Recent Geant4 Developments

D. Wright, A. Dotti on behalf of Geant4 collaboration
CALICE Collaboration Meeting - Argonne National Laboratory
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U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Introduction

Only few **highlights** will be presented

- For a full review of recent versions, see **Technical Forums**:
  - Geant4 Version 9.6 (December 2012): https://indico.cern.ch/event/216885/
  - Geant4 Version 10.0 (December 2013): https://indico.cern.ch/event/284492/

- In this talk concentrate on aspects relevant for CALICE
  - Status of Physics Lists: the general picture
  - Refinements on **EM physics**: improved multiple-scattering
  - Updates on **Hadronic physics**: improvements in models and neutron physics
  - **Technical** Updates: CPU performances and Multi-threading
- **Focus is on Geant4 Version 10.0 and Hadronic Physics**

Happening now…

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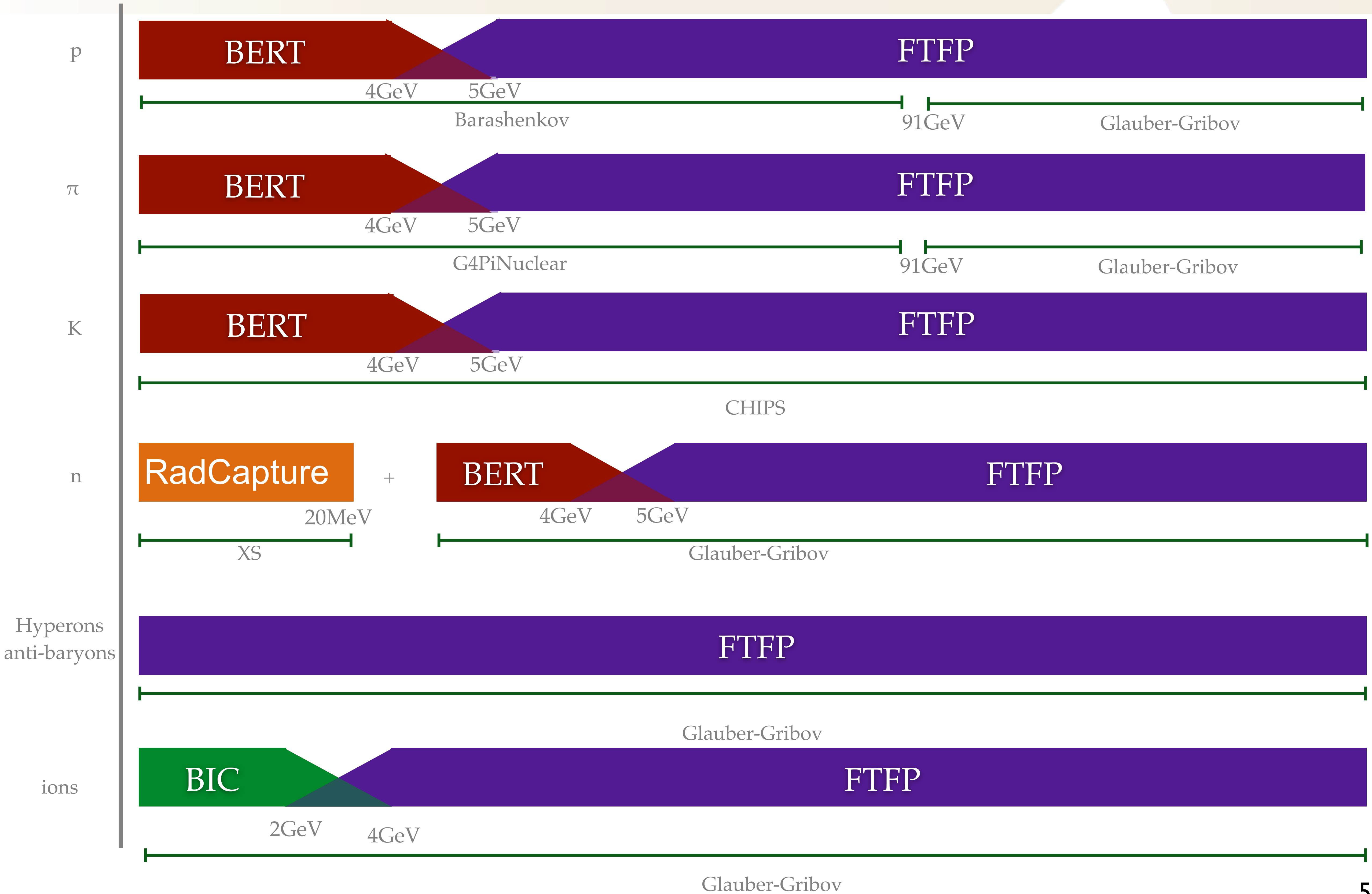
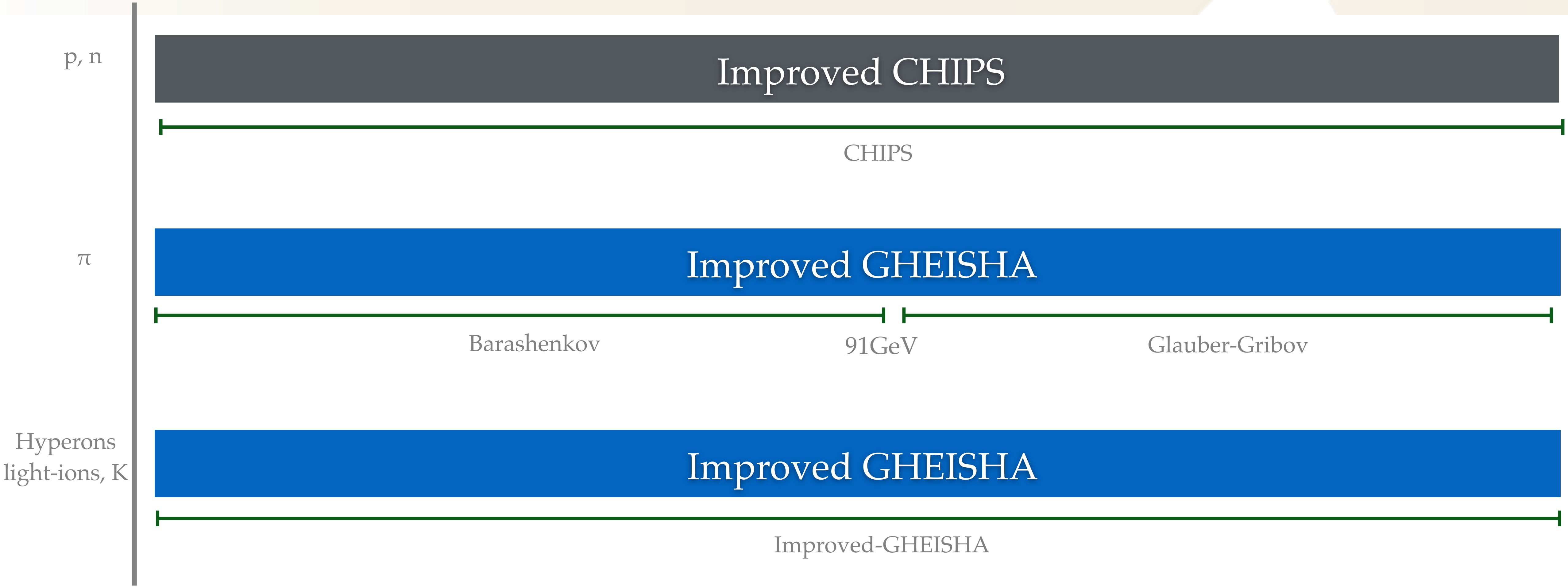
- Second **LPCC Detector Simulation Workshop**
  - https://indico.cern.ch/event/279530/other-view?view=standard
- We did not have time to go thorough all presentations yet, but some relevant summaries are included in the backup slides
- Focus is on LHC, but one contribution from CALICE (E. Sicking)
- Please take a look at A. Ribon's summary
  - **Several times CALICE is mentioned as the source of validation for G4 in the next years**, given the diminished interest for LHC on test-beam data

Summary of performances: Physics List

FTFP_BERT: inelastic interactions



FTFP_BERT: elastic interactions



Physics Lists (hadronic physics)

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- Recent main activities:
  - Removed obsolete models (next slide)
- Use of **"best" cross section set**
  - Proton, Neutron: Barashenkov+Glauber-Gribov
  - Pions: G4PiNuclearCrossSection & Glauber-Gribov
  - Kaons: CHIPS parametrization
  - Ions: Glauber-Gribov
  - Proton elastic: Barashenkov+Glauber-Gribov

Retired Hadronic Models

- **LEP, HEP** (Low and High Energy Parameterized) models
  - Based on the old GHEISHA Fortran models of Geant3
  - Replaced by extended versions of the Bertini cascade and FTF qcd string models

- **CHIPS** (Chiral Invariant Phase Space) models
  - Thermodynamic clustering model of hadron nucleus interactions
  - Formerly used for stopping, electro-, gamma-nuclear reactions
  - Now replaced by Bertini, FTF
  - Some CHIPS elastic and inelastic cross sections retained and made into separate classes

- **Isotope production model**
  - Based on LEP models
  - Now redundant, since all recoil nuclei are kept for tracking

Physics Lists (EM physics)

