

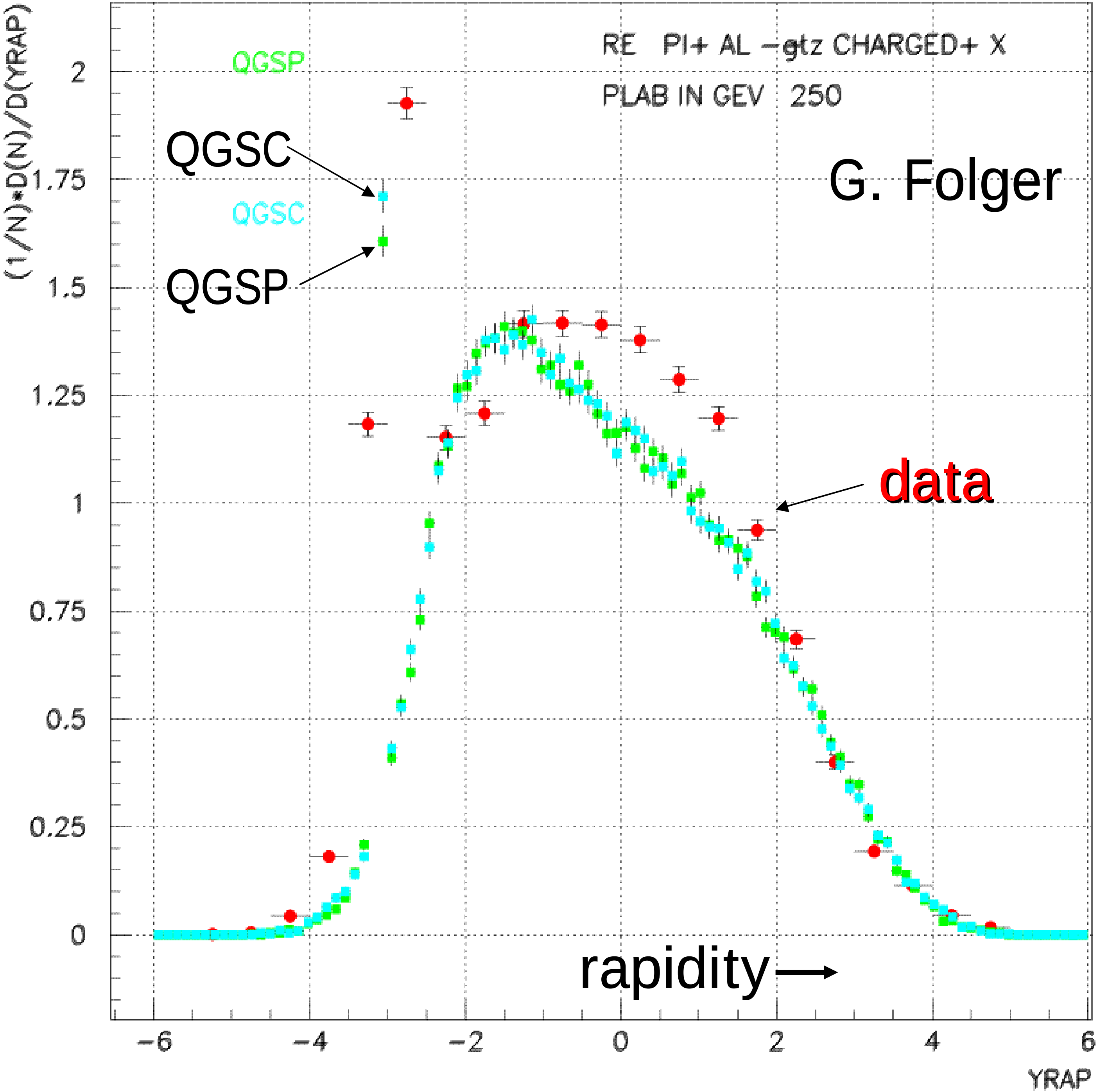
1. Comparing QGSP evolution with LHEP evolution
   - Differences seen in charged π (spectra, multiplicity)
     - Comparisons with data: Agababyan 91, Whitmore 94
2. Analyzing the composition of the shower
   - Particle fluxes
   - Particles depositing energy in each ‘segment’
3. π^0 production
   - isotopic ratio

Note: For each aspect possible we go back to thin-target comparisons to compare with available data

Thin target
250 GeV/c

π^+ Al $\longrightarrow$

Positives X

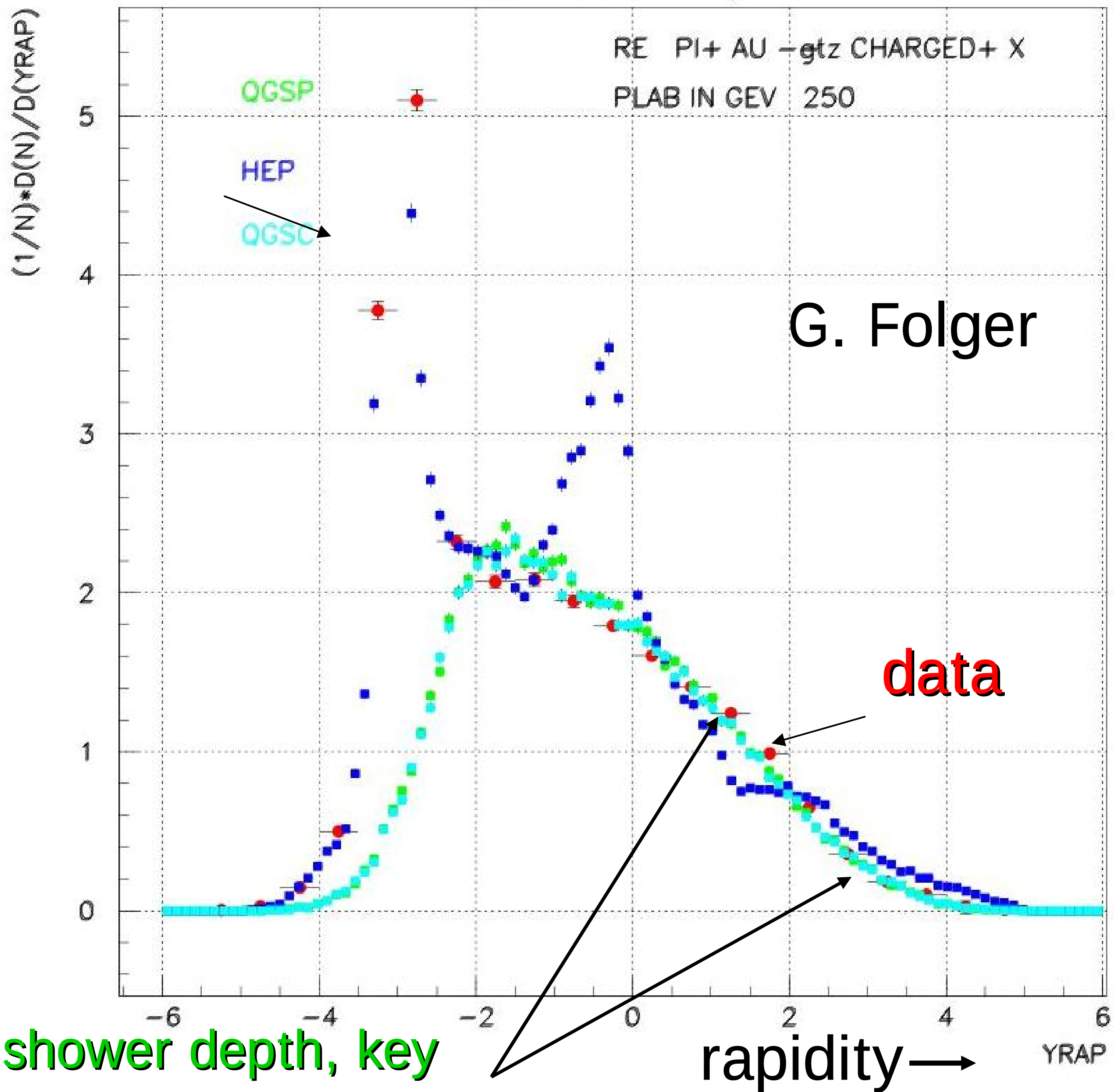


Data:
Agababyan
ZP C50
(1991), 361

Leading particle π

π^+ Au $\longrightarrow$ Positive +X

Data: Agababyan ZP C50 (1991), 361

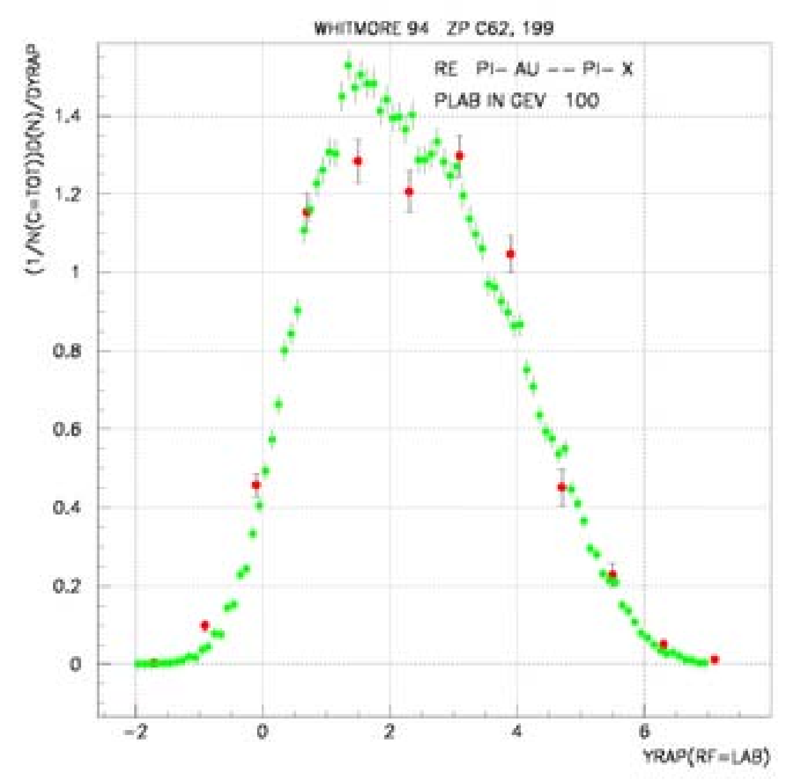


For shower depth, key is the leading particle (π^+)

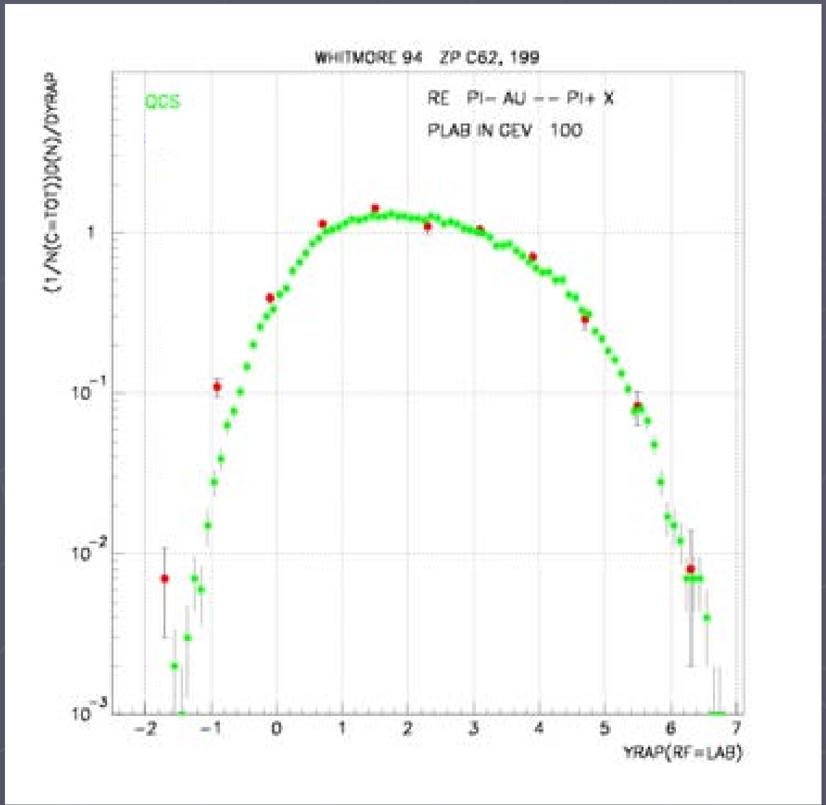
Leading pions

Whitmore ZP C62, (1994) 199

- π- Au → π- X



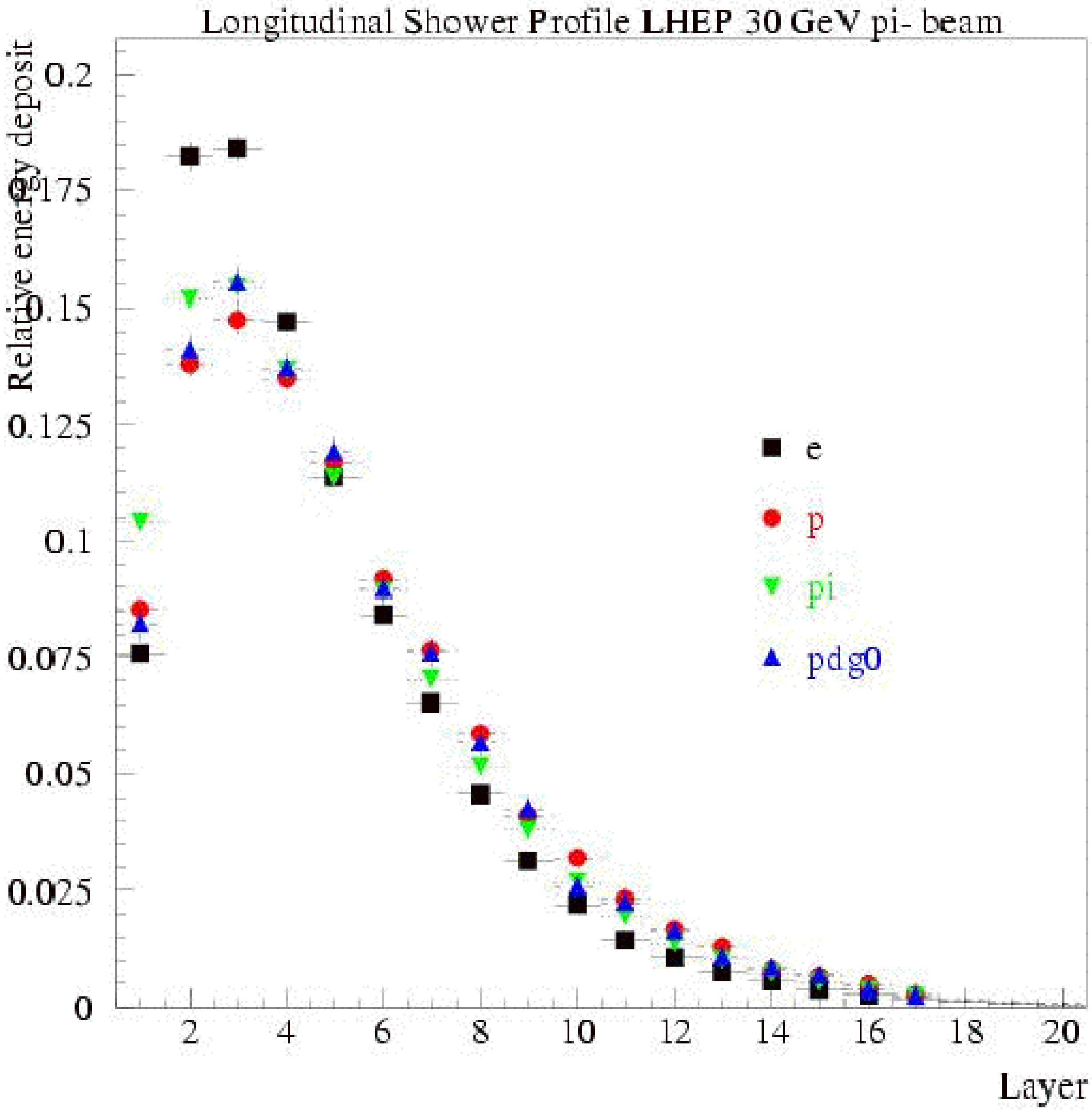
- π- Au → π^+ X



High energy Interactions: Observations

- QGSP/QGSC agree well at large rapidity
  - particles in target rest frame not well reproduced
  - Particle deficit between η= -1 to 2 (for Al)
- LHEP is not as good
  - and has unphysical spectra
    - known feature of Gheisha approach
    - makes it less appropriate for applications where such spectra are relevant
    - makes detailed comparisons QGSx/LHEP less useful.