Constructor	Components	Comments
G4EmStandardPhysics	Default (QGSP_BERT, FTFP_BERT…)	ATLAS, and other HEP productions, other applications
G4EmStandardPhysics_option1	Fast due to simple step limitation, cuts used by photon processes (FTFP_BERT_EMV)	Similar to one used by CMS, good for crystals, not good for sampling calorimeters
G4EmStandardPhysics_option2	Experimental: updated photon models and bremsstrahlung on top of Opt1	Similar to one used by LHCb
G4EmStandardPhysics_option3	standard models when applicable	The most accurate standard
G4EmStandardPhysics_option4	photon models from Livermore and Penelope, Penelope ionisation for e-	The most accurate EM physics
G4EmLivermore	Livermore models when applicable	Livermore
G4EmPenelope	Penelope models when applicable	Penelope
G4EmLivermorePolarized	Polarized models	
G4EmDNA	Example of DNA physics	

- Physics exists for: γ,e,μ,K,p,Σ,Ξ,Ω,τ,B,D,D_s,Λ_c, Σ_c,Ξ_c,d,t,He3,He4, GenericIon
- Using G4PhysicsListFactory just add: `_EMV,_EMX,_EMY,_EMZ,_LIV,_PEN` to physics list name to get EM variant

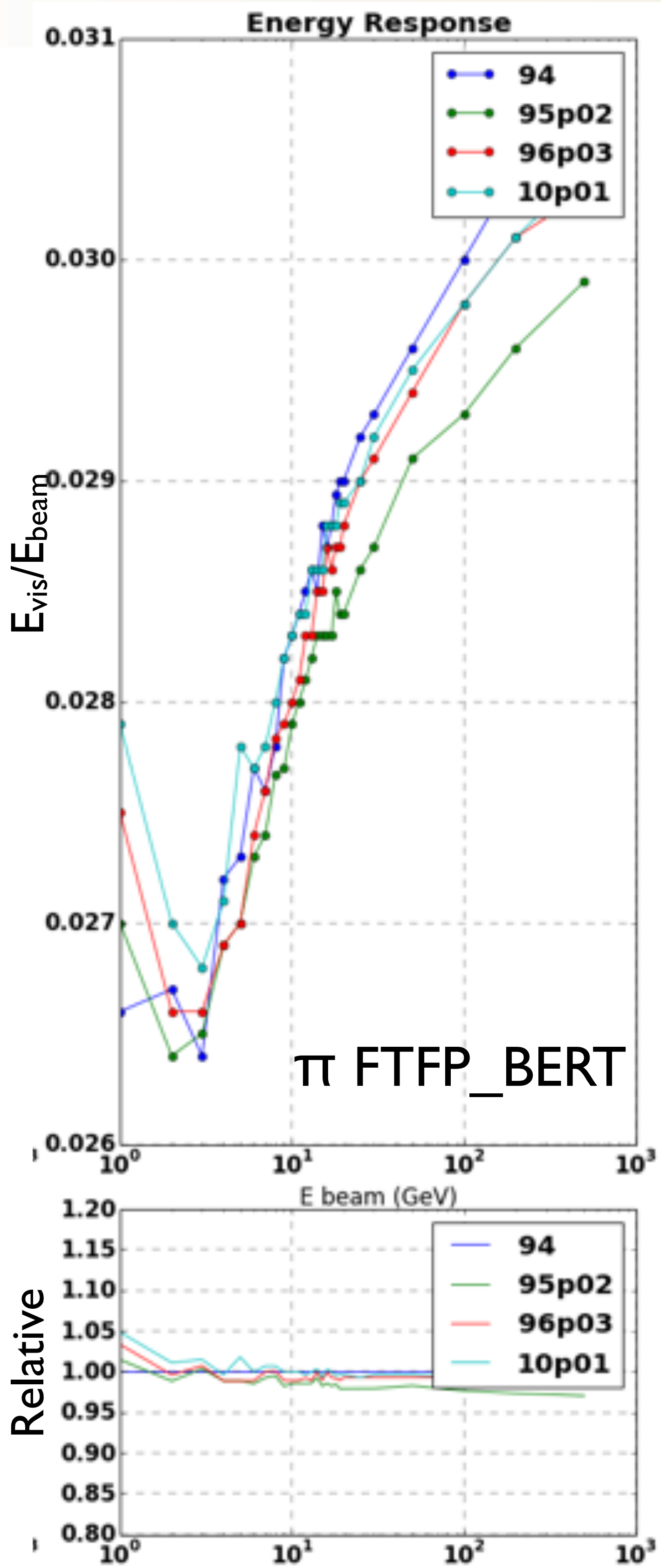
Physics Lists in Version 10

- **Supported** are:
  - FTFP_BERT(_HP),
  - QGSP_BERT(_HP), QGSP_BIC(_HP), QGSP_FTFP_BERT
  - Shielding
  - QBBC
  - G4GenericPhysicsList

- **Experimental** are:
  - FTFP_BERT_TRV
  - FTFP_INCLXX(_HP), QGSP_INCLXX(_HP)
  - FTF_BIC, QGS_BIC

Important note for V10: Since L/H-EP models retired use FTF in "gaps" (e.g. QGSP_BERT = QGS+FTF +BERT)

Simplified Calorimeter: response



- **Showing only Fe/Sci results**
- Similar conclusions for other calorimeters
  - We test: Fe, Pb, Cu, W, Brass as absorber; Sci, LAr, PbWO4 as active material
  - Data available only for response and resolution for Fe/Sci and Cu/LAr cases
- Response: **stable w.r.t. G4 version,** inside experimental (very large) error bars
- **Larger variations in latest release for W** (due to new Neutron Capture)
  - New results closer to _HP: expect to be improvement
  - Need CALICE data

Simplified Calorimeter: resolution

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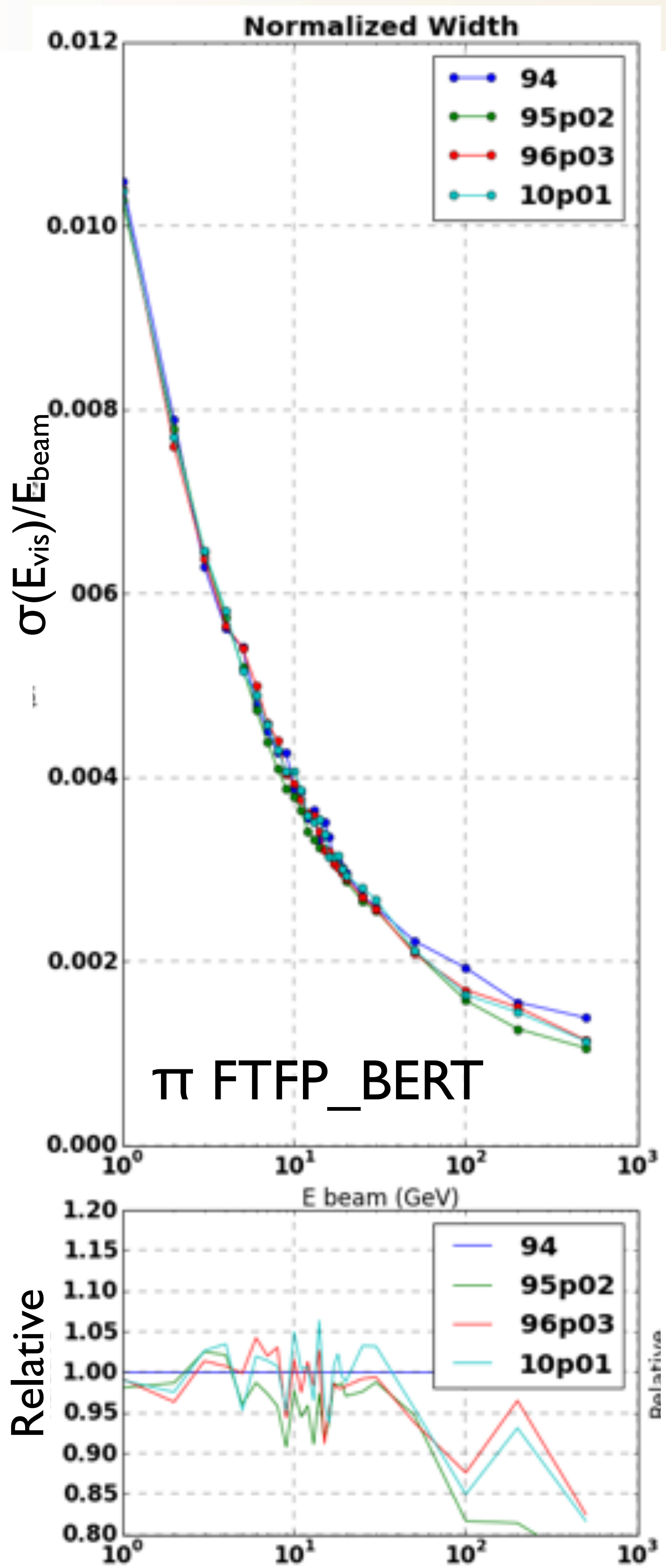
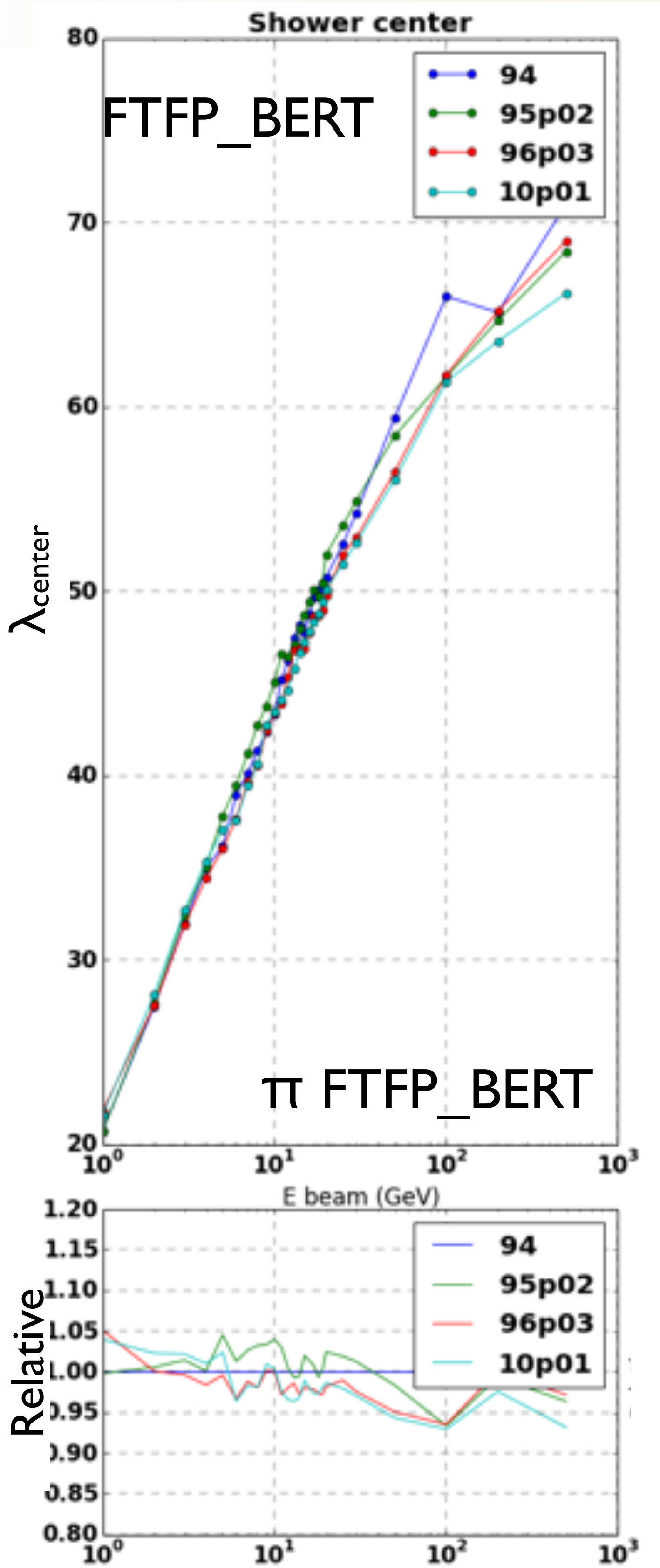