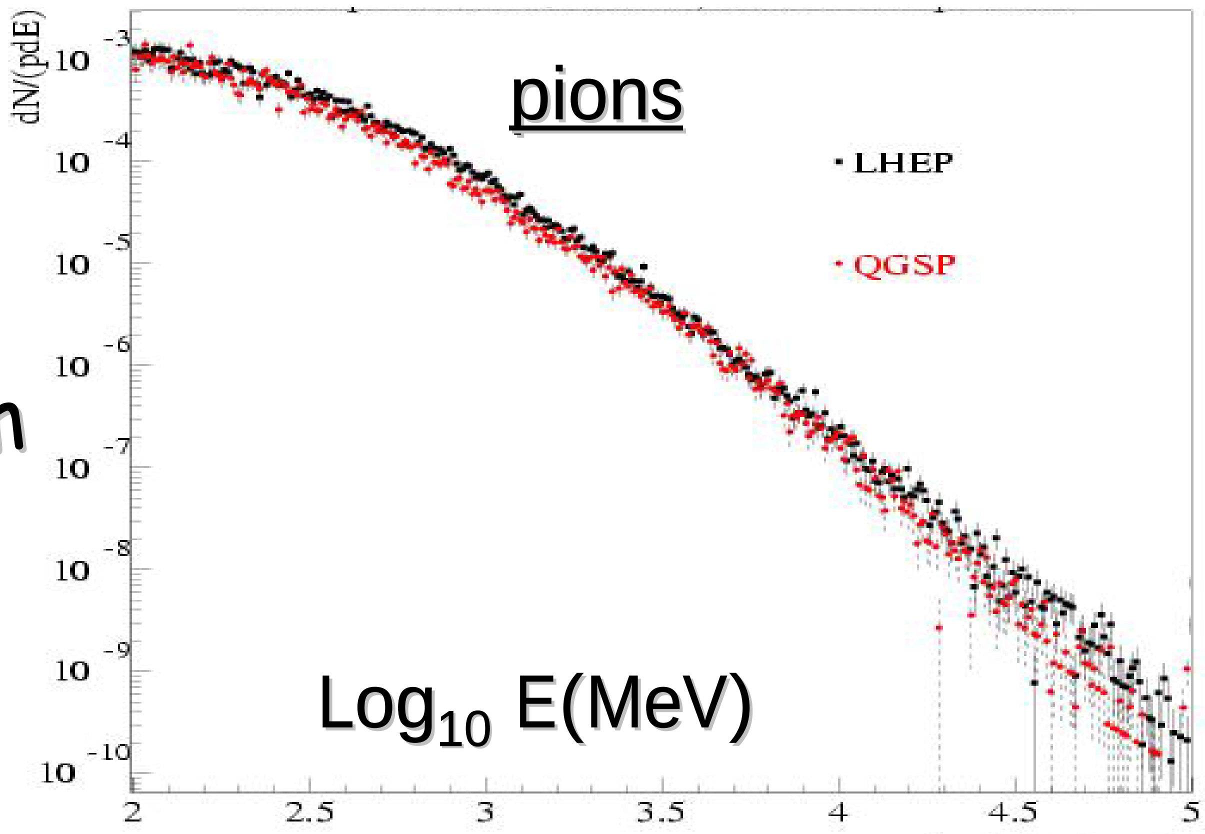
Shower shape, split by Particle type



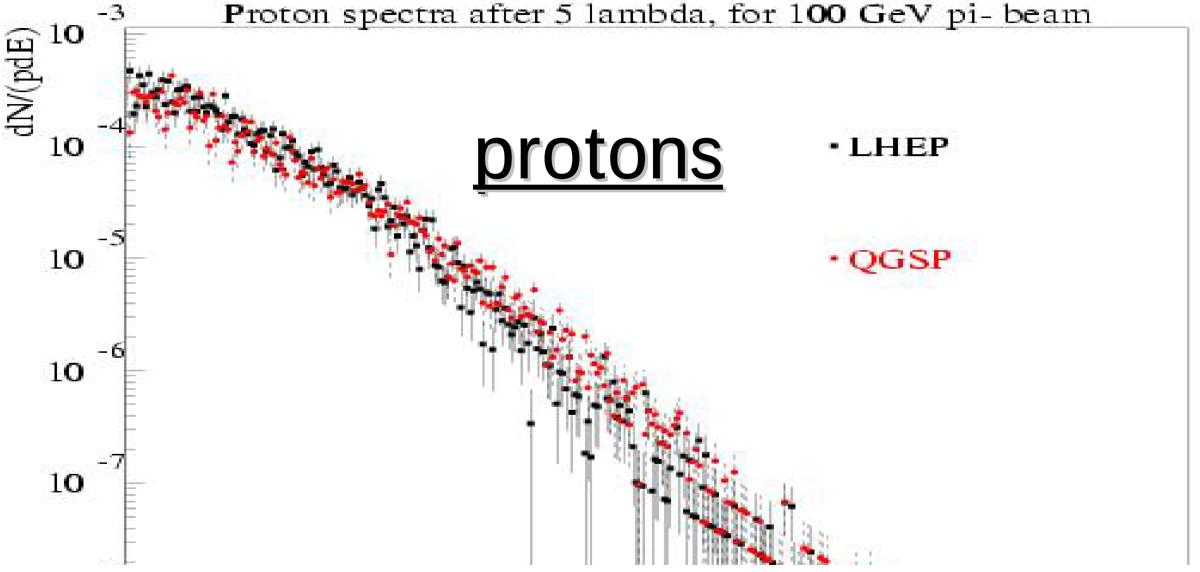
Spectra

100 GeV π- beam

Spectra after 5 λ

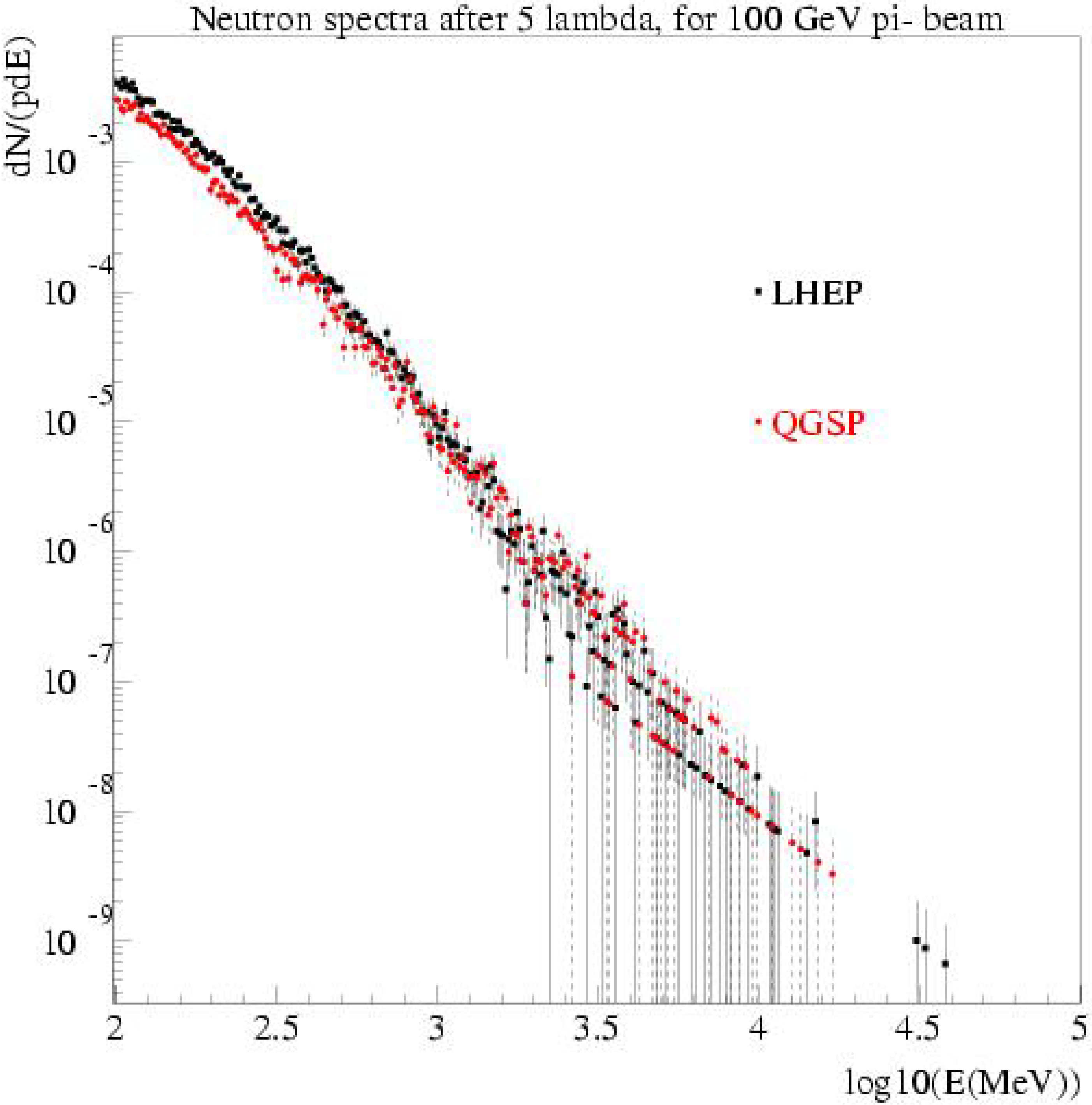


Proton spectra after 5 lambda, for 100 GeV pi- beam



100 GeV π^- beam

Spectra after 5 λ



For more

- For more details on this study see
  - "Hadronic Shower Shape studies in Geant4", A. Ribon, ..
    at Geant4 Physics Verification and Validation mtg, July 2006
    - http://indico.cern.ch/conferenceDisplay.py?confId=4532
- Relevant overview of key aspects, challenges
  - "Toward meaningful simulations of hadronic showers", R. Wigmans at Hadronic Shower Simulation Wrk, FNAL 2006
    - http://indico.cern.ch/contributionDisplay.py?contribId=21&sessionId=9&confId=3734

Shower shape - issues

- Investigated
  - Leading particle
  - Shower composition
  - π^0 production (ratio)
- Key open issues
  - π^0 production (rate)
  - Cross-sections
  - Verification for projectiles 3 GeV/c < p < 50 GeV/c
  - Neutron production (TARC comparisons)
    - Relevant for lateral shower shape
- Need for better coverage in region 3 GeV < E < 20 GeV
  - Extending current models (QGS) ?
  - New models ?

3. Geant4 verification, validation

- Extended verification
  - Thin target comparisons
  - Reaction products (nuclei)

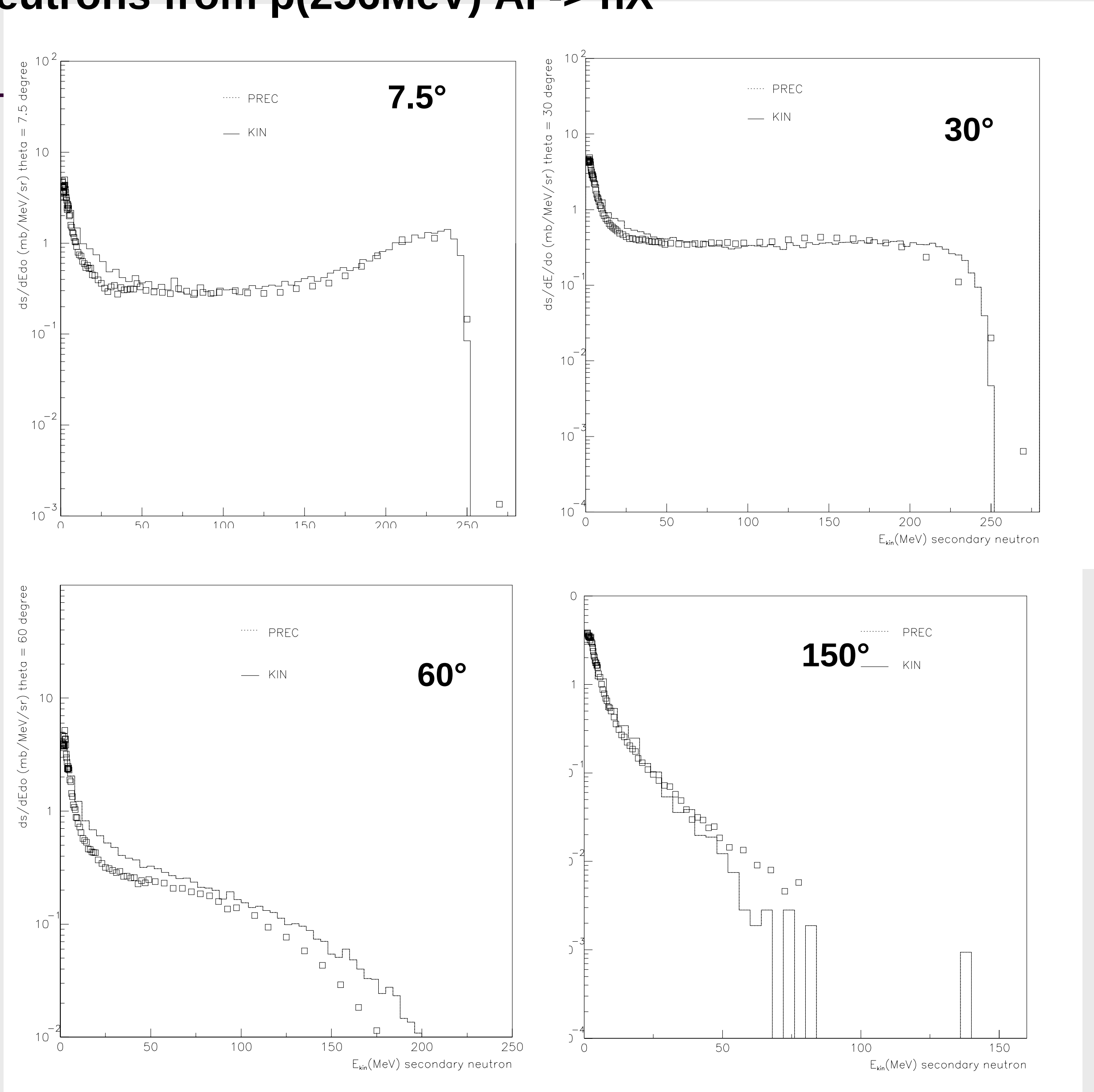
- Tested extensions
  - Bertini-like cascade extended (up to ~10 GeV)
    - Need more verification 3-10 GeV

Verification / validation

- Additional thin-target comparisons
  - For verifying models
- Validation
  - New comparisons (eg CMS TB2004, ATLAS CTB)
  - Revisiting test-beam comparisons
    - Eg Atlas HEC
  - EM calibration below per-cent level
  - Open challenges for hadronic calorimetry
    - Shower shape, energy density (at low values)

Cascade common test suite – few plots

Neutrons from p(256MeV) Al -> nX

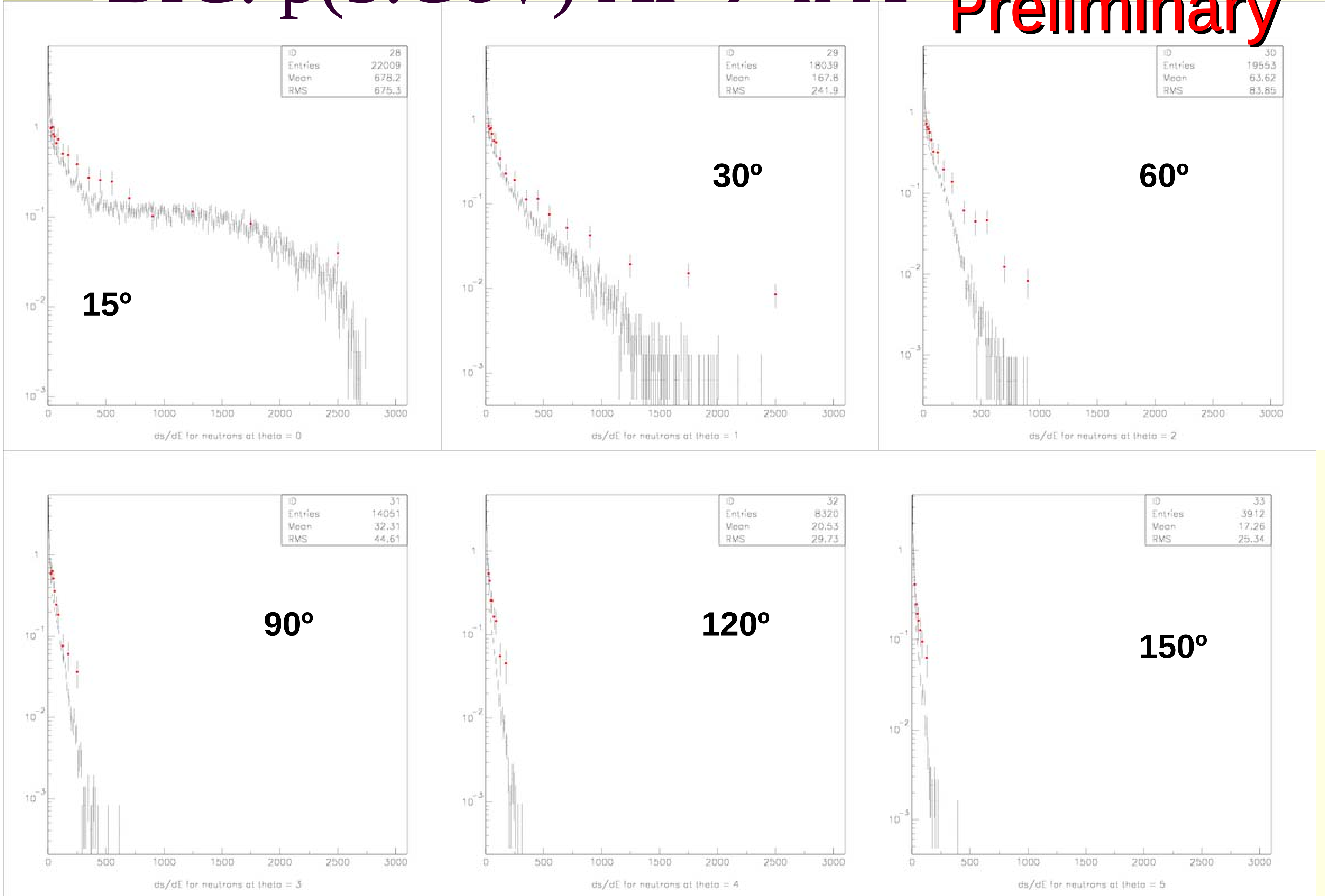


Binary Cascade

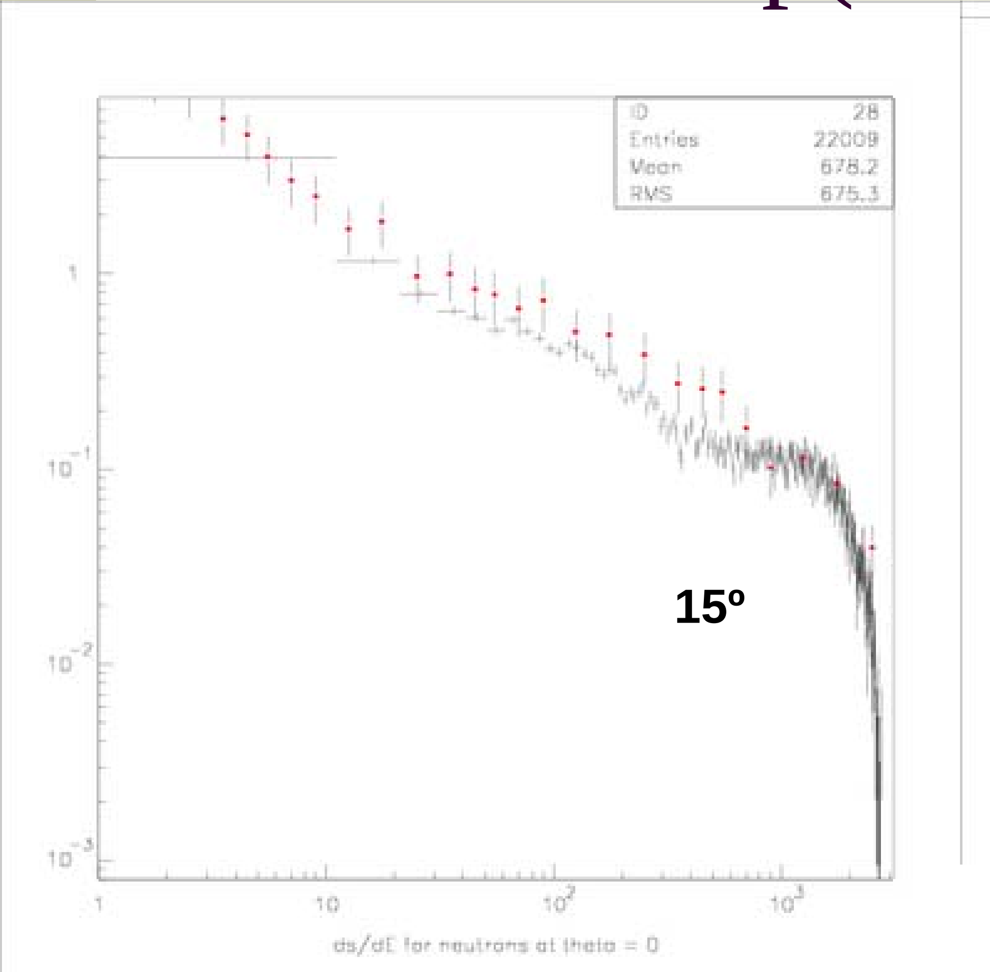
G Folger

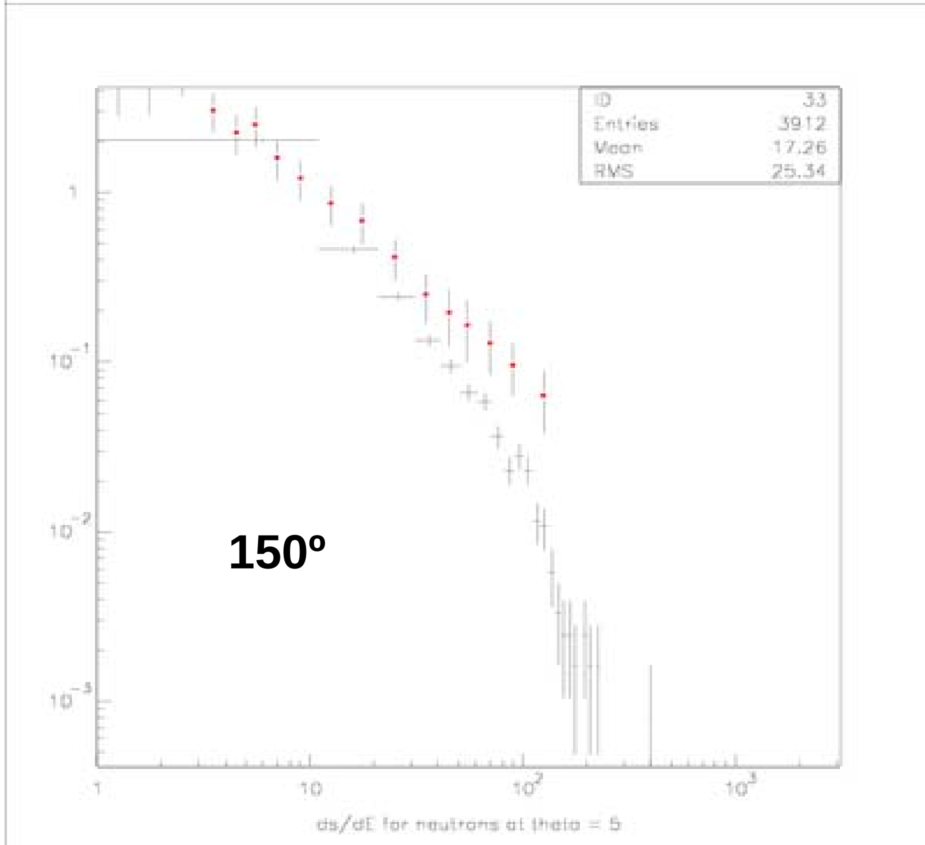
BIC: p(3.GeV) Al → n X

Preliminary



BIC: p(3.GeV) Al → n X





Same – but x log(E)

Preliminary

Experiments data for further comparisons $E_{proj} < 10$ GeV

- 5 GeV/c HARP data (near future)
- McGill et al., Phys.Rev. C29, 204 (1984).
  - 800 MeV p-p, p-d, p-C, p-Ca, p-Pb => $d^2\sigma/d\Omega/dp$
- Shibata et al., Nucl. Phys. A408, 525 (1983).
  - 1.4 – 4.0 GeV/c (pi,pX) on C, Cu, Pb
  - 3.0 GeV/c (p, nX), (π, nX) on Cu => invariant d.d. cross section
- En'yo et al., Phys. Lett. 157B, 1 (1985).
  - 4 GeV/c (p,pX), (p, πX) on Al, Pb => inv.d.d. cross section
- Niita et al., Phys. Rev. C52, 2620 (1995).
  - 3.17 GeV (p, pX) , (p, pi X) on Al => invar. dd cross section
  - 1.5, 3.0 GeV (p,nX) on Pb => dd cross section
- Armutliiski et al., Sov. J. Nucl. Phys. 48, 161 (1988).
  - 10 GeV/c (p, pi- X) on C, Ta => invar dd cross section
- Leray et al., Phys. Rev. C65, 044621 (2002)
  - 0.8, 1.2, 1.6 GeV (p, nX) on many nuclei => dd cross section

D. Wright, SLAC

- New Elastic process

n - H elastic : dσ/dt

'QElastic', **M. Kossov**

- Systematics for cross-section
- t-dependence of σ modeled

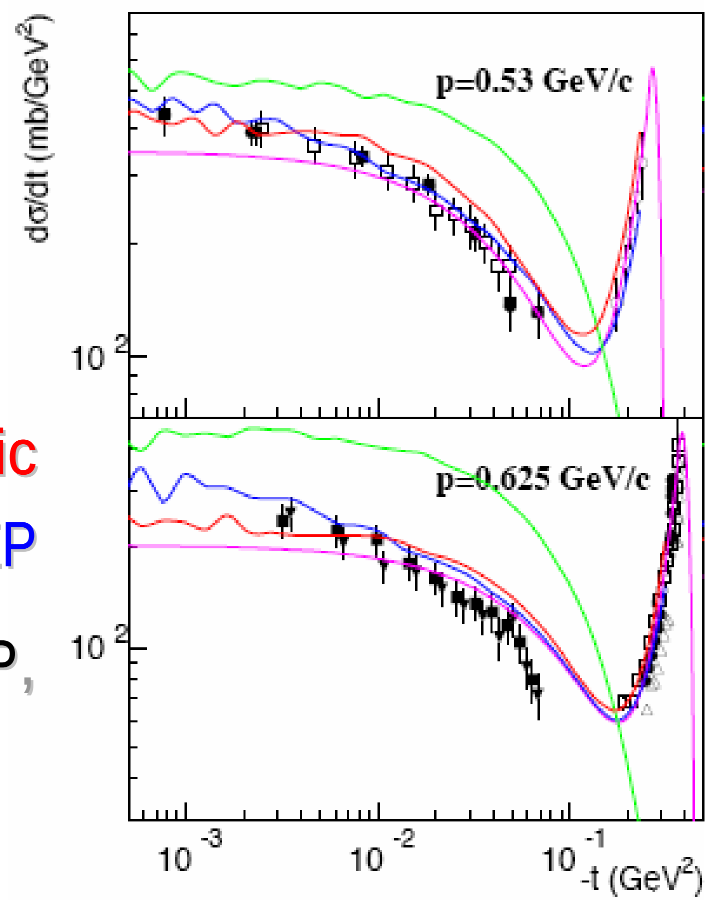
$$\frac{d\sigma}{dt} = A_1 \cdot e^{B_1 \cdot t} + A_2 \cdot e^{B_2 \cdot u}$$

  - p-dependent A_i B_i

Red/pink Qelastic

blue LHEP

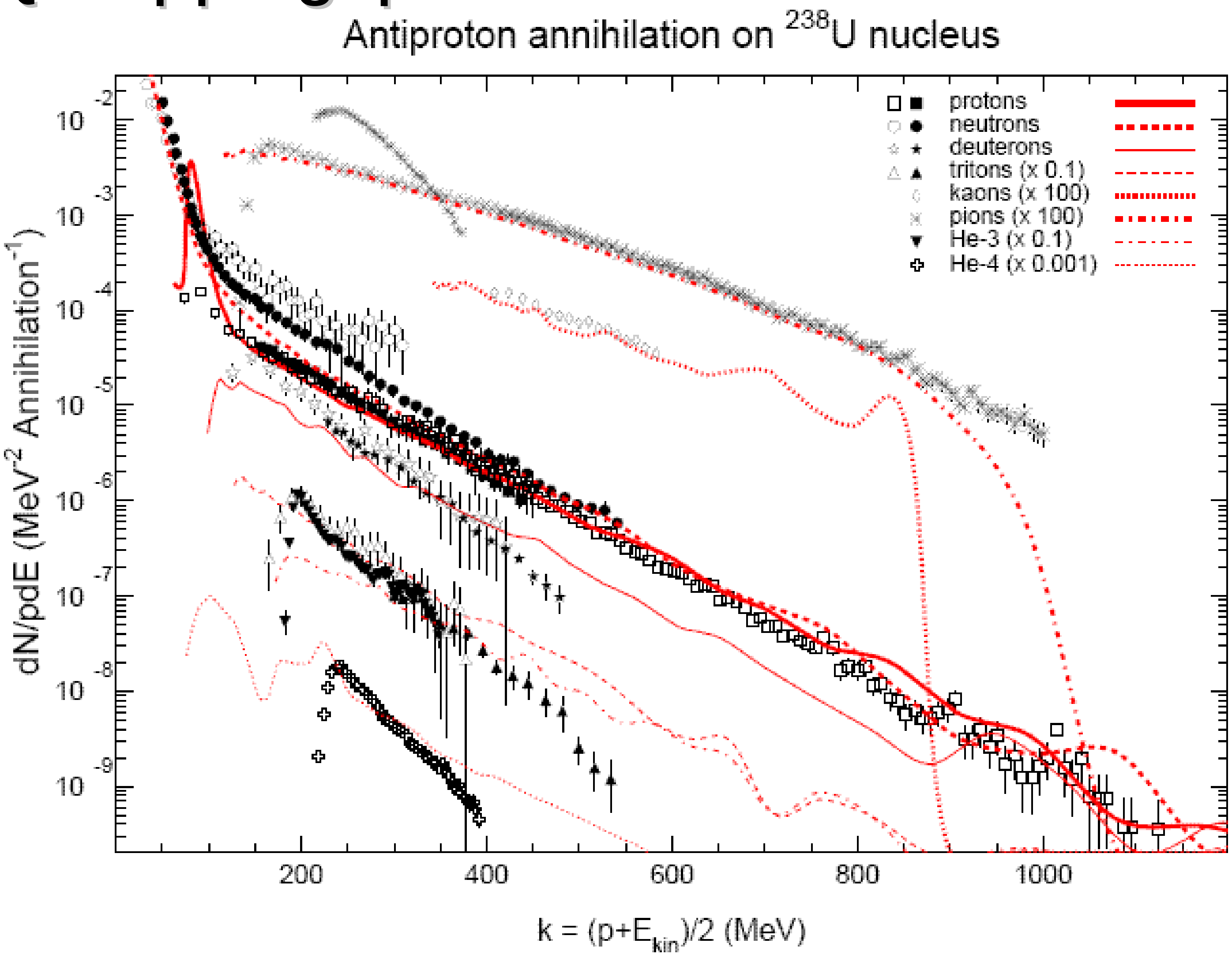
black HP,



Other elastic scattering cases considered:

p with H, d, He4, Be, C, Al, Pb

'QStopping' process



CERN

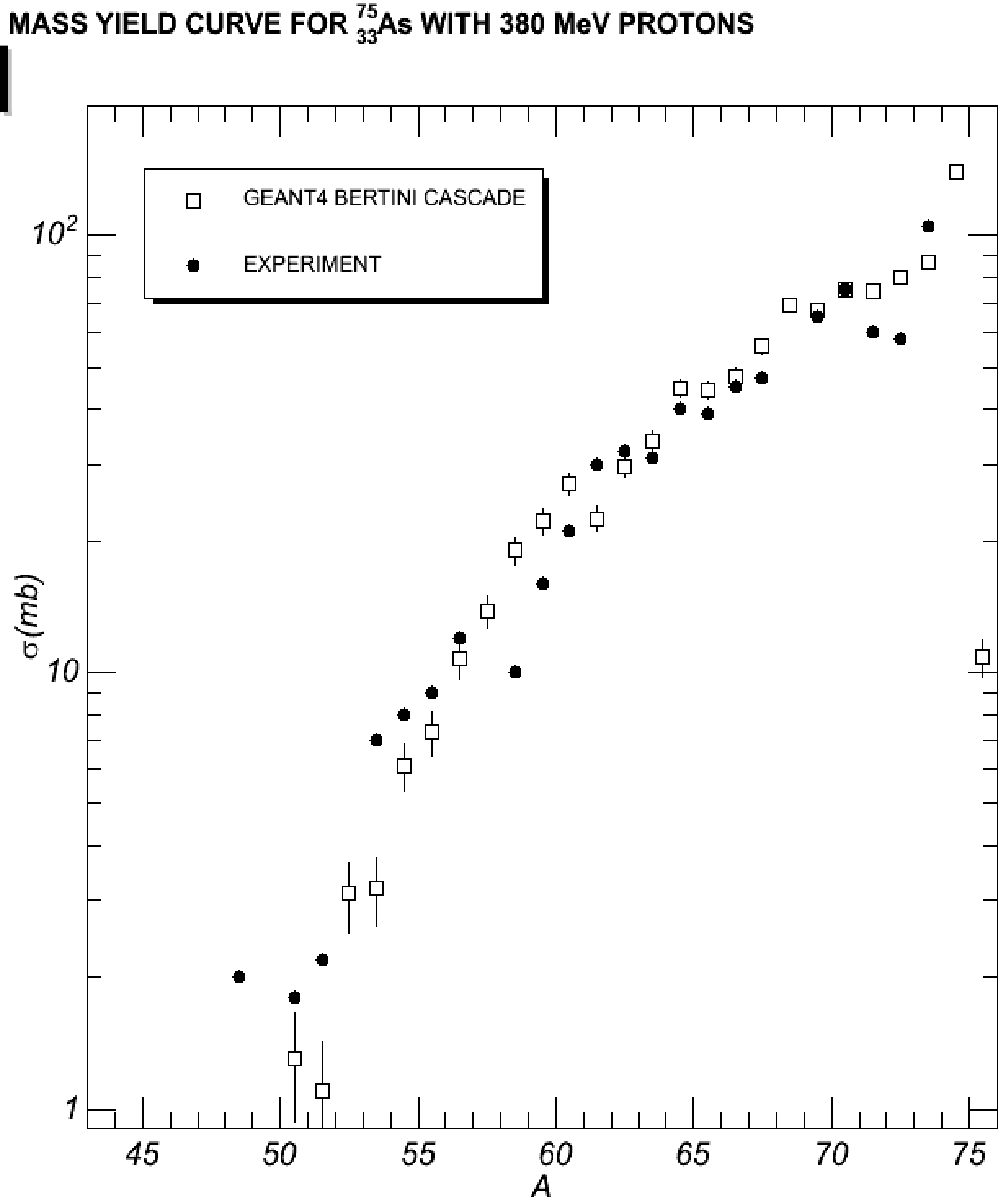
Mass yield curve

Geant4 Bertini

vs

Experiment

A. Heikinen



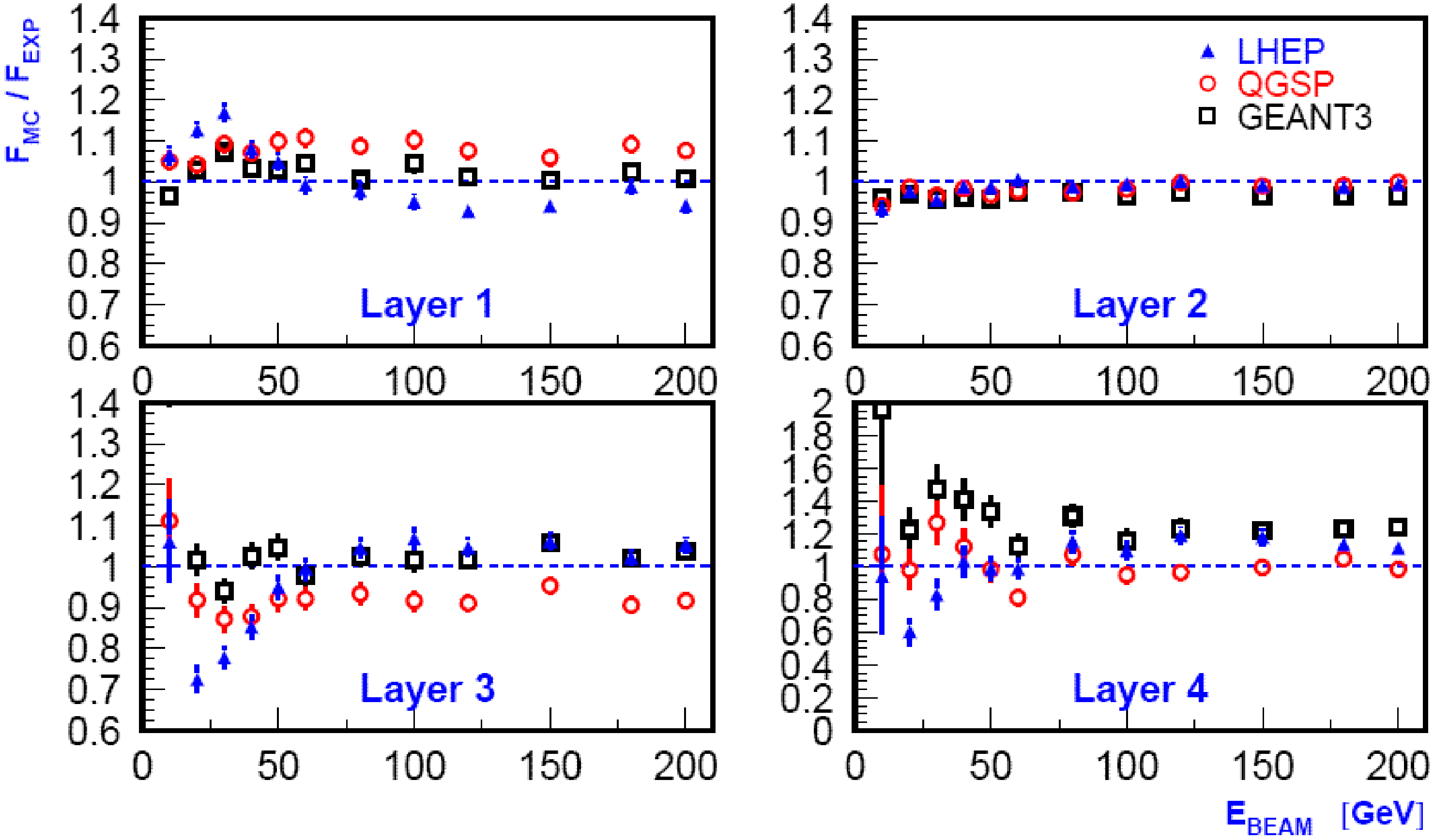
ATLAS HEC: G4 8.0p01 Update, July 2006

Updated comparisons from 5.2

GEANT4 Physics Verification and Validation Workshop July 17, 2006

Energy scans with pions

Fraction of energy in layers: ratio to experimental data



GEANT4 version 8.0, 20 μm cut

Thanks to A. Kiryunin, ATLAS-HEC

4. Geant4 improvements

- Improved stability of EM energy deposition, resolution
  - From revision of electron transport (Multiple scattering)
  - Enables better accuracy at higher cuts - with less CPU
- Extensions to geometry modeler
- Ability to revise many particle properties
- Refinements, improvements in hadronics
- Physics Lists

Additional capabilities

- Fast simulation (shower parameterisation)
  - Originally a framework for users' parameterisations
  - New GFLASH concrete implementation
    - By J. Wang (CMS), E. Barberio (ATLAS)
  - Extending use of 'Regions' to fast simulation
- Handle 'unknown' particles (with no G4 physics)
  - Accept from Event Generator, transport, decay
- Allow user to change particles' properties
  - At initialisation change unstable particles' mass, width, ..