- **Stable results** w.r.t. version at low energy
- New FTF tunings: effect at high energy
- Feedback from LHC: resolution is too good in MC
- One of the main effects comes from pion multiplicity of first interaction(s)

	|
γ de-excitation	~0
p	0.7%
n	0.35%
π	4%
π	2.75%

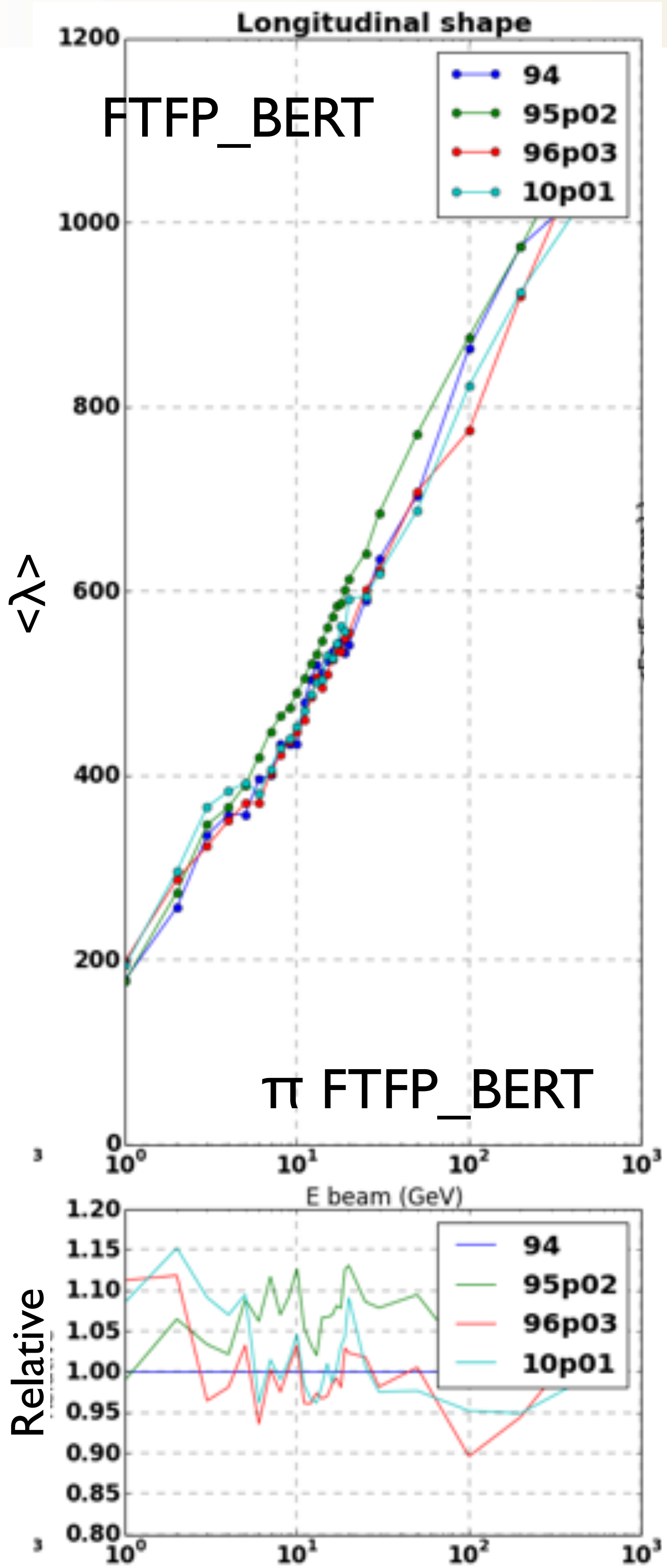
Simplified Calorimeter: shower center



- **Stable results** w.r.t. version at low energy
- Mainly affected by hadronic inelastic cross-section
  - Satisfactory validation against thin target data

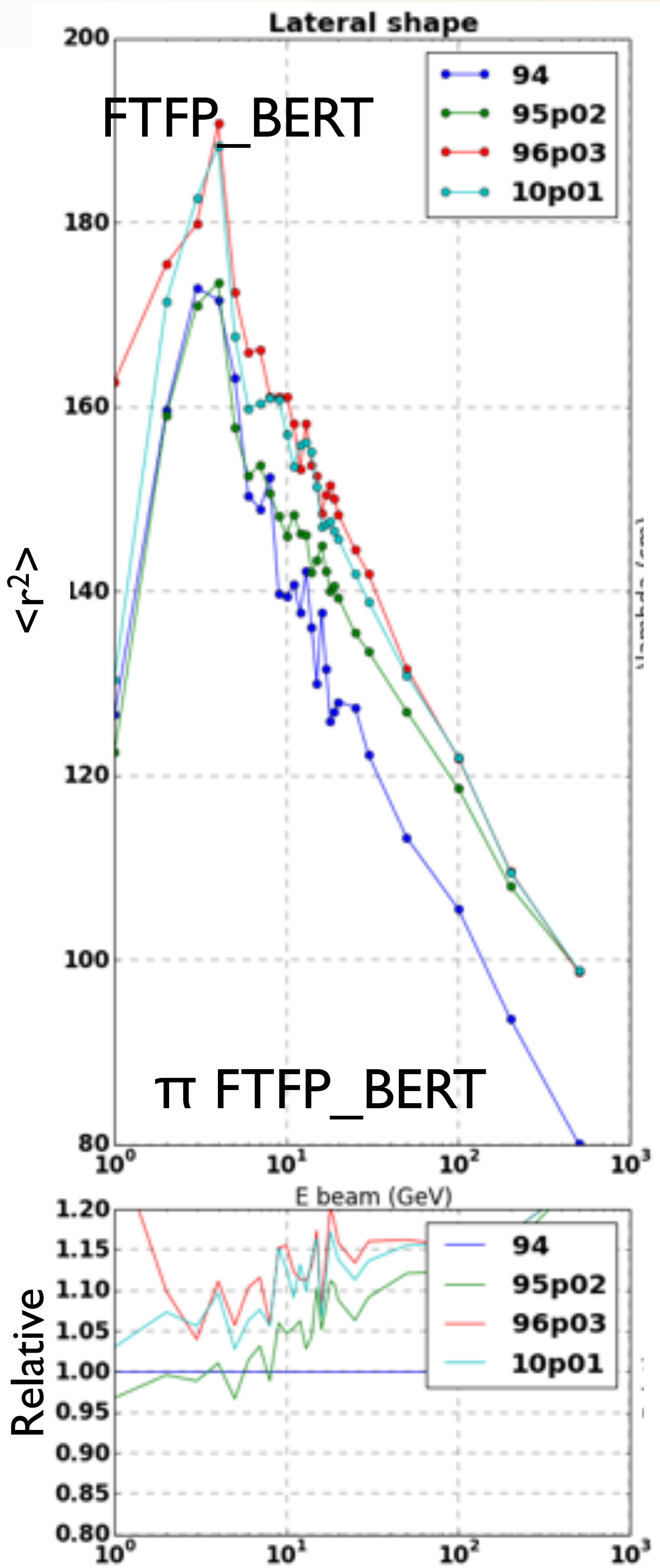
See CERN-LCGAPP-2012-01 for details on *shower moments* definitions (http://sftweb.cern.ch/AAdocuments). Very similar to the one used by you