Geometry improvements

- New solids for unusual shapes
  - Twisted trapezoid, ellipsoid, tetrahedron
- Ability to measure volume (mm^3)
  - Use it to measure also the mass of a setup
- Refinement to support better dynamic geometries
  - Option to only re-optimise parts that change with run
- New ability to detect overlap problems
  - when a user creates each part of geometry setup
- Tool for large regular (‘voxel’) geometries
  - When only material varies in regular structure

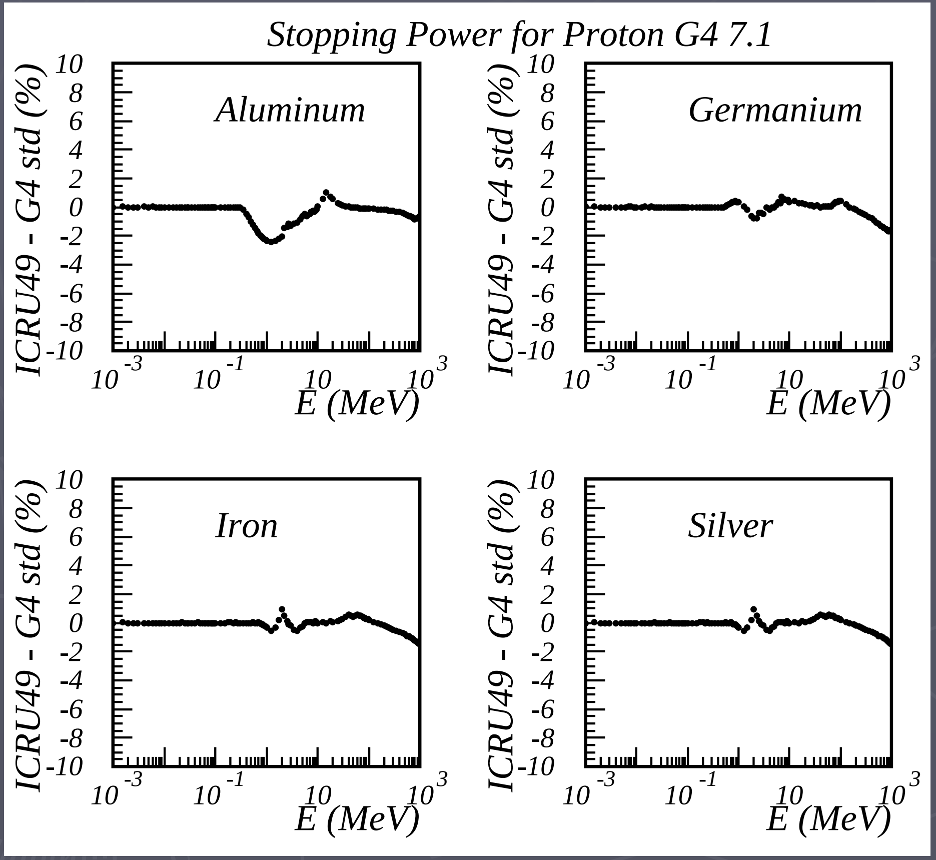
Physics Lists

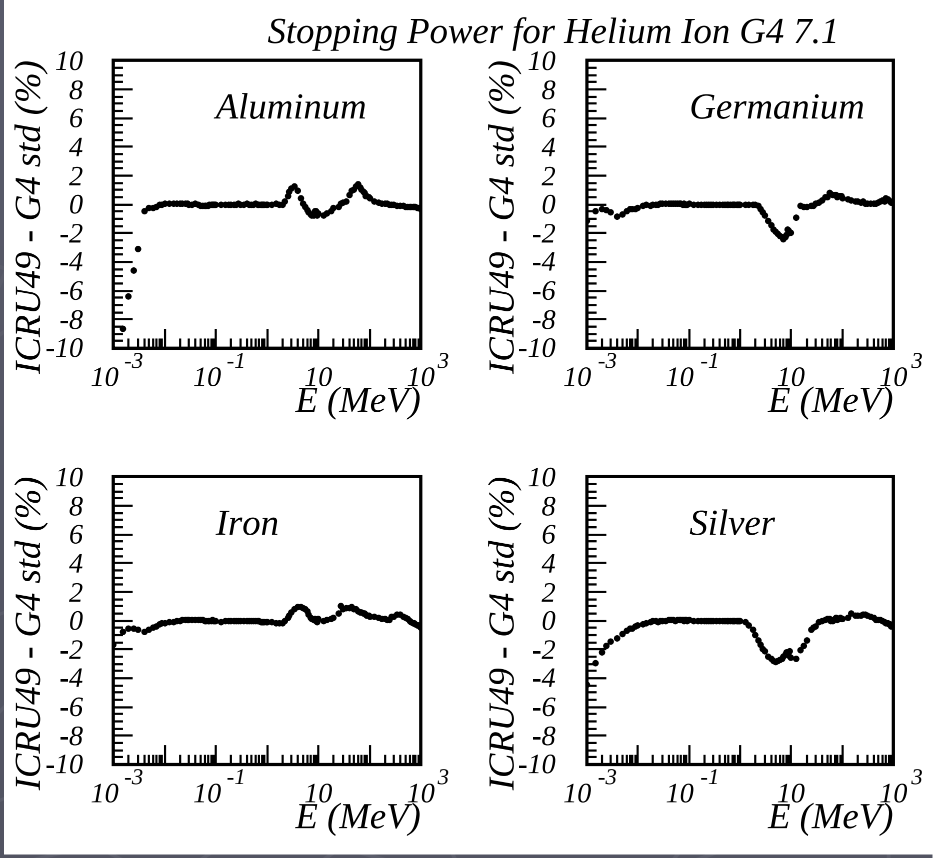
- New Multiple Scattering is used (8.0)
  - 'Old' EM physics, MS, available in variant
    - QGSP_EMV uses multiple scattering without extra steps
- γ-A interactions is default in all PLs (8.0)
  - It is in nature!
    - but it can be switched off easily for studies ..
- Stopping particles simulated with CHIPS (8.1)
  - Verification showed it describes data much better – 'QStopping'
- Elastic interactions (n, H) revised
  - Deployed in QGSx, FTFx versions only
- Other
  - Revised to work with particles revision
  - Utilise EM(std) physics builders provided by EM(std) team

Robustness, testing

- Low rate of problems in production
  - Was <~ 10^{-4} per LHC event with G4 5.x
  - CMS reports 10^{-6} per event (G4-related) with G4 6.2
- New, large-scale, regressions testing
  - Finds rare problems
  - Used LCG/EGEE Grid
    - Need and got > 150 CPU-weeks in 10 days
      - G4 VO: thanks to LCG team, CERN, Imperial C., Nikhef, CIEMAT
  - Identifies physics revisions, finds new software issues
    - For details, see A. Ribon's talks at CHEP 2006, AA meeting

Result of refinement of stopping power – Geant4 and NIST are within systematic uncertainty of the data





Developments Summary

- Improvements in multiple scattering process
  - Addressing issues with 'electron transport'
- Speedups for initialisation/navigation
  - Option to only re-optimise parts that change with run
  - New voxelisation options being studied for regular geometries
- New shapes (twisted, tesselated)
- Overlap checks at geometry construction
- Revised implementation of particles
  - Impacting advanced users, customizing
- Refinements in hadronic physics

Organization

- “New” Geant4 Collaboration
  - Collaboration Agreement (CA) finalized, approved in 2005
  - ‘Launched’ end-January 2006
    - Majority institutions (by FTE) signed CA
  - New Oversight Board
  - New Steering Board
    - chair Petteri Nieminen (ESA), deputy KEK
- Agreed and adopted Geant4 Software License (June 2006)
  - Based on EGEE model
    - Mix of copyleft, BSD
  - http://cern.ch/geant4/license/

G4605 2006/03/31	Development release including new tool for overlap detection at geometry construction and extensions to QGS.
G4606 2006/05/31	Development release. Including new features for parallel navigation enabling scoring charged particles at arbitrary locations, improvements to stability of showering for changes in cuts, and additional verification tests for hadrons between 10 and 50 GeV, as part of potential June 2006 public release of Geant4
G4611 2006/09/30	Geant4 development release. Including developments including redesign of Binary Cascade's field transitions, additional benchmarking for radiation and shielding use cases and refinements to physics lists for low-rate processes.
G4614 2006/12/01	Geant4 development release. Including surface tolerances tuned to model geometry size
G4615 2006/12/31	Investigation of the main physics effects responsible of the hadronic shower development in Geant4 simulations
G4701 2007/06/01	Geant4 development release. Including refined models for EM interactions of exotic particles, first implementation of tessellated BREP solids

Platforms / configurations

- Support for CLHEP 2.0.X series (since 8.0)
    - With Geant4 release 8.1 it is version 2.0.2.3
  - Option to use 1.9.x available
    - Now version 1.9.2.3
    - Expected to retain it for Dec 2006 release
- OS / compilers verified
  - SLC3 with gcc 3.2.3 (IA32)
  - SLC4 with gcc 3.4.5 (IA32 & AMD64) and gcc 4.1.1
  - Win/XP with VC++ 7.1/8.0
  - MacOS 10.4 with gcc 4.0.1
  - SunOS 5.8 with CC 5.5

Tutorials in 2005-2006

- Geant4 Users' Tutorial
  CERN, **25-27 May 2005**.
- 2nd Finnish Geant4 Workshop and Tutorial
  HIP, Helsinki (Finland), **6-7 June 2005**.
- Geant4 short course
  INFN Pisa, Pisa (Italy), **12 January 2006**.
- Geant4 training course
  Austrian Academy of Sciences, Vienna (Austria), **18-20 May 2006**.
- 4-day Geant4 tutorial
  SLAC, Stanford (USA), **7-10 March 2006**.
- 4-day Geant4 tutorial
  Jefferson Lab, Newport News, Virginia (USA), **22-25 May 2006**.
- Geant4 tutorial course, McGill University, Montreal (Canada), **25-28 September 2006**.
- Geant4 Course at the 10th Topical Seminar on Innovative Particle and Radiation Detectors, Siena (Italy), **5-6 October 2006**

Workshops and Symposium

- Workshops
  - 4th Geant4 Developers Workshop on bio-medical applications and physics validation
    INFN Genova, Genova (Italy), **13-20 July 2005**.
  - 10th Geant4 Users Conference and Collaboration Workshop
    Bordeaux (France), **3-10 November 2005**.
    Presentations for the Users Workshop
  - 11th Geant4 Collaboration Workshop, LIP, Lisbon (Portugal), **9-14 Oct 2006**.
- Space Users Workshops
  - Workshop for SPENVIS and Geant4 Space applications
    Catholic University, Leuven (Belgium), **3-7 October 2005**.
  - Geant4-Spenvis Space Users' Workshop, NASA Jet Propulsion Laboratory - Pasadena, CA (USA), **6-10 November 2006**.
- Symposium on the Applications of the Geant4 Simulation Software at the 9th ICATPP Conference, Villa Olmo, Como (Italy), **17-21 October 2005**

User meetings and Topical meetings

- User Meetings
  - Geant4 Users Conference, Bordeaux (France),
    3-10 November 2005, with 10th Collaboration Workshop.
  - Regular Geant4 Technical Forum meetings 4-6/year planned
    - Meetings: 5 in 2005 including 2 at workshops, 3 in 2006 to date
    - Last meeting: 14th G4 TF meeting, CERN, **25 April 2006**
- Geant4 Physics Verification & Validation Meeting
  - CERN, 17-19 July 2006
- **Topical Meetings & Workshops**
  - Monte Carlo MC 2005 Topical Meeting, Chatanooga, TN, 17-21 April 2005
  - Hadronic Shower Simulation Workshop, Fermilab, Batavia, IL, 6-8 Sept 2006.

http://www.in-cites.com/hotpapers/2004/november04-eng.html

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1 Citations: 133

Title: GEANT4-A SIMULATION TOOLKIT

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Summary

- Revised Multiple Scattering
  - improves E_{vis}, σ_E
- Hadronic shower shape issues under study
  - extending thin target verification
  - simple thick target studies to identify isues
- Improved physics models deployed
  - Improved Stopping, n-H, p-H elastic
  - key physics lists revised: QGSP, LHEP
- New capabilities
  - geometry, materials, particle properties, ...

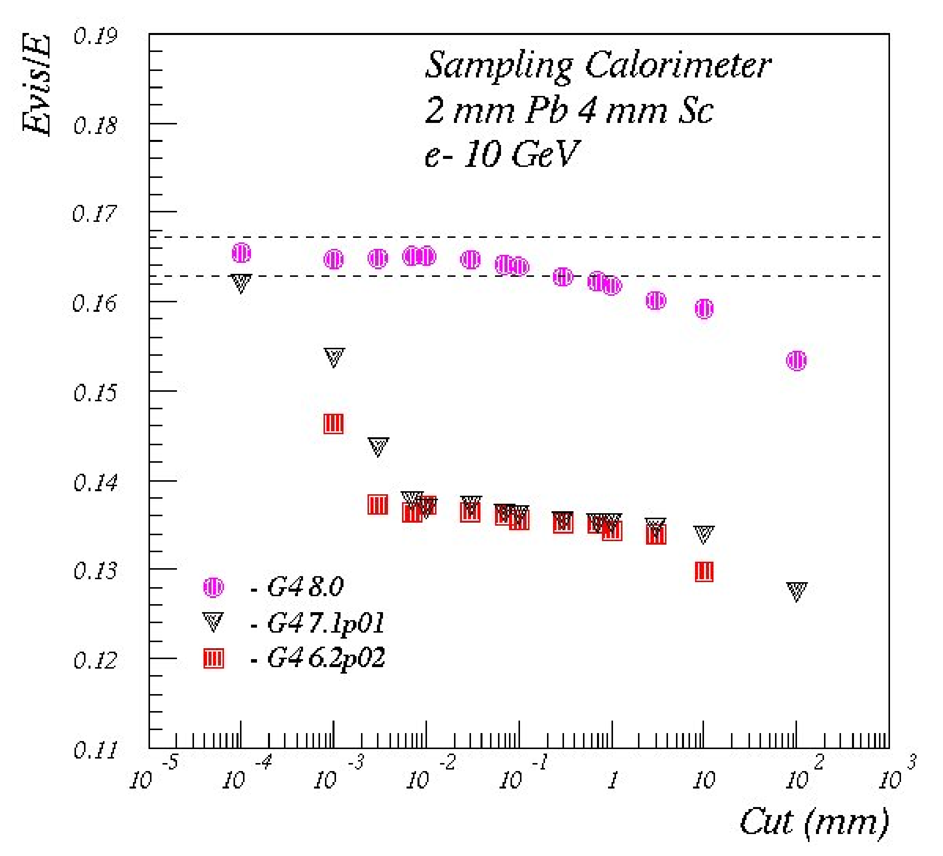
Backup Slides

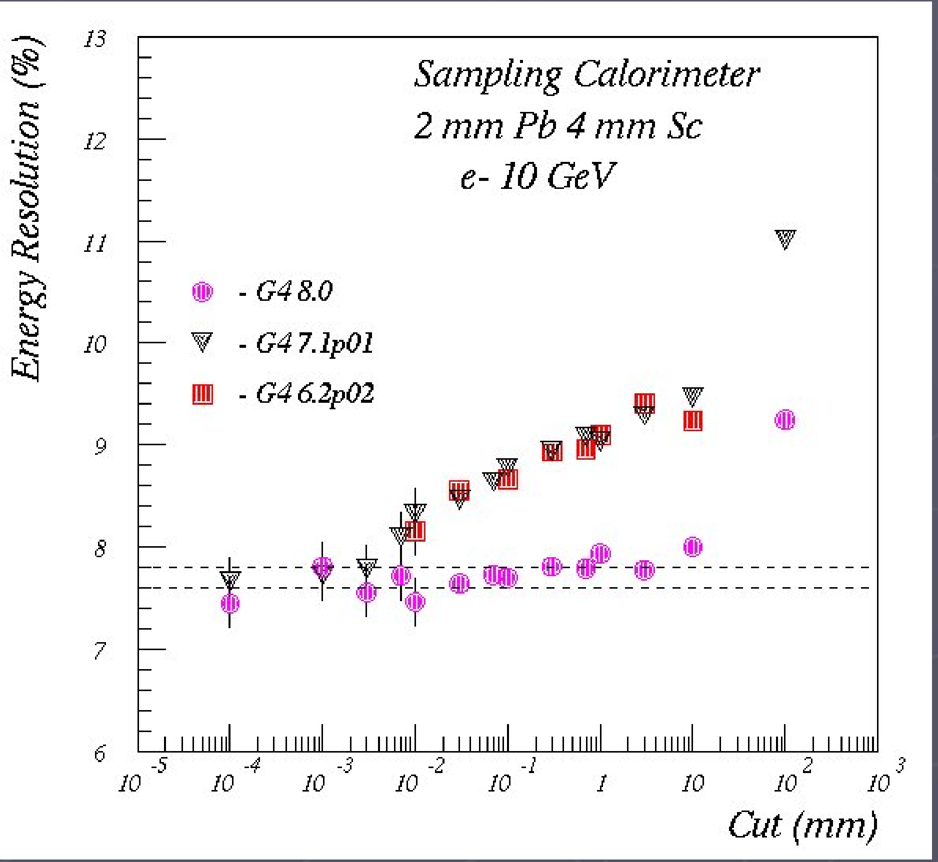
Geant4 Software License
Release 8.1

- Text available from:
  - http://cern.ch/geant4/license/
  - Based on EGEE model
- Key issues considered
  - Need and wish to enable users to use freely, modify and redistribute original or revised versions (with conditions)
  - Need to protect the contributor's reputation from those who might revise the code, but not make clear that they changed it when they published results or when they redistributed revised versions
  - Need to have users give credit to the collaboration for work undertaken utilising Geant4 as a tool (or toolkit)
  - Need to ensure the presence of a strong disclaimer of warranty and liability
  - Wish to enable user in academia, research institutes and commercial contexts to use and/or revise the code in the different manners of use: as users of an application written using Geant4, as developers of applications or toolkits based on Geant4, and as developers of tools that utilise Geant4 as part of another product
  - Need and wish to impose a minimal burden and no significant impediment to commercial use that includes Geant4 software but also includes proprietary revisions that a company developed as significant investment

More slides on EM revisions, performance

Multiple Scattering model upgrade LHCb type calorimeter

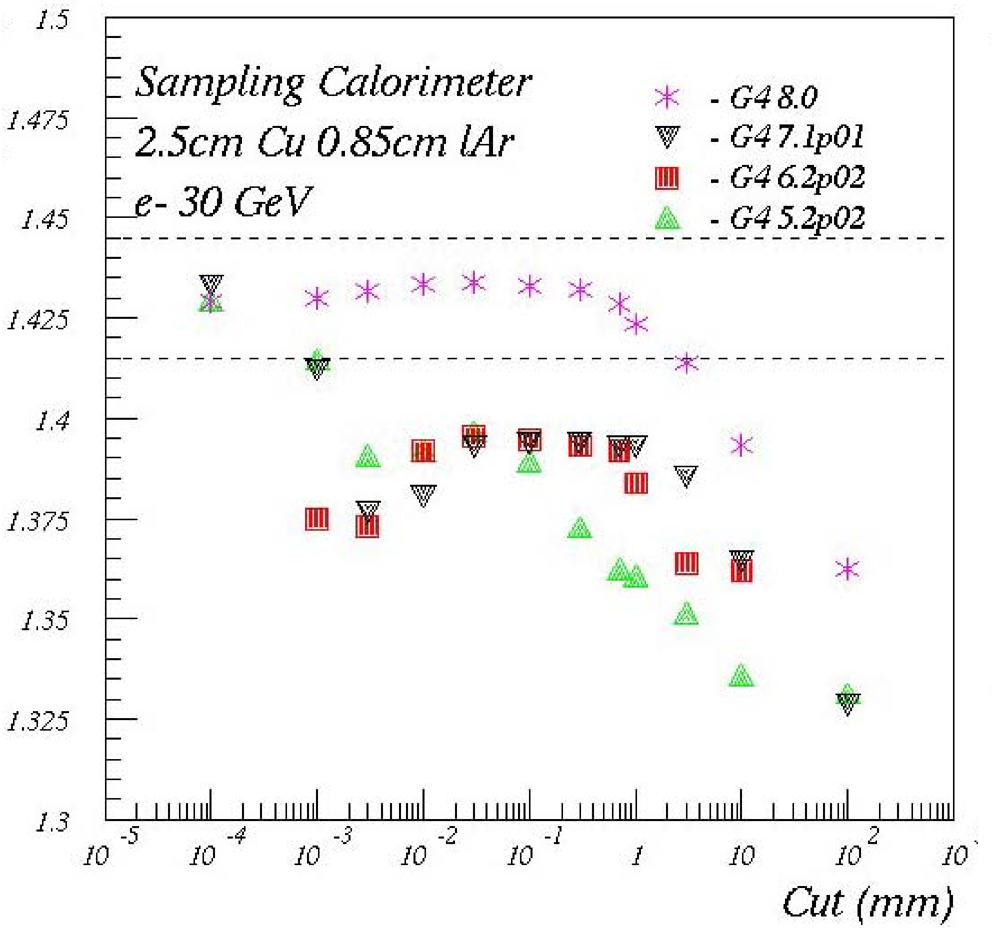




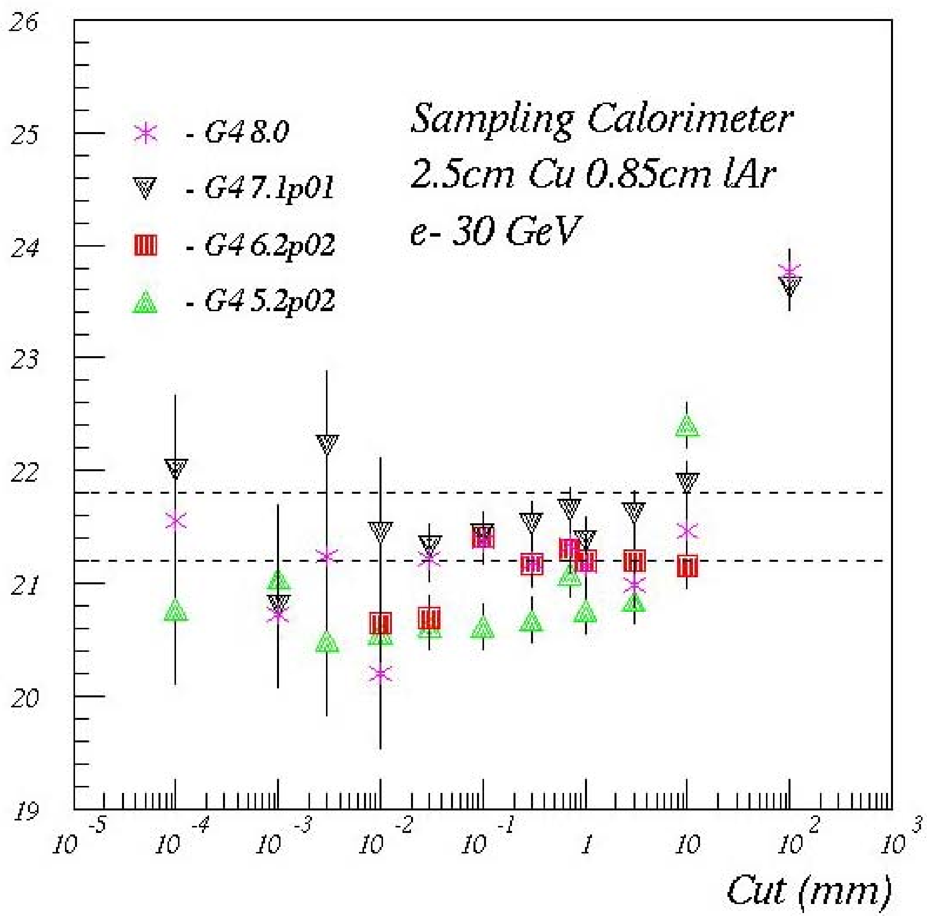
V. Ivantchenko

Atlas HEC : Cu(25mm)-lAr(8.5mm)

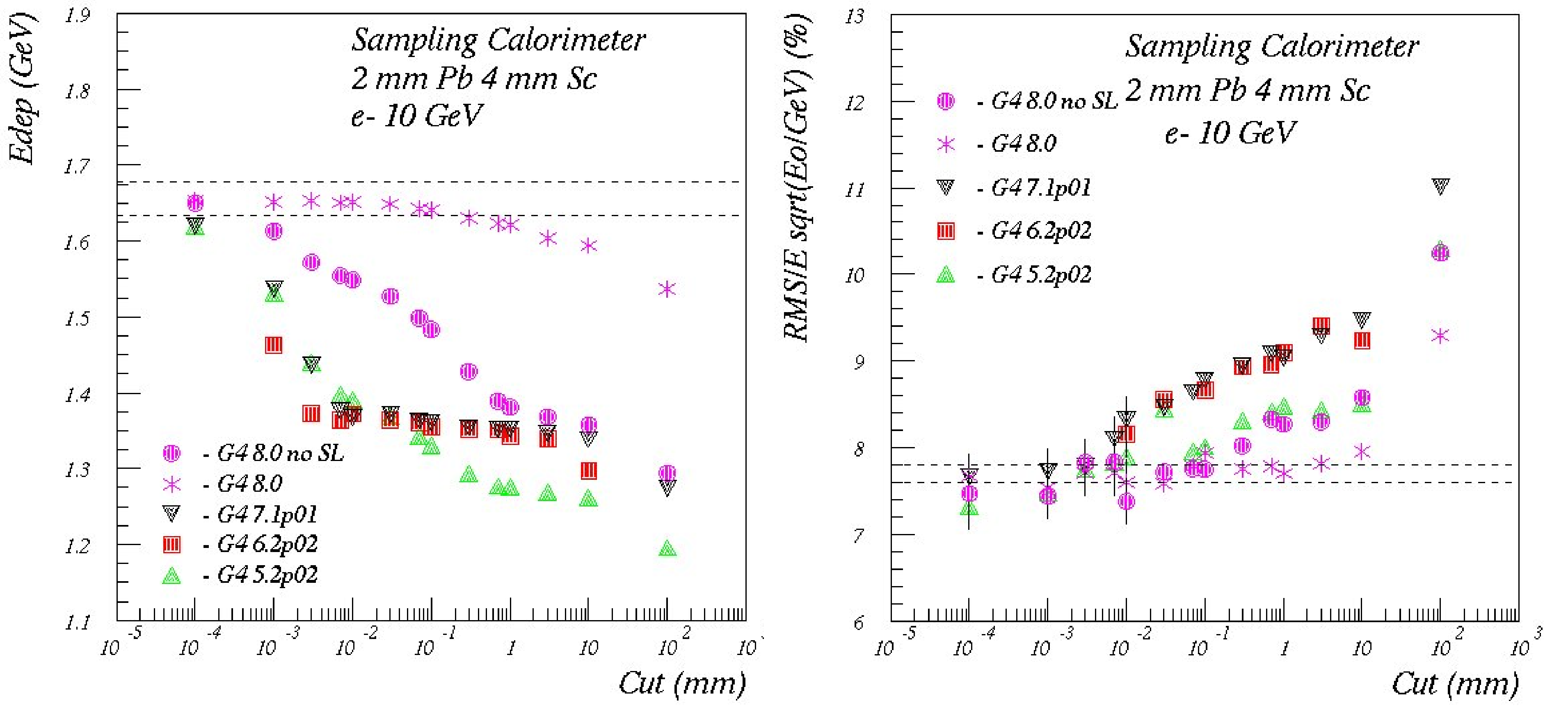
Energy Deposited (GeV)



RMS/ (E * sqrt(E_0/GeV) (%)



LHCb : Pb(2mm)-Sc(4mm)



Energy deposition and cuts (more)

- Electron transport is key to accurate energy deposition, resolution
  - in setups with materials with very different Z
- Users reported results strongly dependent on cut value and step limits
  - Atlas sampling calorimeter (Cu – lAr)
  - In water phantoms with perturbing layer (Poon & Verhaegen)
  - In other hadronic calorimeters (W-Si ILC, Pb-Sci LHCb)
- Cut dependence verified in HEP sampling calorimeters (eg Cu-lAr, Pb-Sci)
  - Energy deposition varied 10%-30% in changing production cuts from 1 µm to 1 mm
    - Effect existed in recent Geant4 releases (5.x, 6.x and 7.x)
- An extensive investigation of cut/step limit effects concluded that the Multiple Scattering process could be improved
  - Revisions provided in Geant4 8.0 address this issue

M. Maire, L. Urban

Energy deposition and cuts: result

Revisions of Multiple Scattering (available in release 8.0)

- Improvements to physical model – calculating displacement and applying it
  - Introduced correlation between scattering angle and lateral displacement
  - Ensure recalculation of geometry 'safety' before sampling the displacement
    - Since the safety value limits the displacement allowed
- Improvements in restricting step:
  - Stricter step restriction
    - using smaller fraction (0.02 vs old 0.2) of particle's range
    - in all volumes, including the starting volume of track
  - Restrict step size using geometrical information
    - Ensures more than one step in each volume

Note: User can switch off the new extra step limitation (for comparison or speed)

For more CHEP 2006 talk "The recent Upgrades in the Geant4 Standard Electromagnetic Physics Package"

M. Maire, L. Urban

More on applications

1. Geant4's in HEP, production

- HEP Experiments in large scale production
  - BaBar (2001)
  - CMS (2003)
  - ATLAS (2004)
  - LHCb (2004)
- Used in many existing experiments
  - KamLAND, Borexino, HARP, ...
- Used to study future experiments
  - ILC, NA48/3 (PA326), ...

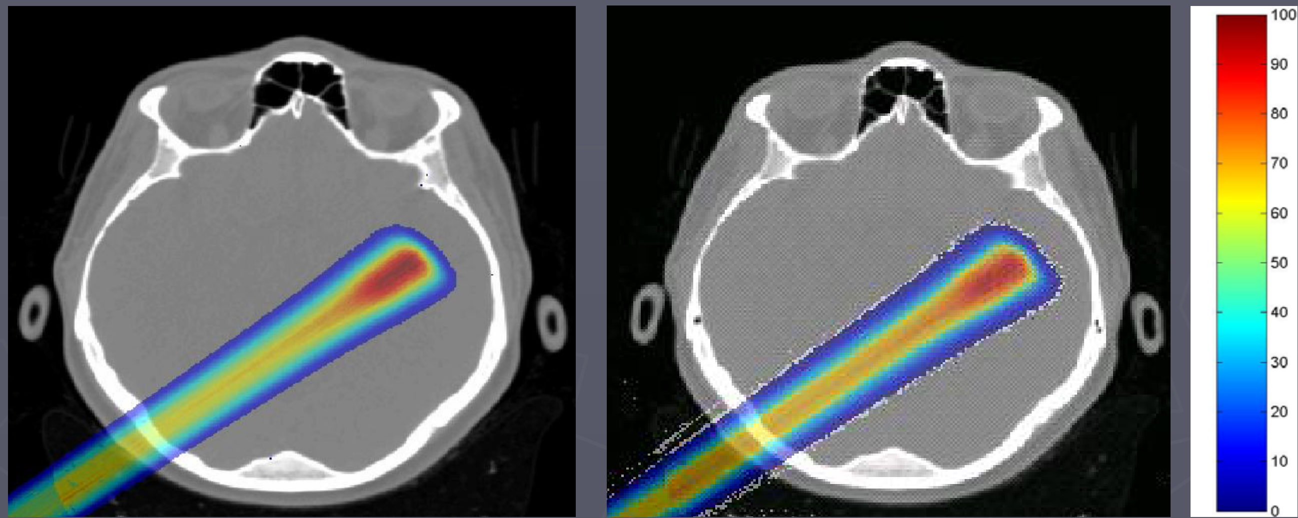
Geant4's widespread use

- Imaging, radiotherapy, dosimetry
  - PET and SPECT imaging (GATE),
  - brachytherapy, hadrontherapy,
- Space: satelites and planetary missions
  - XMM, INTEGRAL, Bepe Colombo, LISA, ...
- Radiation assessment, dosimetry
  - LHCb, Electronics (TCAD), ...

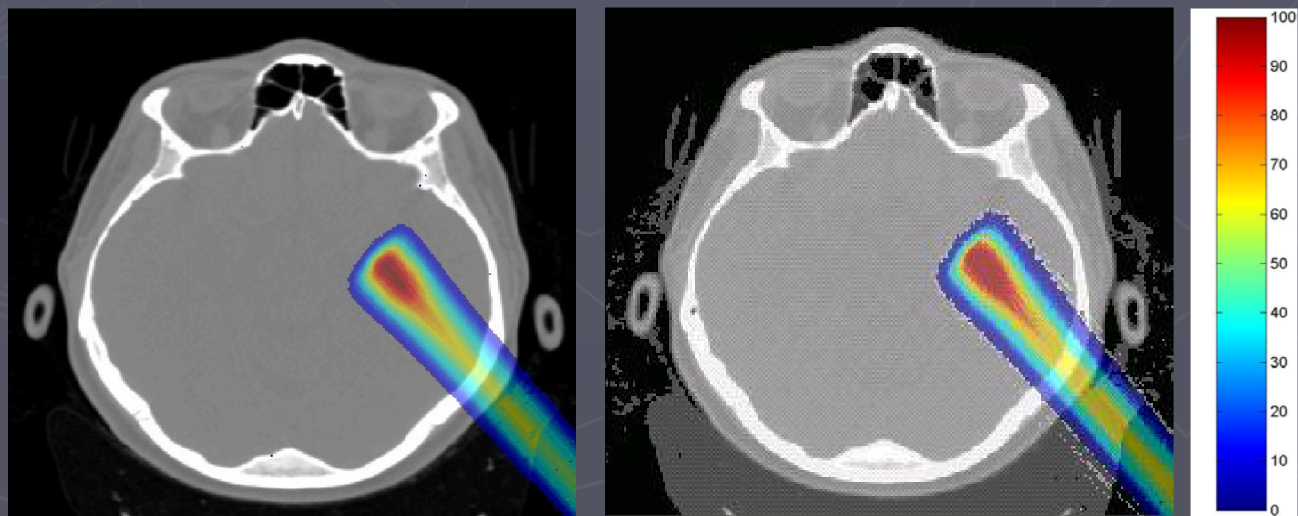
Geant 4

BORDEAUX 2005

Monte Carlo dose calculation, Example 2: Radiosurgery (4 fields)



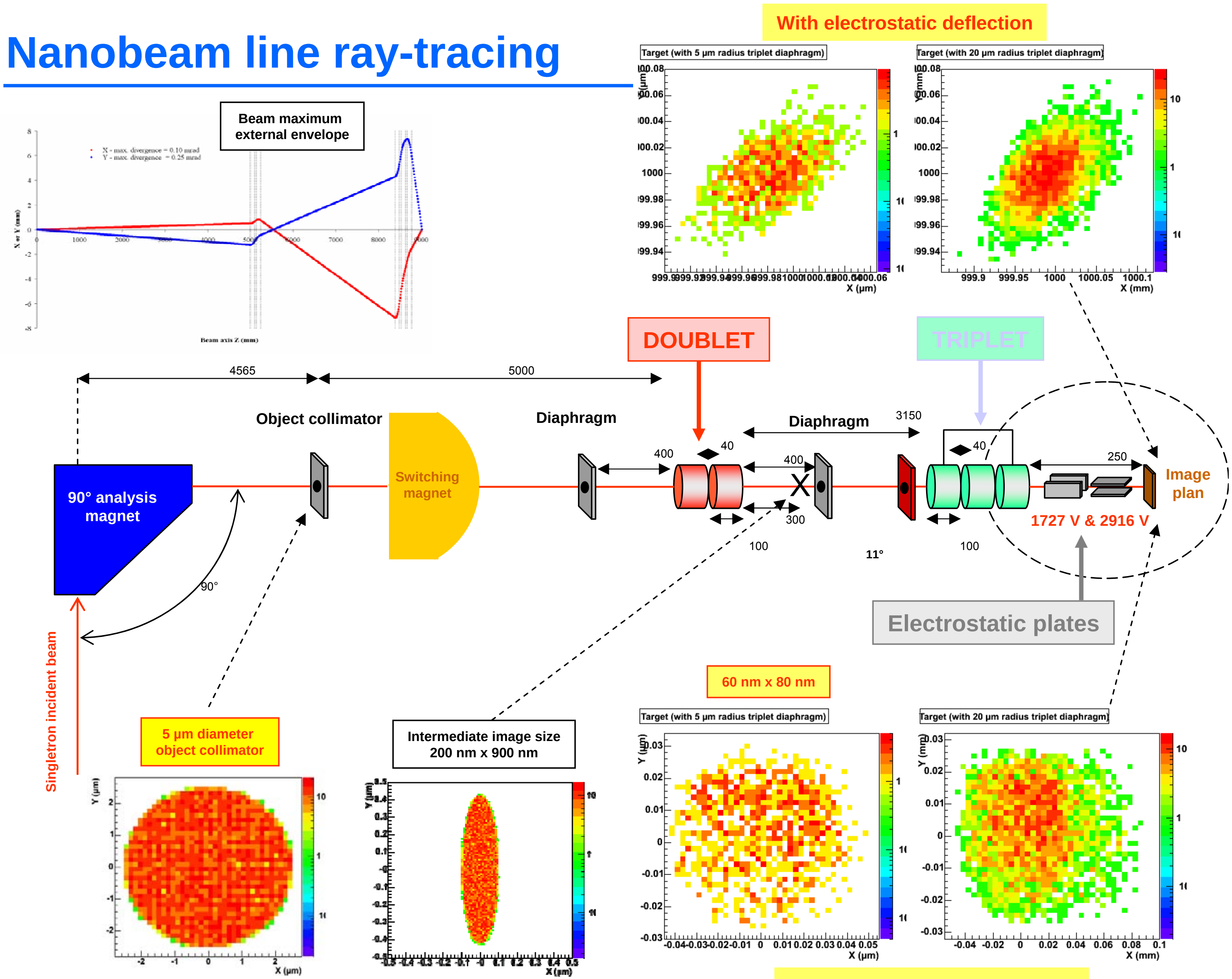
FOCUS Monte Carlo



FOCUS Monte Carlo

Thanks to H. Paganetti, MGH

Nanobeam line ray-tracing



Thanks to S. Incerti, CENBG

Geant4 8.0 developments

Additional information

Geometry: solids and dynamical geometries

- Additional solids
  - Generic twisted trapezoid shape with different endcaps - (O. Link)
  - New ellipsoid (G.Guerrieri, INFN/Genova) and elliptical cone (D. Anninos, CERN/Cornell)
  - Tetrahedron (M. Mendelhall, Vanderbilt Univ.)
- Testing and Improvements (O. Link, CERN)
  - Solid accuracy tests identified problems in torus, sphere (theta)
  - Fix in sphere and improvement of torus (new polynomial solver)
- Localized re-optimization for dynamic geometries
  - Change and re-optimize only part of a large geometry (G. Cosmo)
    - Enables lightweight initialisation for changes in dynamic geometries

Other new features in geometry

- Overlap detection at construction time
  - When a volume is placed it is checked optionally for ‘overlaps’
    - If it overlaps sister volumes or protrudes from its mother
    - Points on its surface are sampled
    - An exception is generated if a point is outside the mother or inside a sister volume
  - Applicable for placement and parameterised volumes
- Extended use of G4Region:
  - Was used for G4ProductionCuts and G4VUserRegionInformation,
  - Can now create User Limits for Regions (7.1)
  - Now enabled its use with parameterisation / Fast Simulation
    - All these data members are optional

Nested parameterization

- In the past G4VPVParameterization::ComputeMaterial() method used to take only the copy number of the immediate physical volume
  - There was no way to get a copy number of its (grand)mother volume
- To implement boxes in 3-Dimensional alignment with varying material (e.g. DICOM), one parameterization has to take care of three dimensions.
  - One big mother volume filled by one tiny cell with 3-dimensional parameterization
- With newly introducing nested parameterization, a touchable instead of naïve copy number is provided to ComputeMaterial() method.
  - Material of a box can be indexed not only with the copy number of the immediate volume but also with copy numbers of its (grand)mother volumes
  - The big mother box can be replicated twice in first and second axes, and then parameterized only along the third axis.
  - Performance improvement in both voxelization and navigation/tracking

Non-static particle definition

- In Geant4 8.0, all particle definition class objects are instantiated when GenerateParticle() method of physics list is invoked
  - Until now, most particle definition objects were static and the GenerateParticle() method ensured they were linked in the executable
- A side effect is foreseen if your physics list has physics processes/models as data members of your physics lists.
  - such processes or models may not been instantiated properly.
- Released revised physics lists to address this
- What to do
  - In case processes/models are defined as data members, they are actually instantiated at the moment your physics list itself is instantiated, i.e. before GenerateParticle() method is invoked.
  - If you use your own copy/customized physics list you will need to migrate
    - For example if you derived from one of the "educated guess" physics list,
    - How to do this
      - define pointers for such processes/models as the data members, and make sure all processes/models are actually instantiated in your GenerateProcess() method.