Simplified Calorimeter: longitudinal dimension



- With the exception of Version 9.5 longitudinal dimension **stable within 5%**
- Driven by string-model
- In particular:
  - Projectile/Target diffraction
  - Quasi-elastic (known to play important role)
  - Re-scattering at high energy
  - Elastic
- All the above will be **further tuned** in 2014+
- QGS model is theoretically more solid for high energies, tuning in program for 2014

Simplified Calorimeter: lateral dimension



- **Lateral shape is the observable with larger variations**
  - Recent versions give wider showers (exception W)
- Mainly driven by cascade model
- Feedback: showers are too compact w.r.t. data
- Transport/absorption of low-E neutron plays most important role
- **Summary**:
  1. Wider showers for Fe and Cu
  2. Narrower showers for W (n-Capture)
  3. Nearly stable for Pb

See, for some more details: CERN-LCGAPP-2012-02 (http://sftweb.cern.ch/AAdocuments)

Neutron Effect at low-E

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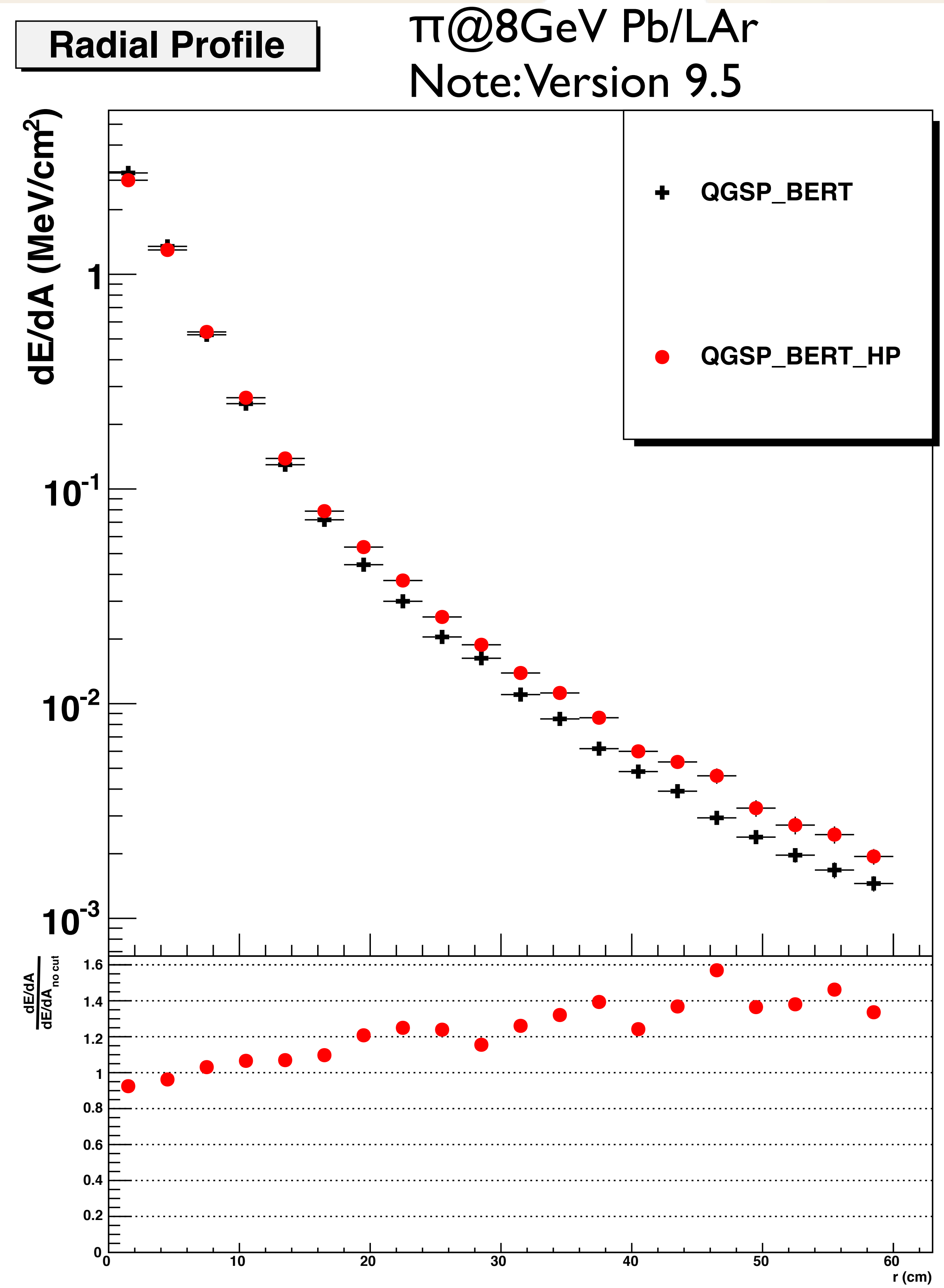
- Precise neutron description plays an important role in describing lateral shower shape
- In particular time-structure of showers seems more correct when using HP capture (CALICE T3B results)
- **We studied a new capture model (see later)**



Summary (G4 9.4.p01)

	Response	Resolution	Smoothness	Lateral Shape	Longitudinal Shape @10λ	Notes
QGSP_BERT	+(1-3)%	-(10-5)%	Bad	-(20-10)%	π: -10% p: -20%	anti-nucleons, hyperons via LHEP
FTFP_BERT	+(3-5)%	-(7-3)%	Good	π: -(20-10)% p: -(10-3)%	π: +10% p: +(10-20)%	anti-nucleons, hyperons via CHIPS(*)
CHIPS	+(10-5)%	-(20-10)%	Very Good	π: -(10-3)% p: -(20-10)%	π: -10% p: -20%	native anti-nucleons, hyperons
FTF_BIC(**)	+(3-5)%	-(6-2)%	Bad	-	π: +10%	Implements re-scattering

(*): Native FTF model under development
(**): Much less tested at LHC

OLD results @ LHC first beam
Since then we expect improvements in FTFP_BERT
Obtained with Test-Beam data

EM Physics Updates

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Photo Credit: Peter Ginter

Multiple Scattering

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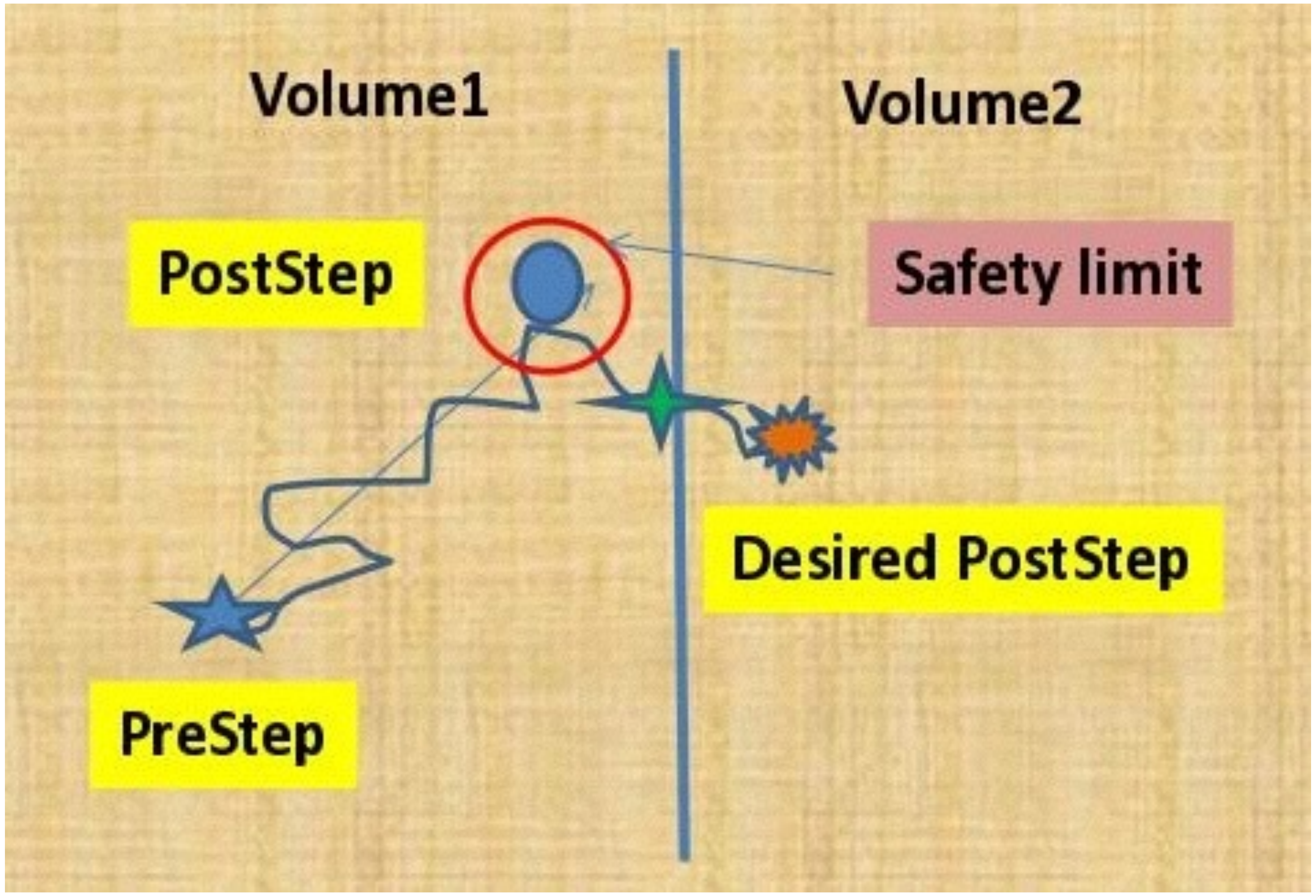
- Multiple scattering process has **improved near-boundary** behavior
  - coming from fix of reported problems with electron range

- New multiple scattering model: G4UrbanMscModel
  - Urban multiple scattering model tuned to larger set of data
  - **Replaces** all previous versions: Urban 90, 93,95, 96
  - New default for e+, e-, hadron multiple scattering below 100 MeV
  - Currently used for LHC production
  - **More accurate and stable vs. step size**

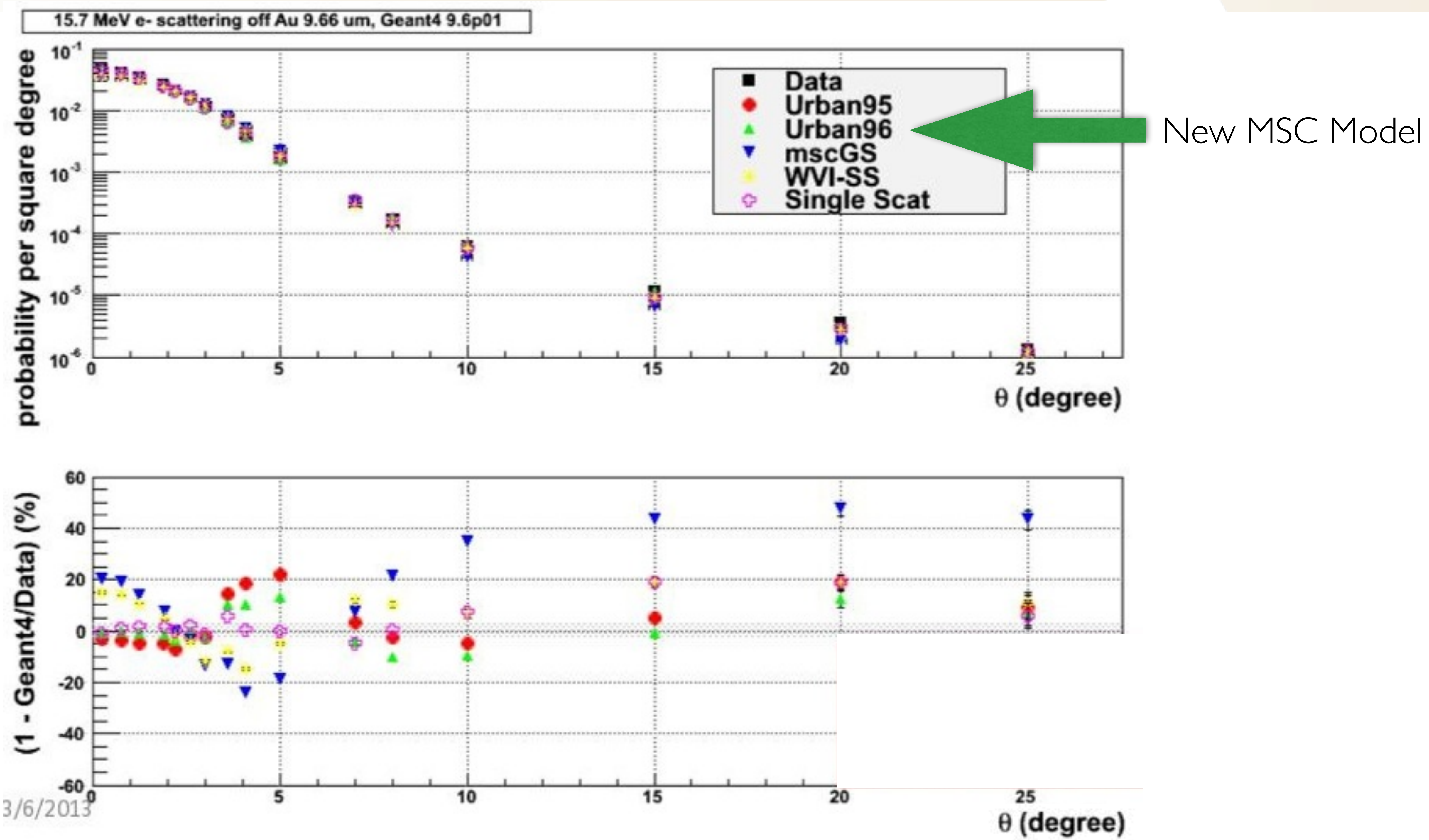
Refinement of MSC implementation

- Electron ranges seen to be too short in certain geometries
  - Cause: MSC process senses a boundary and limits step due to safety
- Solution: sample MSC AlongStep instead of PostStep, shift end-point to boundary, correct the true path length