Concrete sensitivity classes

- Until 7.1 Geant4 provided only an abstract class (G4VSensitiveDetector) for the user to define his/her detector sensitivity.
  - Various example detector classes are provided.
    - Good to store hits in their detectors (HEP experiments).
  - But is not convenient for radiation applications (Space/medical/HEP)
    - Where the main interest is scoring dose/flux.
- G4 8.0 introduces G4MultiFunctionalDetector
  - In it you can register concrete 'scorers' to build a custom scoring detector.
  - Now provide scorers for EnergyDeposition, Surface Flux, Dose, Track Length
    - additional concrete classes are under development.
  - Note: G4MultiFunctionalDetector is a G4VSensitiveDetector.

Concrete sensitivity classes

- Each G4VPrimitiveSensitivity class generates one hits collection per event. By registering more than one classes of G4VPrimitiveSensitivity, G4MultiFunctionalDetector generates more than one collections.
- G4THitsMap template class (an alternative to G4THitsCollection) introduced. It is also a derived class of G4VHitsCollection.
  - It is more convenient for scoring purposes, and simpler
- New class G4VSDFilter introduced. Can be attached to G4VSensitiveDetector and/or G4VPrimitiveSensitivity to define which kinds of tracks are to be scored.
  - E.g., surface flux of protons of more than 1 GeV/c can be scored by G4PSSurfaceFluxScorer with a filter.
- Current G4Scorer and its related classes are kept, for the time being
  - Expect these to be declared obsolete.

Bertini Cascade

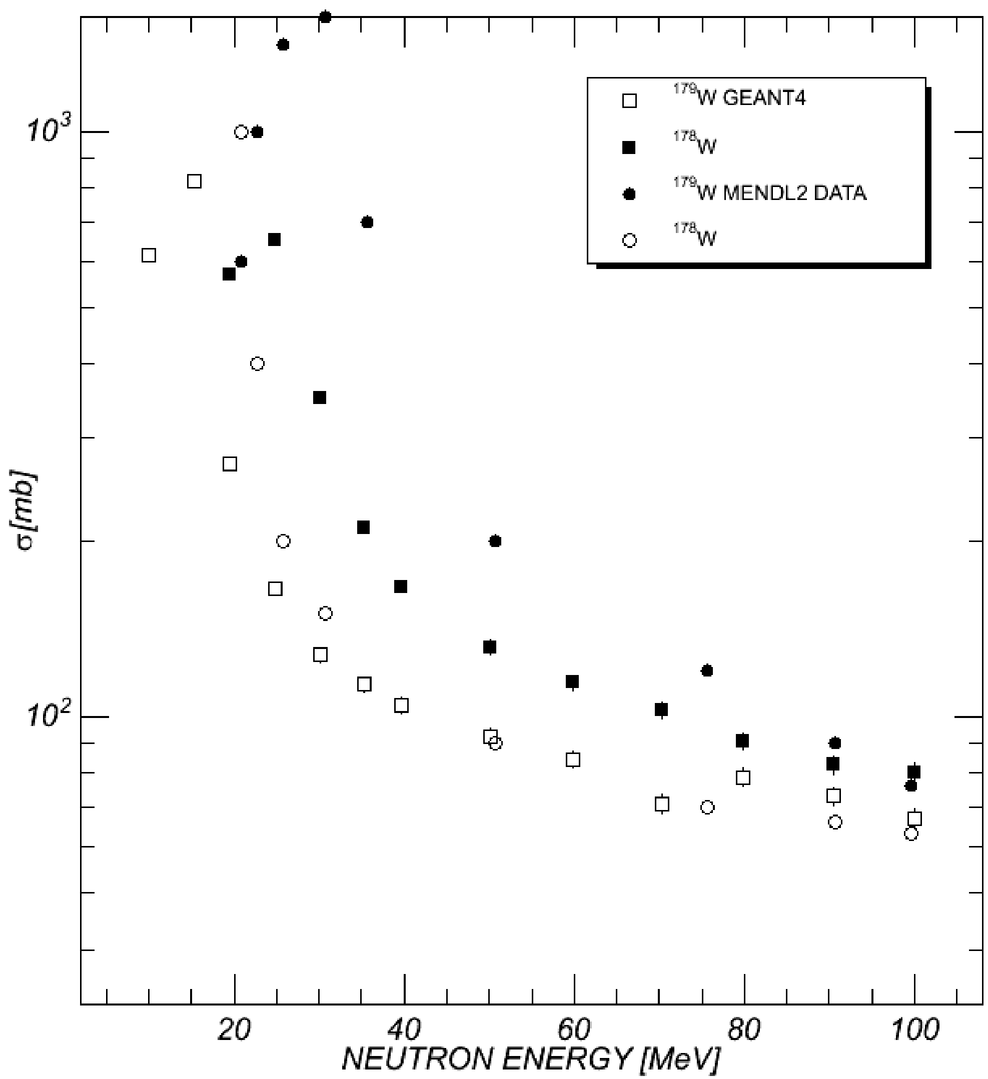
- Isotope production
  - Proton and neutron induced
- Elastic scattering interface (release 7.1)
  - G4CascadeElasticInterface (for < 1 GeV)
- Kaon extensions
- Validation
- Optimization for speed, model tuning

A. Heikkinen (HIP), D. Wright (SLAC)

Bertini hadronic models in Geant4 7.1

- Submodels implemented for proton, neutron, pion bullets:
  - `G4ElementaryParticleCollider`
  - `G4IntraNucleiCascader`
  - `G4NonEquilibriumEvaporator (pre-equilibrium)`
  - `G4EquilibriumEvaporator`
  - `G4Fissioner`
  - `G4BigBanger`
- Latest Bertini extension (June, 2005)
  - First partial release providing elastic part of intra-cascade treatment for kaon, lambda, sigma, and xi by Dennis Wright (SLAC)
    - Now stable and available at CVS (use `KAON`-flag)
    - This SLAC-tag was to be released fully in next Geant4 (8.0) release

ISOTOPES PRODUCED BY NEUTRONS ON $^{180}_{74}W$



Low-energy neutron induced isotope production is usually treated with Geant4 isotope production model using of evaluated data libraries

Yet in some cases Bertini model performs quite well and might be useful

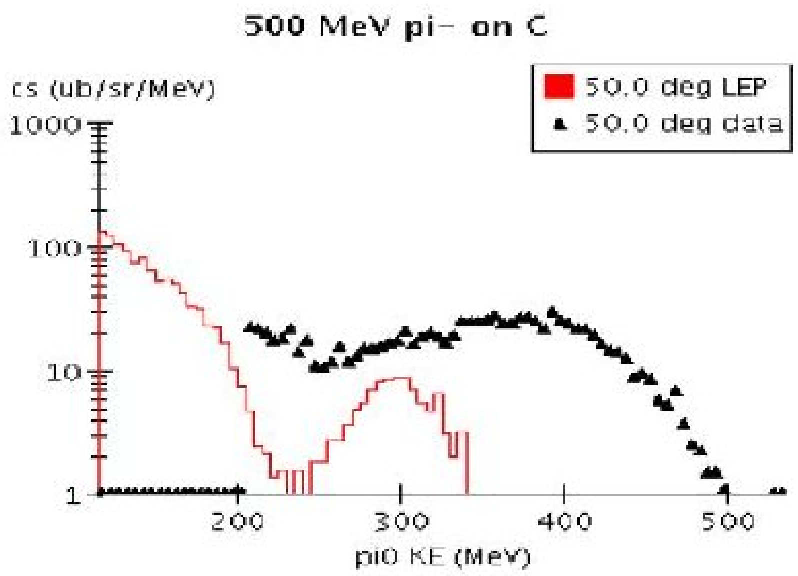


Figure 1: Current GEANT4 LEP physics list setting against data (Ouyang, Peterson 1992)

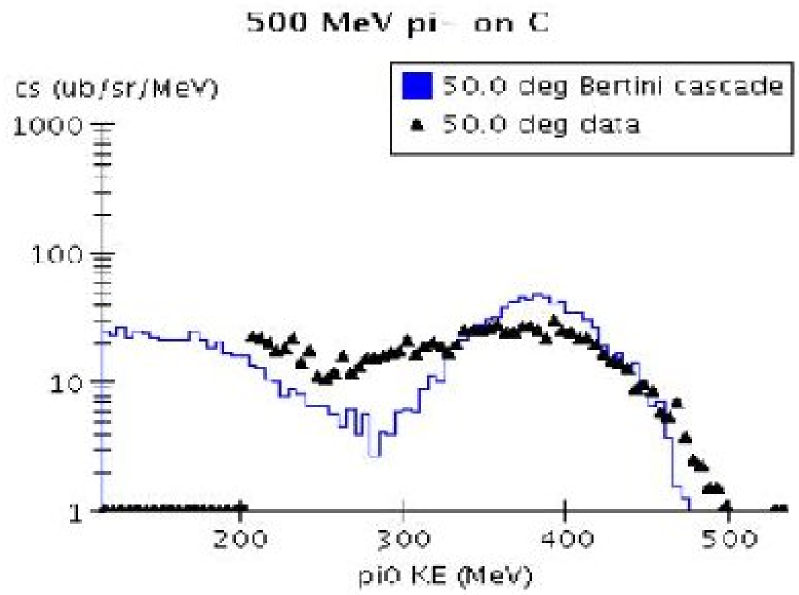
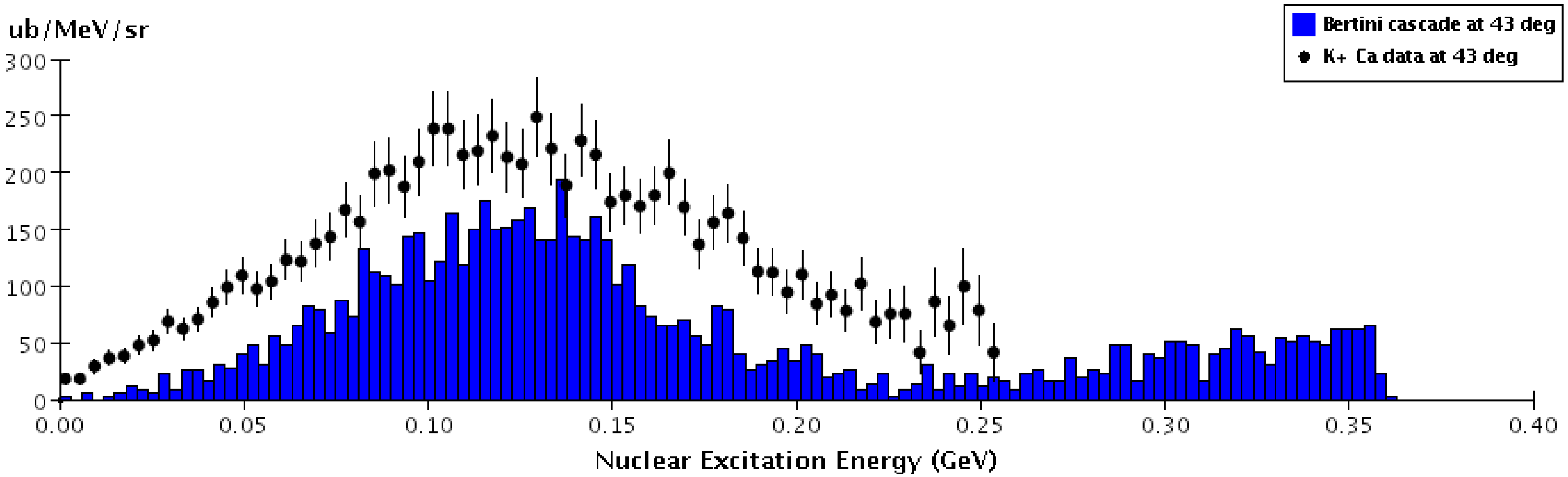
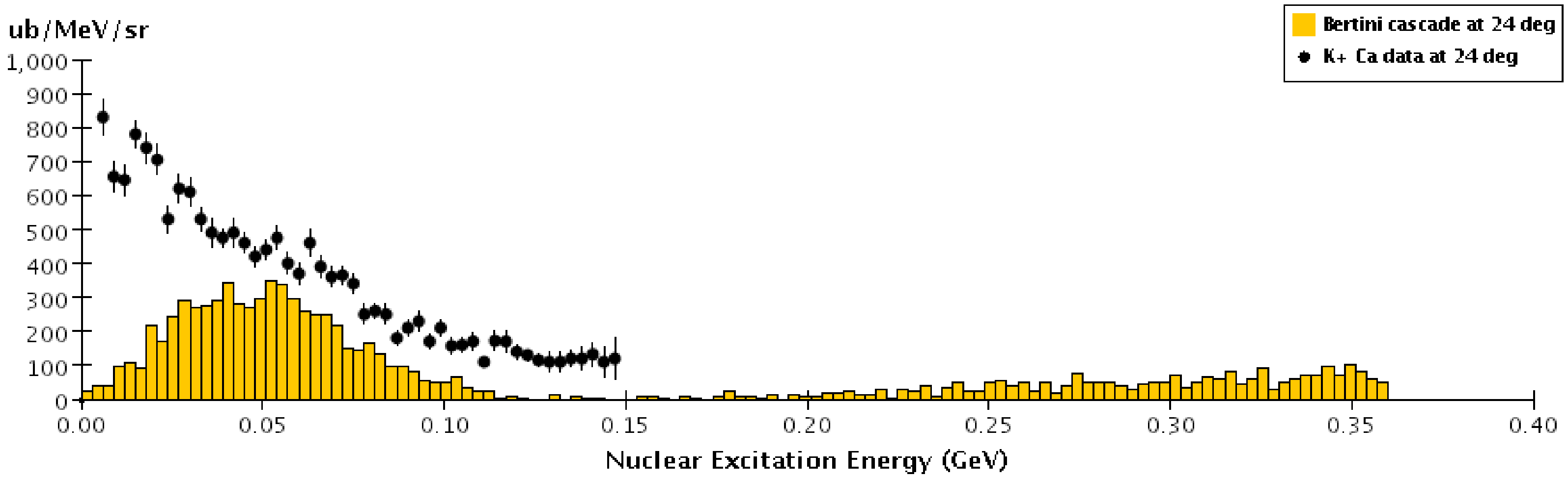


Figure 2: Bertini cascade model

705 MeV/c K+ quasi-elastic scattering from Ca



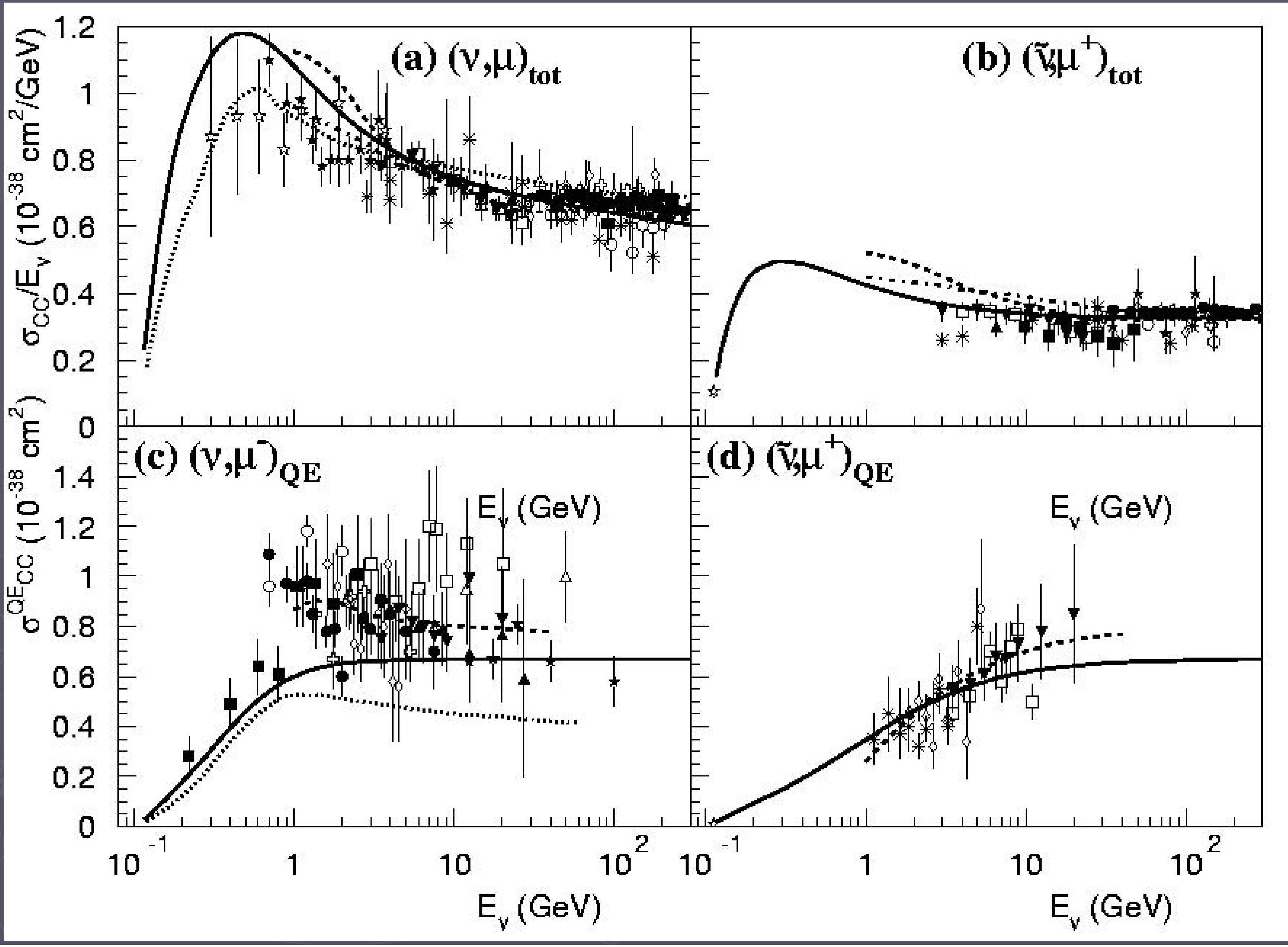


New Developments in CHIPS

- G4QCaptureAtRest for nuclear capture
  - of negative hadrons, muons, and low energy neutrons/antineutrons.
- G4QCollision for photo- and lepto-nuclear reactions
  - with DIS simulation of neutrino-nuclear reactions.
- Process level tests for comparison of simulated parameters with experimental data
  - Validation tests for at rest and in-flight (test19/test29).
- New fixed version of CHIPS for QGSC and FTFC.

M. Kosov

Neutrino-nuclear interactions for CNGS



Physics Lists

- Revised to work with Geant4 8.0
  - Co-work with particles revision
- Utilise EM(std) physics builders
  - Tested by EM(std) WG on HEP calorimeter setups
- Now γ-A interactions is default in all PLs
  - QGSP_GN is now QGSP, includes γ–nuclear
  - A few ‘engines’ suppressed
    - LHEP_GN, ..
- New variant with ‘old’ EM physics
  - QGSP_EMV uses multiple scattering with 7.1 parameters

Migrations

- Migrations:
  - Use of <sstream> instead of <strstream>
  - Support for CLHEP-2.0.X (compatible with 1.9.X series)
- Changes required in User Code
  - Fast parameterisation
    - Region replaces 'envelope'.
  - Creating and instantiating physics lists : impact of the revised, "non-static", particle definitions
  - G4VProcess base class
    - StartTracking() now has argument const G4Track*

http://top25.sciencedirect.com/index.php?subject_area_id=21

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INTRODUCTION

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1. Nanoscience and engineering in mechanics and materials • **Article**
   Journal of Physics and Chemistry of Solids, Volume 65, Issue 8-9, 1 August 2004, Pages 1501-1506
   Chong, K.P.
2. Geant4-a simulation toolkit • **Article**
   Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 506, Issue 3, 1 July 2003, Pages 250-303
   Agostinelli, S.; Allison, J.; Amako, K.; Apostolakis, J.; Araujo, H.; Arce, P.; Asai, M.; Axen, D.; Banerjee, S.; Barrand, G.; Behner, F.; Bellagamba, L.; Boudreau, J.; Broglia, L.; Brunengo, A.; Burk
3. Radiation pneumonitis and pulmonary fibrosis in non-small-cell lung cancer: Pulmonary function,

Other EM / materials issues

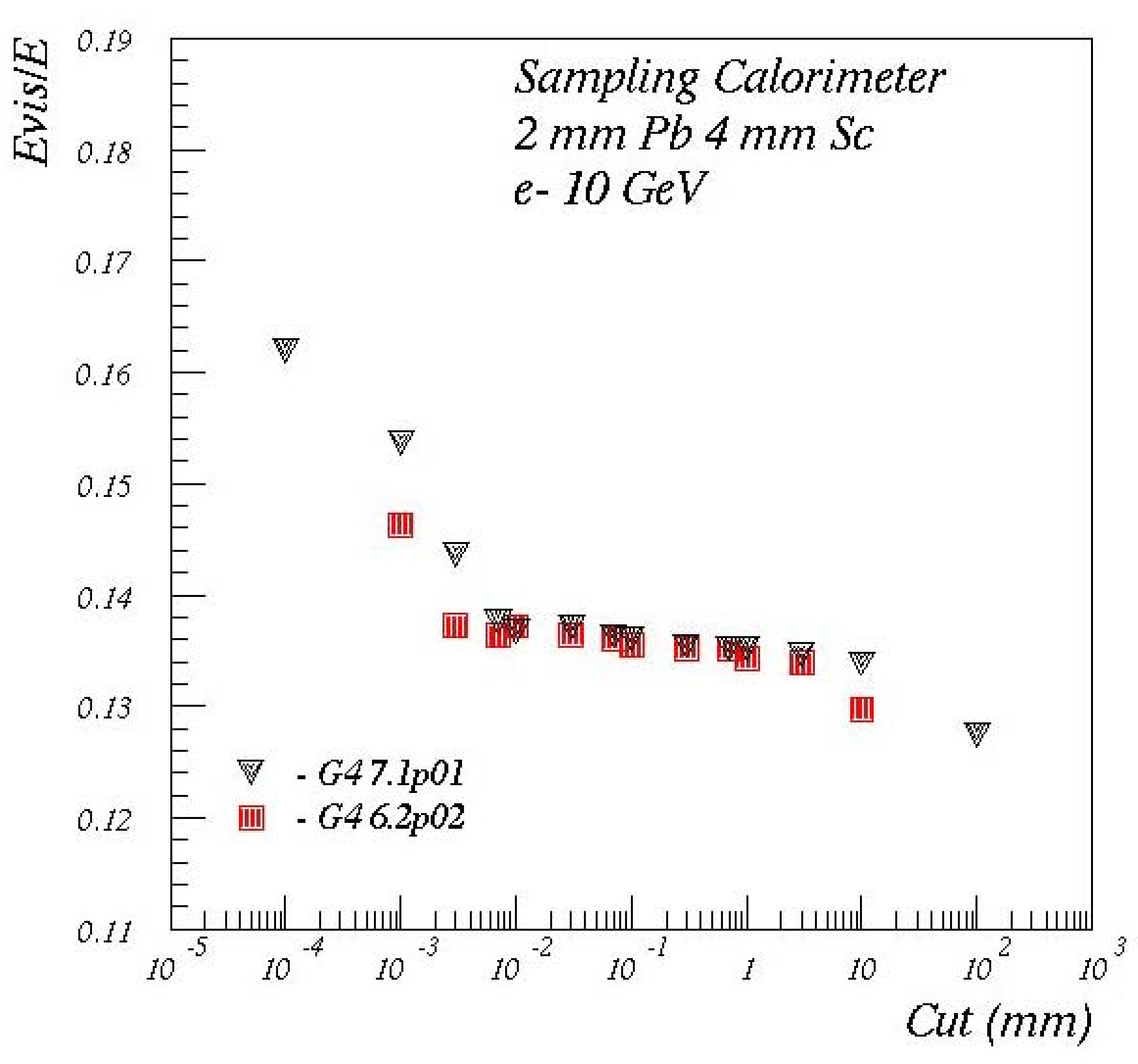
- Other new developments
  - revised Physics models
  - materials
- Infrastructure
  - design and testing

Standard EM Package: complete EM physics for HEP

- ***Standard***
  - basic EM processes for HEP: γ, e^-, e^+, charged leptons/hadrons
  - Cuts used for singularities, efficiency
    - A cut is production threshold,
      - Express in length – it is minimum value for range of produced particle
- ***Xrays***
  - Processes for producing xrays and optical photon
- ***Muons***
  - basic set of muon EM processes for HEP
- ***High-energy***
  - processes at high energy (new development relevant to LHC, Linear collider, astrophysics)

Issue with Stability of visible energy

- Users reported that results in some cases
  - depended on cuts
  - depended on step limits
- Precise simulation for thin layers (medical applications, shielding, fine granular calorimeters...)
  - could require simulation with very small cuts
- Investigated cut/step limit effects
  - concluded that Multiple Scattering process is key



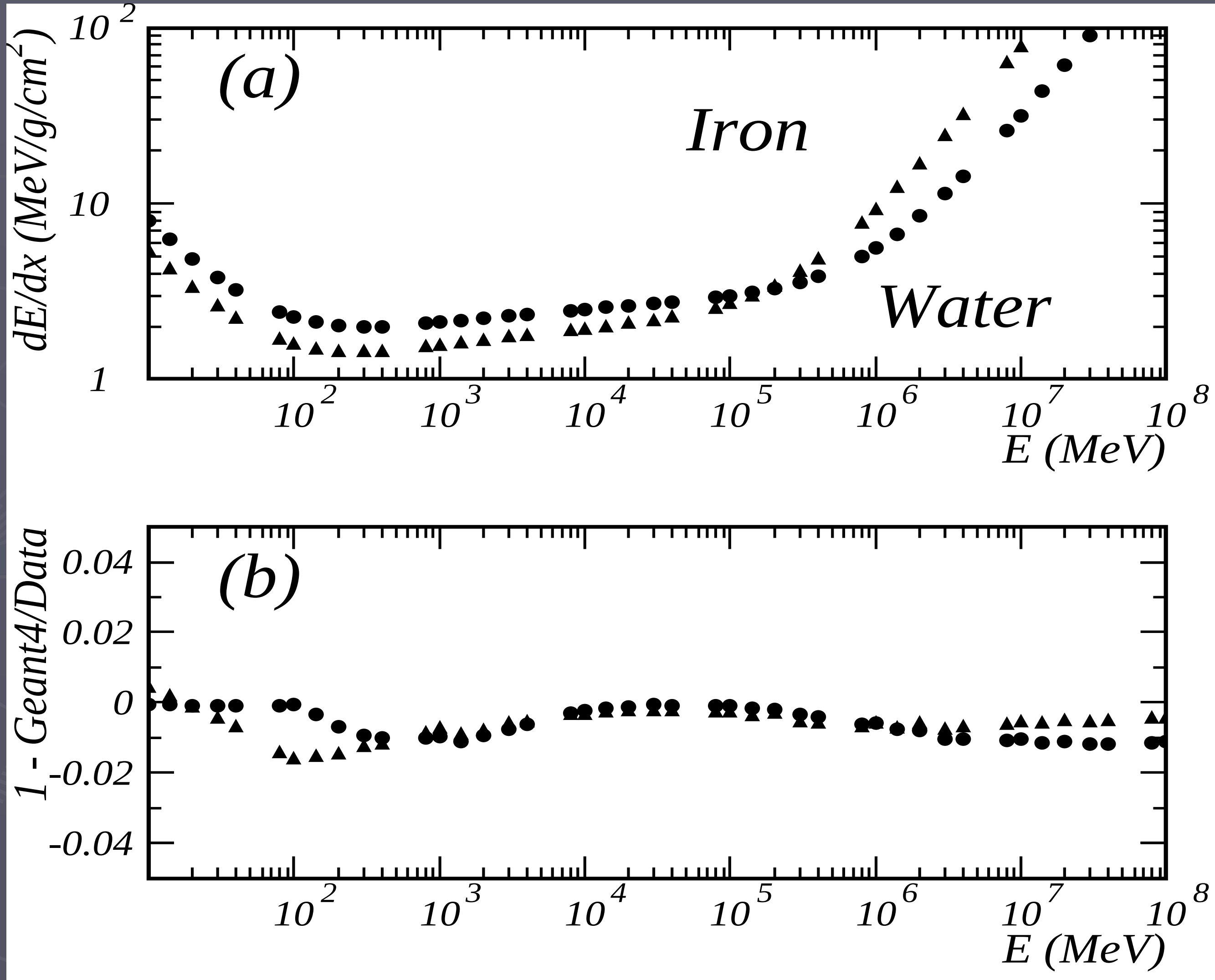
Test suite for EM physics

- The test suite
  - covers 120 test cases from single material to model calorimeter
  - uses the 16 'extended' EM examples
  - 23 key test cases run in regression
- Large statistics tests for simplified LHC calorimeters:
  - ATLAS Barrel Pb/lAr
  - ATLAS HEC Cu/lAr
  - CMS crystal calorimeter $PbWO_4$
  - LHCb Pb/Sc calorimeter
- Results for key test cases kept for each G4 version
  - from Geant4 release 5.1 (April 2003)

In addition these setups serve as starting points for user applications.

Stopping powers validation for muons against evaluated data from *Atomic and Nuclear Data Tables 78, 183 (2001)*

G4 7.1

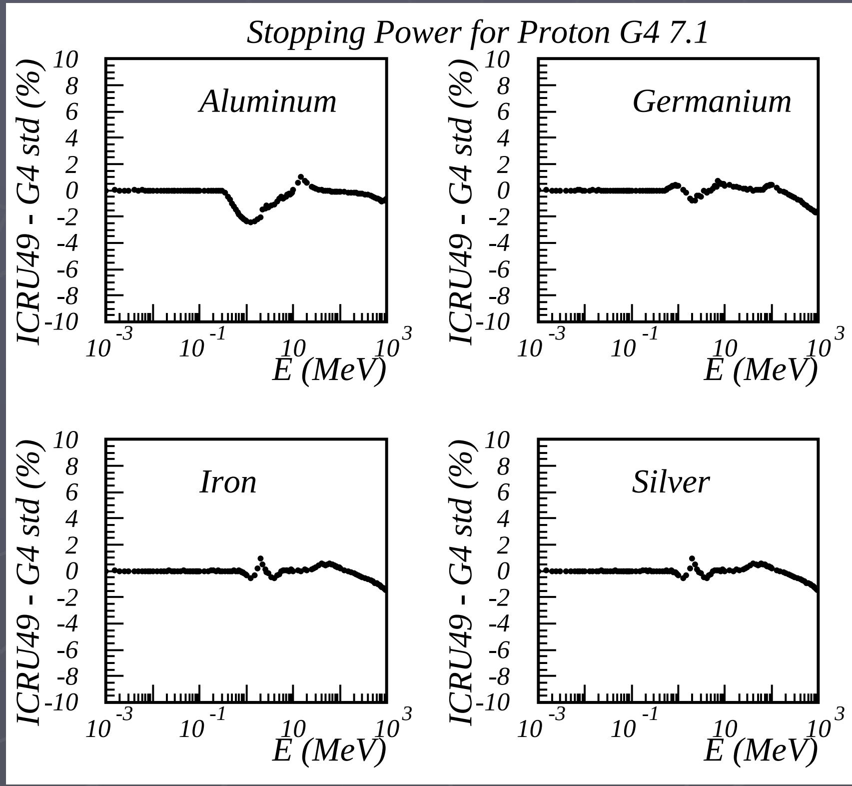


MC/Data
Within 2%

Physics models improvements

- Revision of corrections to hadron/ion ionization
- TRD models
  - specialised models for key LHC use cases
  - Key change
  - X-rays generated as a collective effect at a point in the TR volume
- New process for ionization of exotic hadrons
  - G4hhIonisation

Stopping power within 2%



‘Infrastructure’: Design Iterations

- The goals of the design iterations:
  - Enable extensions (eg with high energy models)
  - Ability to trigger special models per ‘Geometrical Region’
  - Improved bookkeeping, maintenance
- New components and user interfaces:
  - G4EmProcessOptions – enable common options
  - G4EmCalculator – access cross sections
  - G4EnergyLossForExtrapolator – average effects for ‘swimming’ tracks
- Completes design evolution started in release 5.1

‘Infrastructure’:
Database of materials, elements, and isotopes

- Ensure accuracy for key properties of materials:
  - Values from NIST
    - Density
    - Mean excitation potential (I)
    - Chemical formula
    - Element composition
- and (for hadronic processes):
  - Natural isotope composition
- New interfaces
  - Old constructors kept
- Can also access via UI commands

```
#   Elementary Materials from the NIST Data Base
 Z  Name  ChemFormula  density(g/cm^3)   I(eV)
------------------------------------------------------
1    G4_H    H_2              8.3748e-05       19.2
…
6    G4_C                     2                81
7    G4_N    N_2              0.0011652        82
8    G4_O    O_2              0.00133151       95

#   Compound Materials from NIST Data Base
 N Name      ChFormula       density(g/cm^3)
     I(eV)
------------------------------------------------------
95  G4_Air                    0.00120479       85.7
           6      0.000124
           7      0.755268
           8      0.231781
          18      0.012827
96  G4_CsI                    4.51             553.1
          53      0.47692
          55      0.52308
```

Summary

- The Geant4 Multiple Scattering was significantly revised
  - More precise and more stable results for different use cases
  - In typical cases achieves high-quality physics results for less CPU
- A physics testing suite has been deployed
  - 120 cases, 20 used monthly, 4 in high-statistics regression
- Models, infrastructure improved
  - Improvements in high-energy, TRD physics models
  - Cycle of design revision of Std EM package is complete
  - NIST materials database with density, ionisation potential, ...
- Standard EM group continues to
  - focus on validation / verification, and model updates
  - be open to user feedback and new requirements

Cache for materials

NIST materials in Geant4

```
=====================================
###   Elementary Materials from the NIST Data Base
      =====================================
 Z Name  ChFormula        density(g/cm^3)  I(eV)
=====================================
1    G4_H    H_2              8.3748e-05       19.2
2    G4_He                    0.000166322      41.8
3    G4_Li                    0.534            40
4    G4_Be                    1.848            63.7
5    G4_B                     2.37             76
6    G4_C                     2                81
7    G4_N    N_2              0.0011652        82
8    G4_O    O_2              0.00133151       95
9    G4_F                     0.00158029       115
10   G4_Ne                    0.000838505      137
11   G4_Na                    0.971            149
12   G4_Mg                    1.74             156
13   G4_Al                    2.6989           166
14   G4_Si                    2.33             173
```

```
====================================
###   Compound Materials from the NIST Data Base
====================================
 N Name      ChFormula       density(g/cm^3)  I(eV)
====================================
13  G4_Adipose_Tissue              0.92             63.2
        1    0.119477
        6    0.63724
        7    0.00797
        8    0.232333
       11    0.0005
       12    2e-05
       15    0.00016
       16    0.00073
       17    0.00119
       19    0.00032
       20    2e-05
       26    2e-05
       30    2e-05
4  G4_Air                          0.00120479       85.7
        6    0.000124
        7    0.755268
        8    0.231781
       18    0.012827
2  G4_CsI                          4.51             553.1
       53    0.47692
       55    0.52308
```