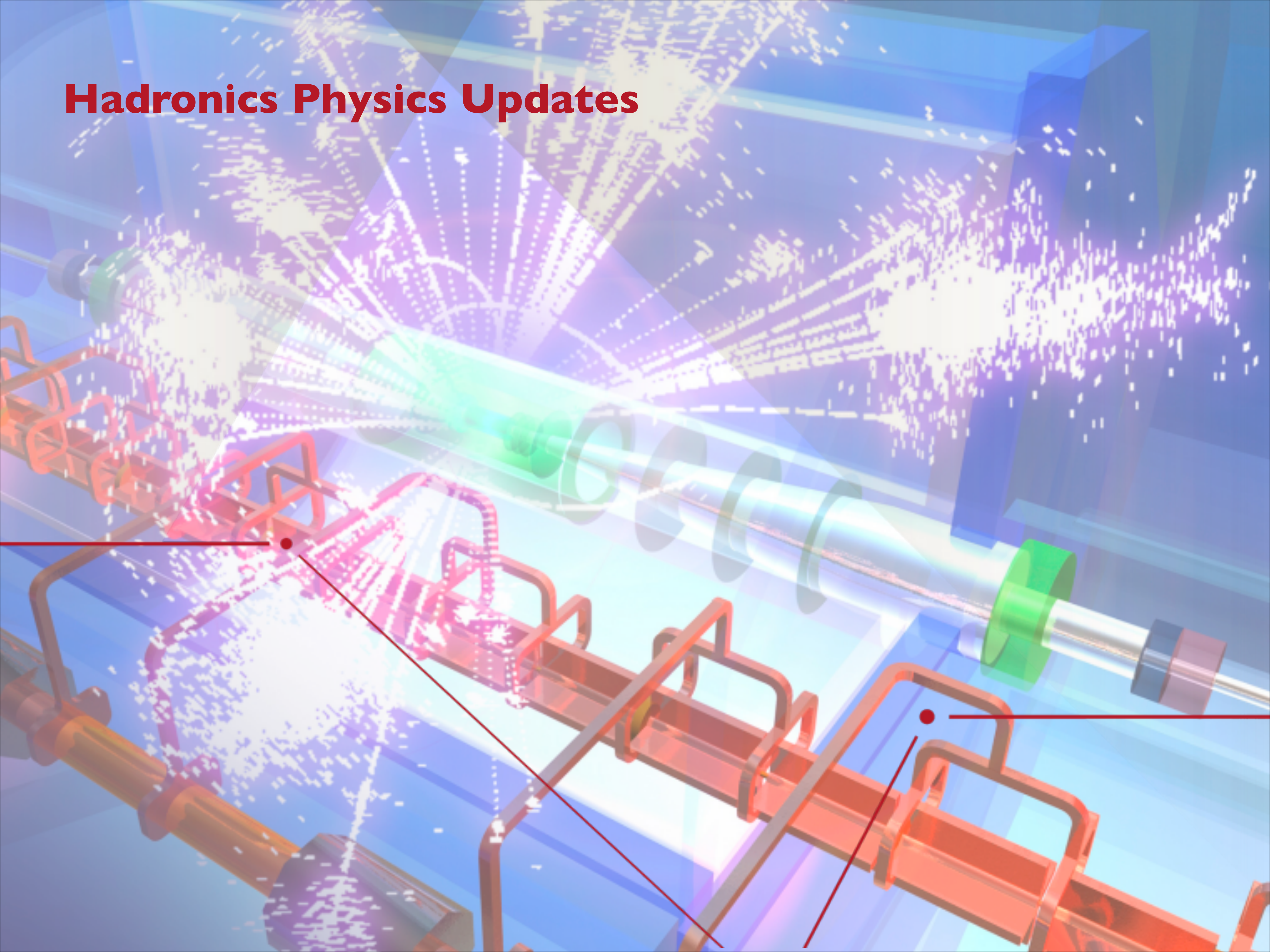
Version 10.0

Validation

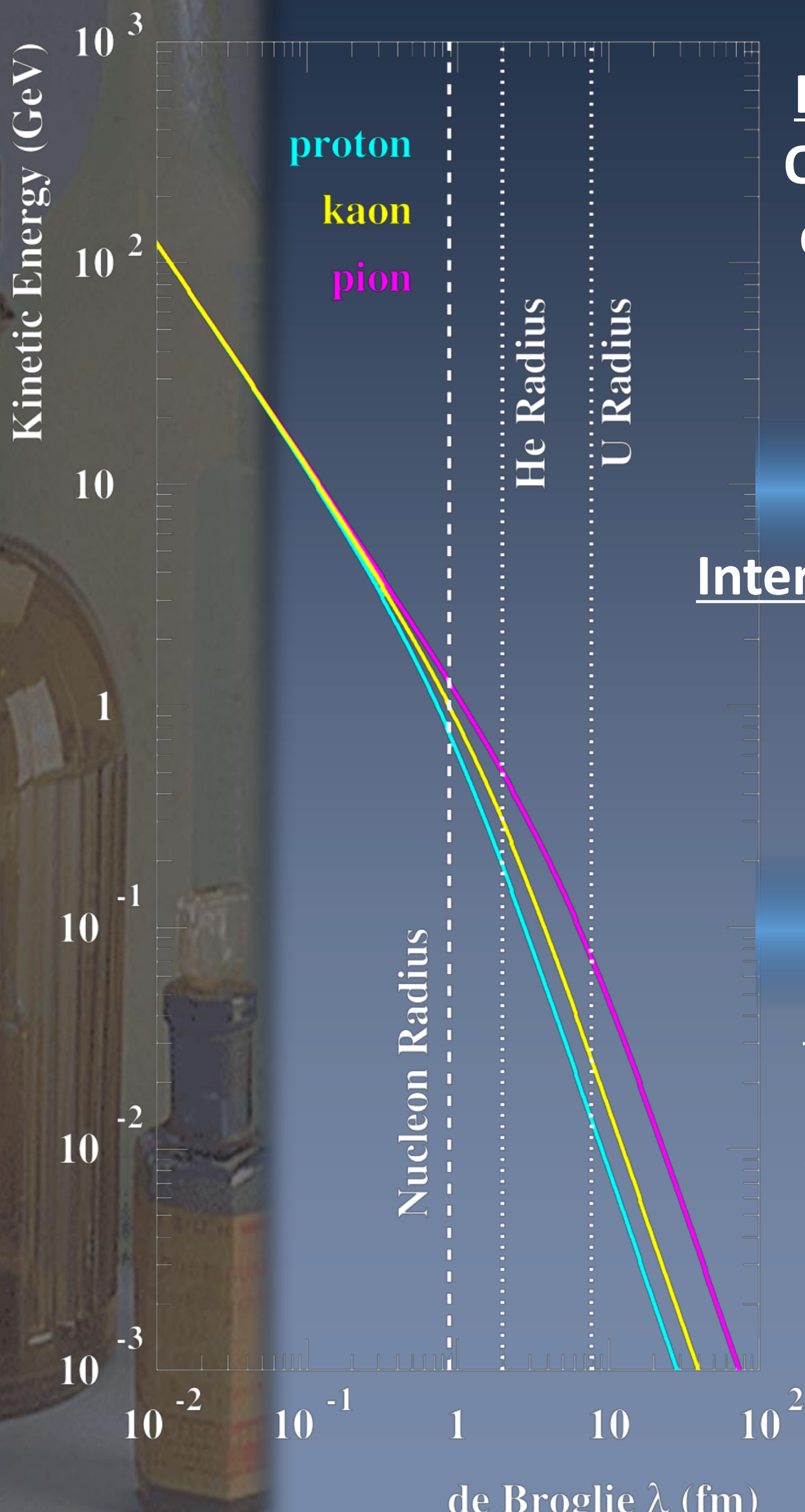


Version 10.0

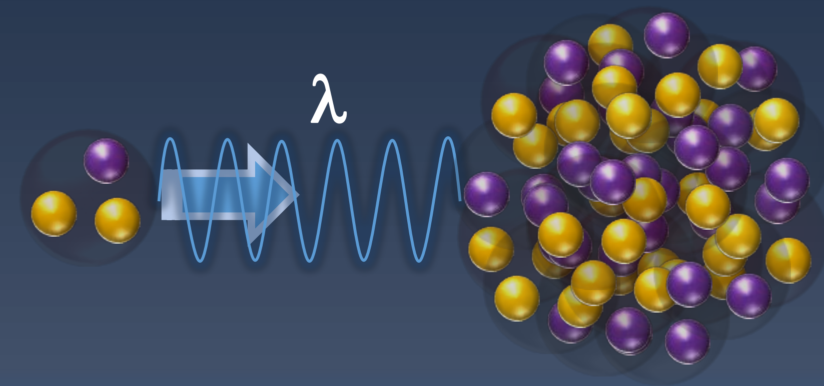
Hadronics Physics Updates



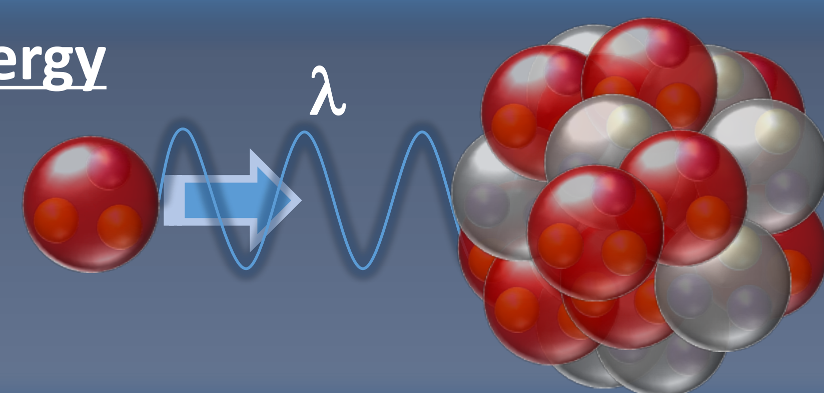
Variety of Hadronic Physics Models



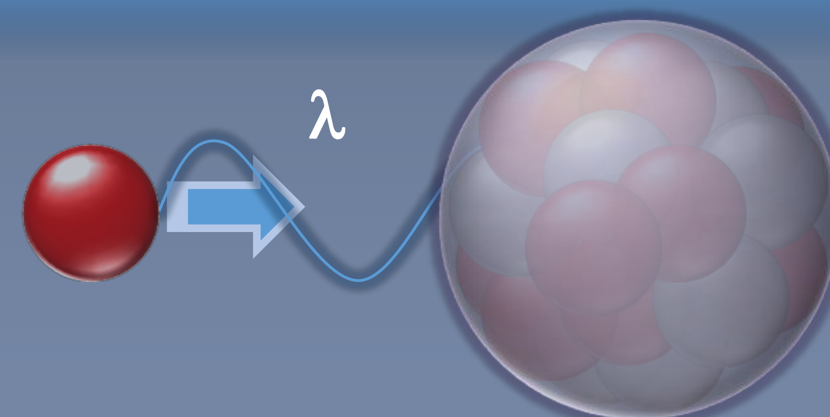
High Energy
Quark/gluon dominating behavior



Intermediate Energy
Nucleon dominating behavior



Low Energy
Nucleus dominating behavior



Main Models

String Models: Quark Gluon String, Fritiof

Intra-Nuclear Cascade Models: Binary, Bertini

Precompound

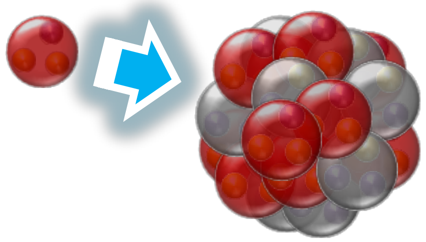
Fission / evaporation

γ evaporation

Radioactive decay

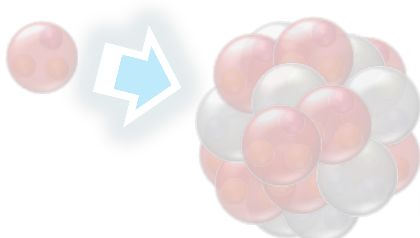
Capture at rest

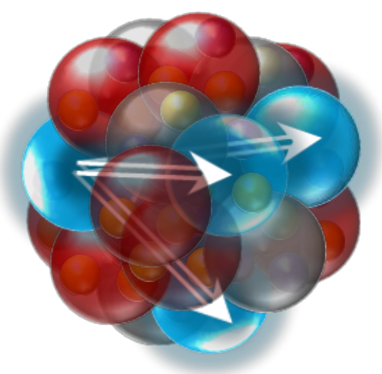
One hadronic collision = sequence of many hadronic interactions