Material Types:
- NIST Elementary Materials
- NIST Compounds
- Nuclear Materials

How to use the Material Manager

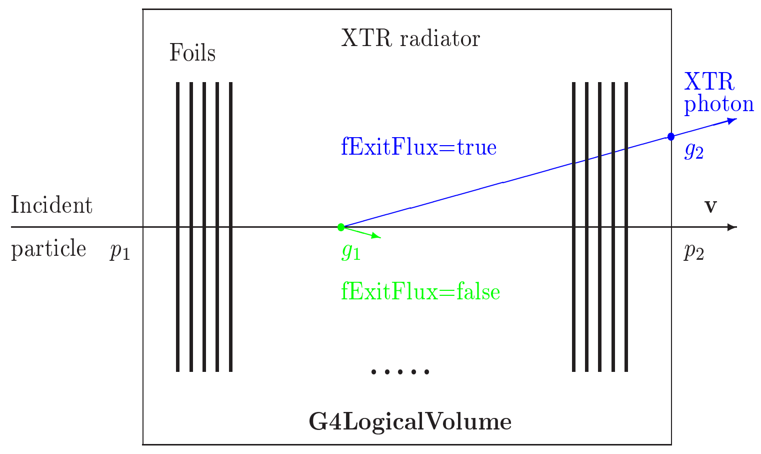
- A user simply requests the element or material
  - does not need to define elements and materials by their properties
- Main new user interfaces:

```
G4NistManager* manager = G4NistManager::GetPointer();
G4Element* elm = manager->FindOrBuildElement("symb", G4bool iso);
G4Element* elm = manager->FindOrBuildElement(G4int Z, G4bool iso);
G4Material* mat = manager->FindOrBuildMaterial("name", G4bool iso);
G4Material* mat = manager->ConstructNewMaterial("name",
                            const std::vector<G4int>& Z,
                            const std::vector<G4double>& weight,
                            G4double density, G4bool iso);
G4double isotopeMass = manager->GetMass(G4int Z, G4int N);
```

TRD Processes and Models Upgrade

- X-ray transition radiation in different radiators became to be discrete process
- It allows to simulate inclined and curved tracks
- The two groups of models are available:
  - Models describing the XTR photons starting from the particle track (fExitFlux=false)
  - Models describing the flux of XTR photons after the radiator (fExitFlux=true)
- The models support foam, fiber and regular radiators
- A new model for the generation of XTR inside straw tube gas detector is available

Production of secondaries is performing at the exit of the Logical Volume



The diagram of the XTR generation according to dE/dx and flux models

0-0

NIST Element and Isotopes Example

Z		A	m	error	(%)	A_{eff}
14	Si	22	22.03453	(22)		28.0855(3)
		23	23.02552	(21)		
		24	24.011546	(21)		
		25	25.004107	(11)		
		26	25.992330	(3)		
		27	26.98670476	(17)		
		28	27.9769265327	(20)	92.2297 (7)	
		29	28.97649472	(3)	4.6832 (5)	
		30	29.97377022	(5)	3.0872 (5)	
		31	30.97536327	(7)		
		32	31.9741481	(23)		
		33	32.978001	(17)		
		34	33.978576	(15)		
		35	34.984580	(40)		
		36	35.98669	(11)		
		37	36.99300	(13)		
		38	37.99598	(29)		
		39	39.00230	(43)		
		40	40.00580	(54)		
		41	41.01270	(64)		
		42	42.01610	(75)		

Verification/Validation Strategy

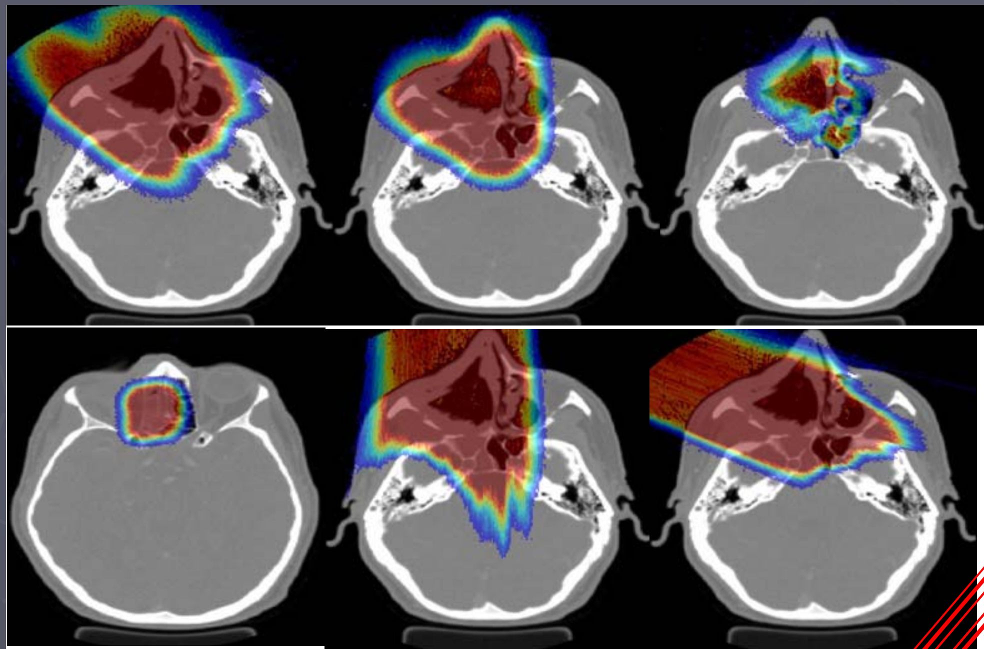
- Unit tests by developers
  - Cross sections, stopping powers
- Fast automatic test on main platform
  - Low statistics test for each tag
  - large statistics test for reference tags
  - Comparison with previous version
- Geant4 system- integration testing
- Selected tests (LHC-like setups) with large statistics
  - Each reference tag
  - Comparisons between different reference tags

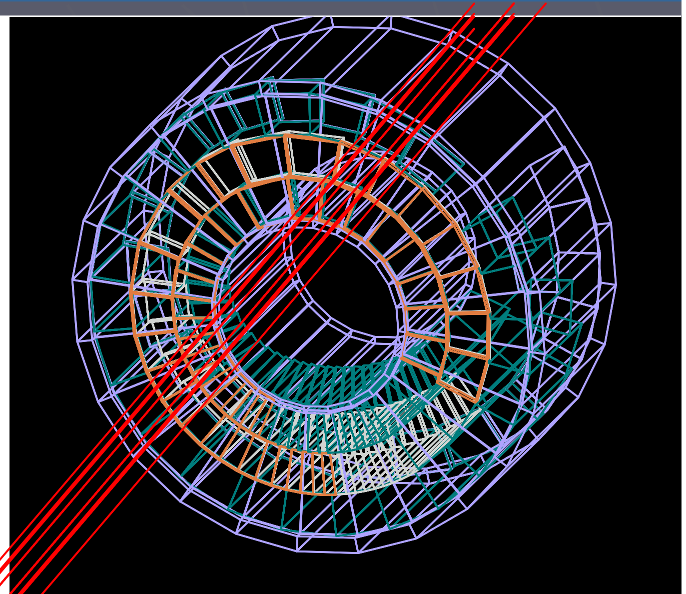
3. Users apply and extend G4

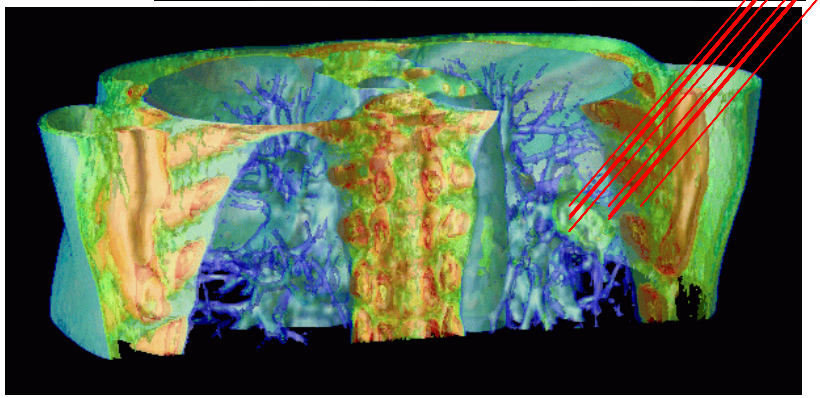
- Tools using Geant4 for class of related applications
  - GATE tool
    - "Geant4 Application for Tomographic Emission"
  - BDSIM for beam-line simulations
- Users extend Geant4
  - Special solids for own geometry (many -> G4)
    - Atlas endcap solid (fan), twisted tube (KEK), Tet (vanderbilt)
  - GFLASH shower parameterisation (Atlas, CMS -> G4)
  - 'Regular' navigation (10-100 mil volumes at one level)
  - Use of 2,500 materials

Key strengths exploited: architecture, open source

GEANT4 based proton dose calculation in a clinical environment: technical aspects, strategies and challenges







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MASSACHUSETTS GENERAL HOSPITAL

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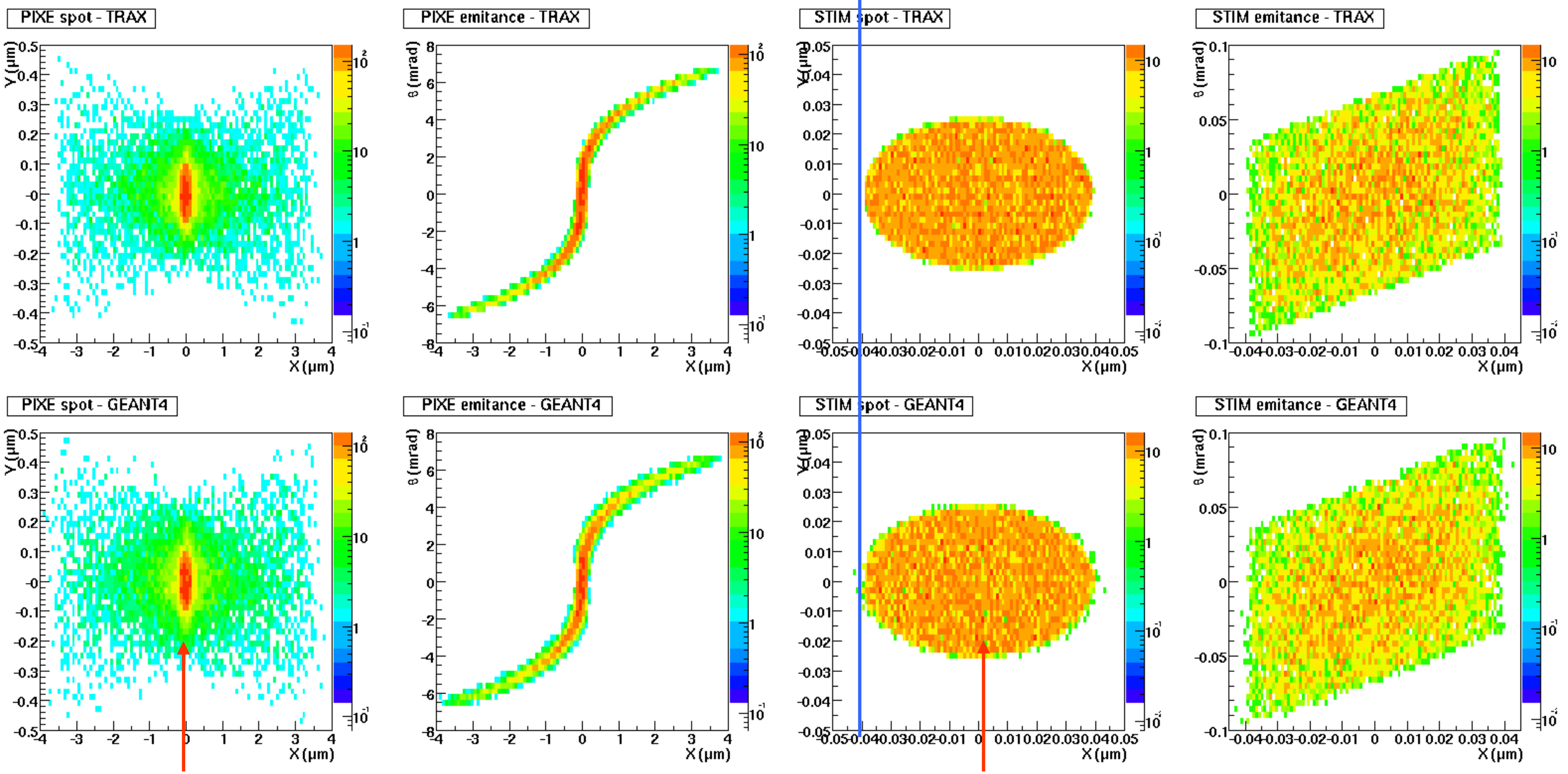
Microbeam simulation: Comparison in high (PIXE) and low flux (STIM) modes

Geant4 versus TRAX (reference)



300 nm x 200 nm **90 nm x 50 nm**

- Nice agreement between TRAX and Geant4 (square field model, no map)
- Sharp STIM image, distorted PIXE image (chromatic and spherical aberrations)
- Compatible with probe size requirements
- Pure vacuum, no collimators

Sept 19th, 2006

Thanks to S. Incerti

Users extend Geant4

- For regular voxel phantom geometries
  - Tens of millions of volumes at one level!
  - Revising one/two navigation class(es)
    - K. Sutherland, H. Jiang
- To simulate thousands of materials
  - Varying in density
  - storing physics tables for tens/hundreds
    - H. Jiang / H. Paganetti
- Utilise toolkit and open source
  - And customise for own application requirements / constraints

Geant4 collaboration

2006 planned developments

Provided for reference.

Covers non-LCG resources in addition to CERN/LCG resources.

Geant4 Collaboration: Planned developments & releases in 2006

- *Items in this list are related to new developments scheduled for the current year. Improvements, fixes, studies and maintenance items are not mentioned here as part of routine activity* . From http://geant4.web.cern.ch/geant4/support/planned_features.shtml
- **Geometry**
  - Generic tessellated solid - *(1)*
  - Parallel navigator, first implementation - *(1)/(2)*
  - Re-factoring and revision of biasing/scoring processes - *(1)/(2)*
  - Tunable geometrical tolerance - *(2)*
  - Identification of the first/last step in a volume - *(2)*
  - Optimized navigation for voxelised phantom geometries - *(2)*
- **Hadronic Physics**
  - Evaluate and improve hadronic elastic scattering - *(2)*
  - Study effects of new multiple scattering on shower shape of hadronic showers and on e/pi ratio - *(2)*
  - Extension to G4NDL data library and repackaging using ENDF - *(2)*
  - Development of sub-models of Bertini cascade and application to ions - *(2)*
  - Binary cascade interface to string models - *(2)*
  - Extensions to CHIPS
    - Neutrino-nuclear interactions at low energies including neutrino-electron process - *(1)*
    - New muon-nuclear and tau-nuclear processes (catastrophic muon interaction) - *(1)*
    - Application to hadronic interactions at energies E < A**.33 GeV - *(1)/(2)*
    - Quasmon String model (hadronic CHIPS at high energies) on the process level - *(2)*
    - Inelastic scattering of hadrons on atomic electrons (reverse kinematics of electro-nuclear reactions) - *(2)*
    - Coherent charge exchange process with corresponding cross sections for different hadrons - *(2)*
  - Review of total, elastic, inelastic cross sections - *(2)*

G4 Coll. Planned developments 2006 (cont)

Standard Electromagnetic physics & optical processes

- Updates to ionization processes
  - Spin and mass effects for pions, muons, kaons
  - Ability to plug in user data for stopping powers
  - Improve kinematics of final state sampling of PAI models - *(2)*
- Implementation of an alternative model for synchrotron radiation
- Alternative multiple-scattering processes for different particle types - *(1)/(2)*
  - e+,e-, muons, hadrons, and ions
- Review of the Bremsstrahlung models including LPM effect - *(2)*
- Development of elastic Coulomb scattering process - *(1)/(2)*
- Extension of e+ annihilation to hadrons
  - Addition of 3pi and K+K- production *(1)/(2)*
- Updates to optical processes
  - Micro-facet extensions - *(1)*
  - Specular and diffuse component transmitted photon - *(1)*
  - Modeling transport in volumes with different optical treatments on different sides/faces - *(2)*
  - Extend usage of optical processes to boolean solids - *(2)*
- Introduction of K-L shell X-rays in photo-electric process - *(*)*

Materials, Generic Processes and Parameterisations

- Ability to change temperature and density of gaseous materials - *(1)*
- Migration of ghost envelope for fast simulation to the parallel navigation facility - *(1)/(2)*
- Review for performance improvement of fast-simulation - *(1)/(2)*
- Allow for more informations/methods to be provided for atomic shells class - *(2)*
- Improvement of verbosity for materials - *(2)*

Low-energy Electromagnetic physics

- Low energy extensions in water - *(2)*
- Evaluation of Penelope multiple scattering - *(2)*
- Low energy extensions in silicon - *(2) (*)*
  - NOTE: *Items marked with (*) may or may not be achieved in 2006.*

G4 Coll. Planned developments 2006 (cont)

- **Particles & Track**
  - Update of PDG encoding and particle names for resonances - *(1)*
  - Review of GetVelocity() method for optical photons - *(1)*
  - Addition of magnetic moment to particle properties - *(2)*
- **Run, Event & Detector Response**
  - First implementation of parallel navigation - *(1)/(2)*
  - Unification of scoring mechanism - *(1)/(2)*
  - Modular user actions - *(2) (*)*
  - Physics list (or process manager) per region - *(2) (*)*
    - NOTE: *Items marked with (*) may or may not be achieved in 2006.*
- **Tracking**
  - Selective verbosity: requirement analysis - *(1)/(2)*
  - Support for scoring in parallel geometries - *(1)/(2)*
  - Support for identification of the first/last step in a volume - *(2)*
- **User and Category Interfaces**
  - Prototype of Python interface - *(1)*
  - Prototype of a platform for Geant4 Web service - *(2)*
  - Prototype of a ui-vis joint GUI desktop - *(2)*

G4 Coll. Planned developments 2006 (cont)

- **Visualisation and Graphics Representations**
  - Support visualization of G4Polyhedra with generic constructor - *(1)*
  - Addition of commands to allow interactive editing of geometry volume visualization attributes such as visibility and color - *(1)*
  - Extensions to G4RichTrajectory and provide examples - *(1)*
  - Provide convenient visualization tools for new Scorers - *(1)*
  - Provide example for generating volume data file suitable for rendering with the GRAPE visualizer (intended for medical apps) - *(1)*
  - Add more commands for modeling trajectories (*drawByInteractionType*, *drawByInteractionVolume*, ...) - *(1)*
  - Extend handling of text to more visualization drivers - *(2)*
  - New commands to cut trajectories based on various attributes - *(2)*
  - Output same event (or event set) to multiple visualization drivers by automatically re-running simulation with same random seed - *(2)*
  - Ability to copy view information from one visualization driver to any another - *(2)*
  - Support 2D Text - *(2)*
  - Implementation of an advanced example geometry - *(2)*
  - Provide solution integrated into normal visualization system for visualization of DICOM files - *(2)*
  - Full support for visualization of boolean shapes - *(2) (*)*
  - Extend ability of generic sections and cuts - *(2) (*)*
  - Support visualisation of regions/envelopes/parallel geometries - *(2) (*)*
  - Create HepRepFile to DAWNFile converter - *(2) (*)*
  - Develop immediate-mode for HepRep to WIRED or FRED - *(2) (*)*
  - Integrated visualization of field-lines - *(2) (*)*
  - Support for dynamic loading of visualization drivers - *(2) (*)*