Projectile hitting
a target nucleus

One hadronic collision = sequence of many hadronic interactions

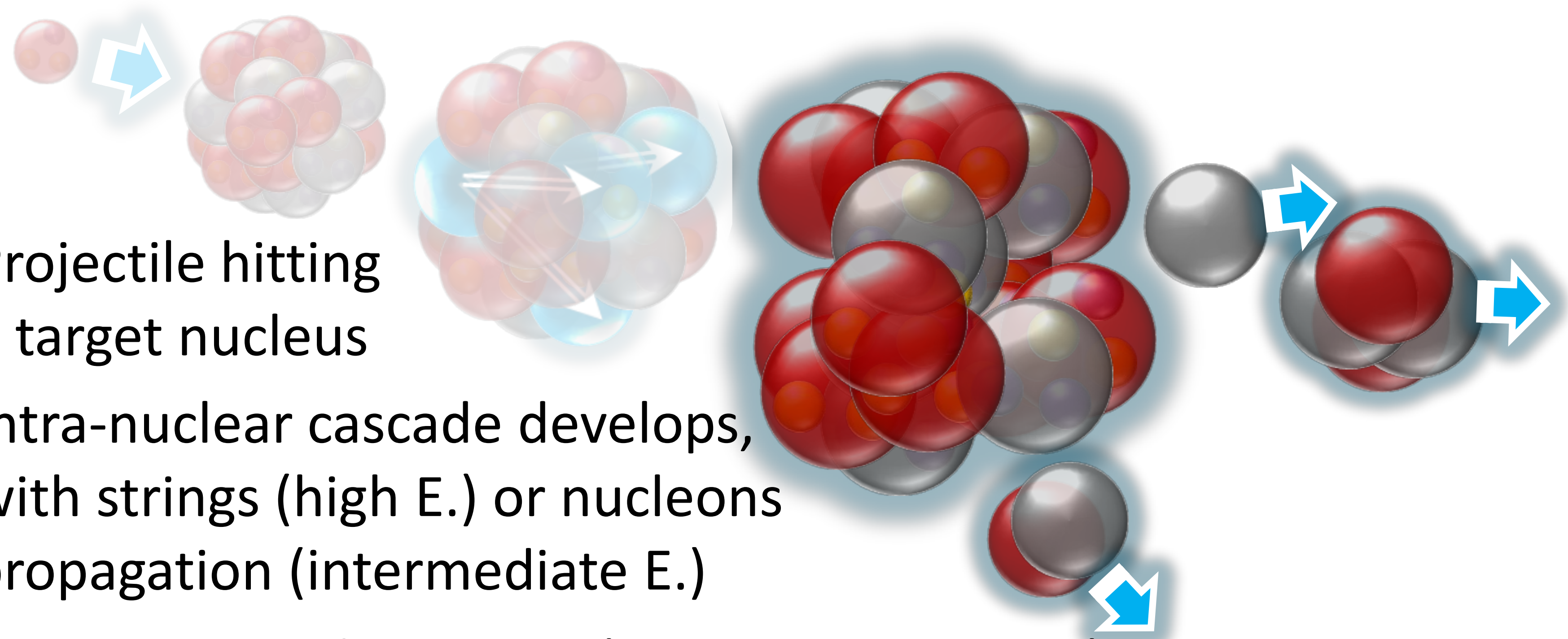




Projectile hitting a target nucleus

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

<u>One</u> hadronic collision = sequence of many hadronic interactions

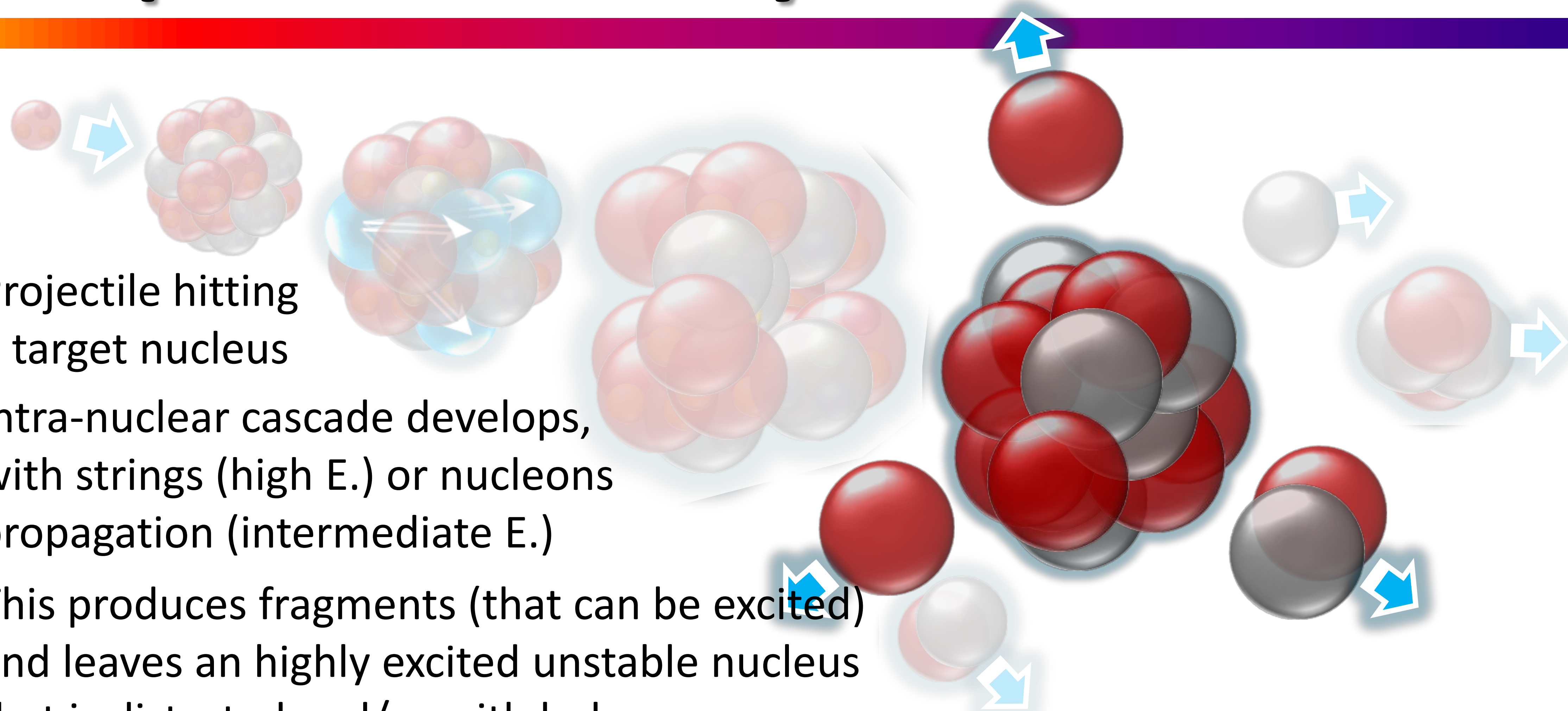


Projectile hitting a target nucleus

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

This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.

<u>One</u> hadronic collision = sequence of many hadronic interaction<u>s</u>



Projectile hitting
a target nucleus

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

This produces fragments (that can be excited)
and leaves an highly excited unstable nucleus
that is distorted and/or with holes.

Nucleus rearranges itself by evaporation* and/or fragmentation :
this leads to a still excited nucleus, but stable (metastable), and
with no memory of the collision history.

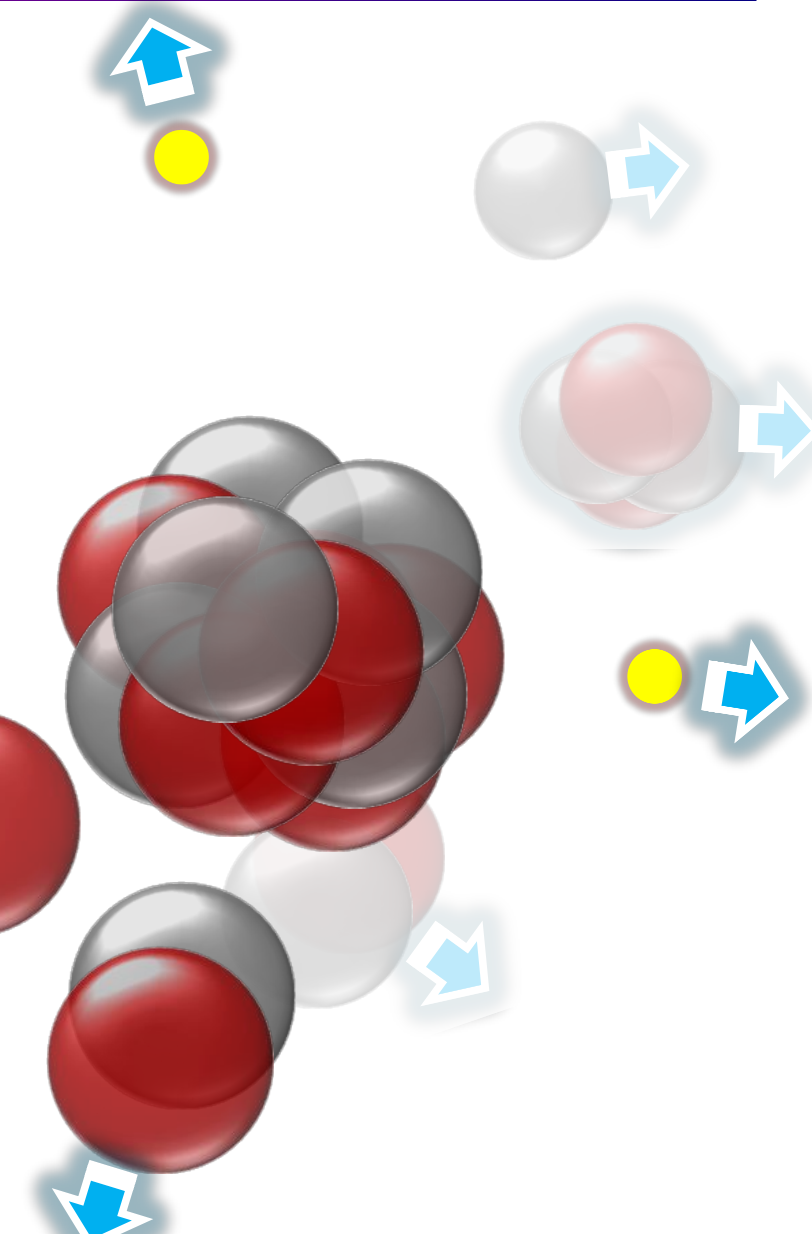
(*) **Evaporation** = de-excitation by emission of light nuclei ∈ {n, p, d, 3d, 3He, a} or photon

One hadronic collision = sequence of many hadronic interactions

Projectile hitting a target nucleus

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

This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.



Nucleus rearranges itself by evaporation* and/or fragmentation : this leads to a still excited nucleus, but stable (metastable), and with no memory of the collision history.

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

(*) **Evaporation** = de-excitation by emission of light nuclei $\in$ {n, p, d, t, 3He, α} or photon

High Energy interactions

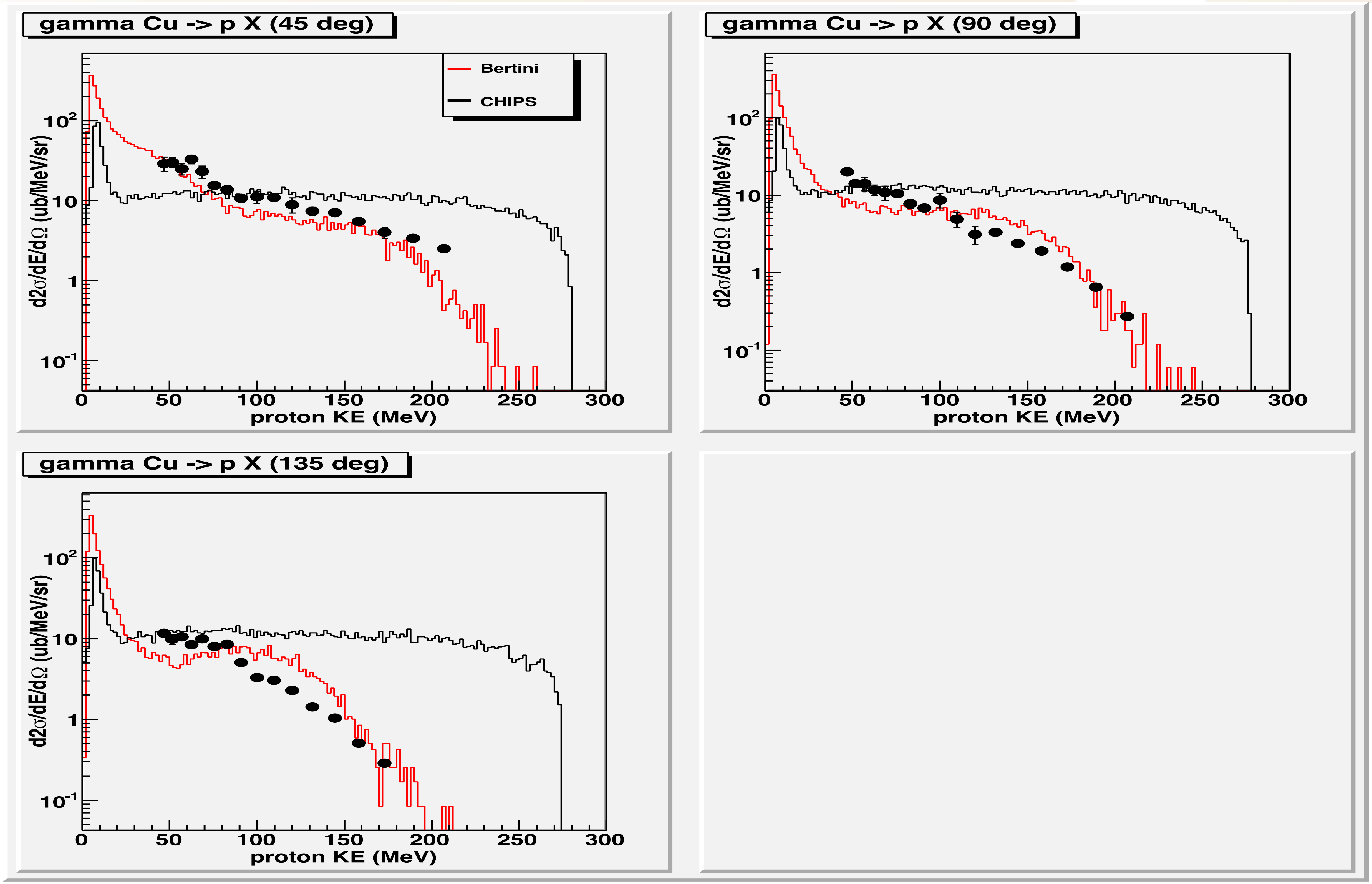
- Fritiof (FTF) high energy model
  - Recently **re-tuned** to a larger set of thin-target data
  - lower limit of applicability now 2 GeV (was 3 GeV)
  - Now handles anti-proton
  - Can now do ion-nucleus and anti-ion-nucleus reactions
  - Improvement of hadron-nucleon diffraction

- Quark-gluon string (QGS) high energy model
  - No development last few years
  - Plans this summer for:
    - Addition of Reggeon cascade (quark-level cascade which helps to broaden hadronic showers)
    - Improved diffraction
    - Expected to extend validity down to 2-3 GeV as for FTF

Intermediate Energies: Bertini cascade

- Added **detailed** two-body nucleon final state angular distributions (from SAID) to replace old Barashenkov parameterizations
  - Not much change observed in thin target validations
- Also added SAID **angular distributions of π-nucleon**
  - Not added in time for v 10, but will be available in June
  - Significantly different from old Barashenkov parameterizations
  - Expected to affect lateral shower shape
- **Electro-nuclear, muon-nuclear, gamma-nuclear models** now all based on Bertini cascade
  - General improvement over previous CHIPS-based models

γ Cu → pX (300 MeV)

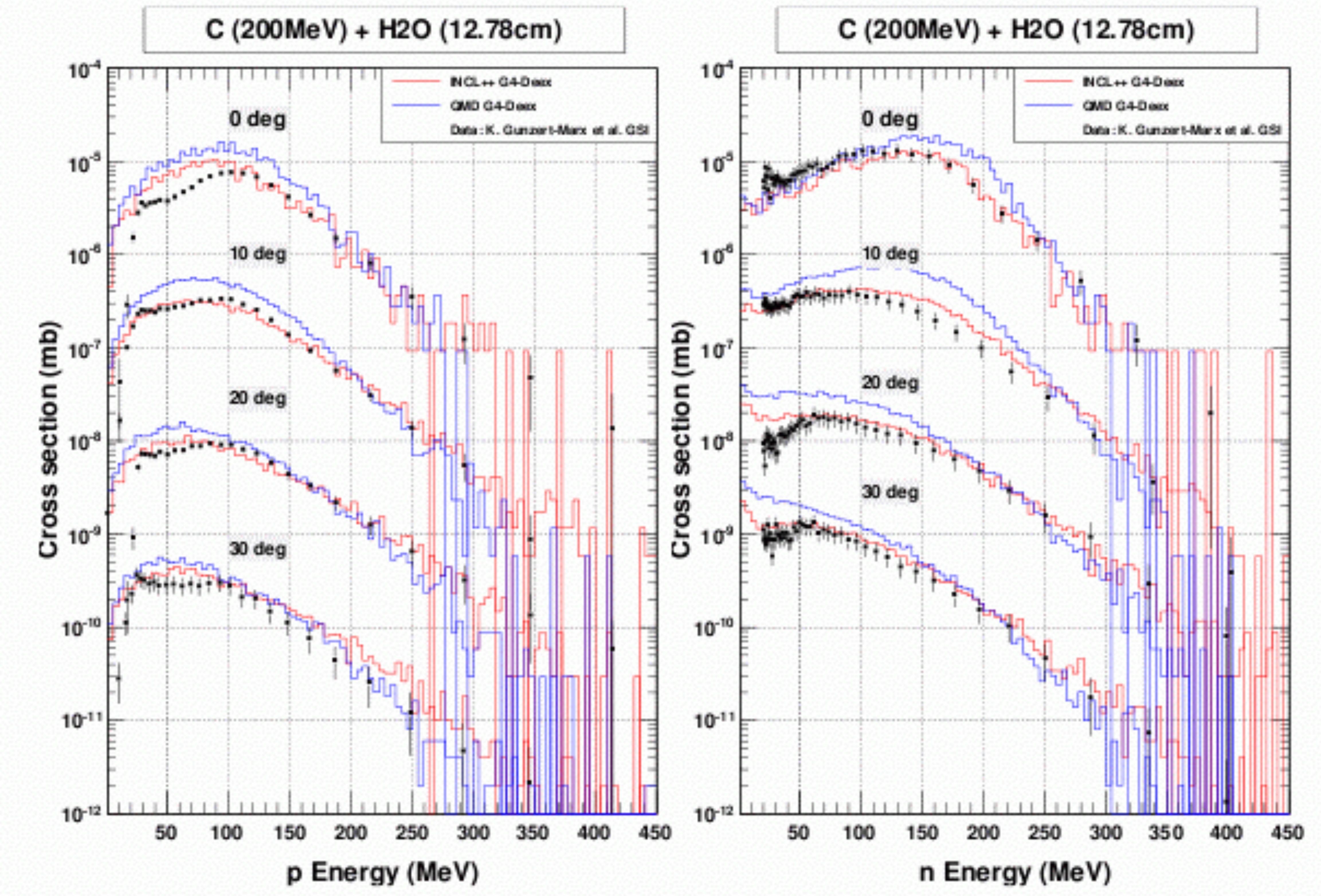


Liege Cascade (INCL++)

- Latest Geant4 version contains many improvements
  - Originally for pion- and nucleon-induced cascades between 100 MeV – 3 GeV
  - Now completely re-designed, written in C++
  - Can now do light ion projectiles (up to and including 12C)
  - Uses Geant4 de-excitation package to bring residual nucleus to ground state, improve light cluster emission

- An **alternative** to Bertini cascade, G4BinaryCascade or G4QMD
  - Especially good for spallation energies
  - Physics lists available to use this model

Ion-ion collisions with INCL++



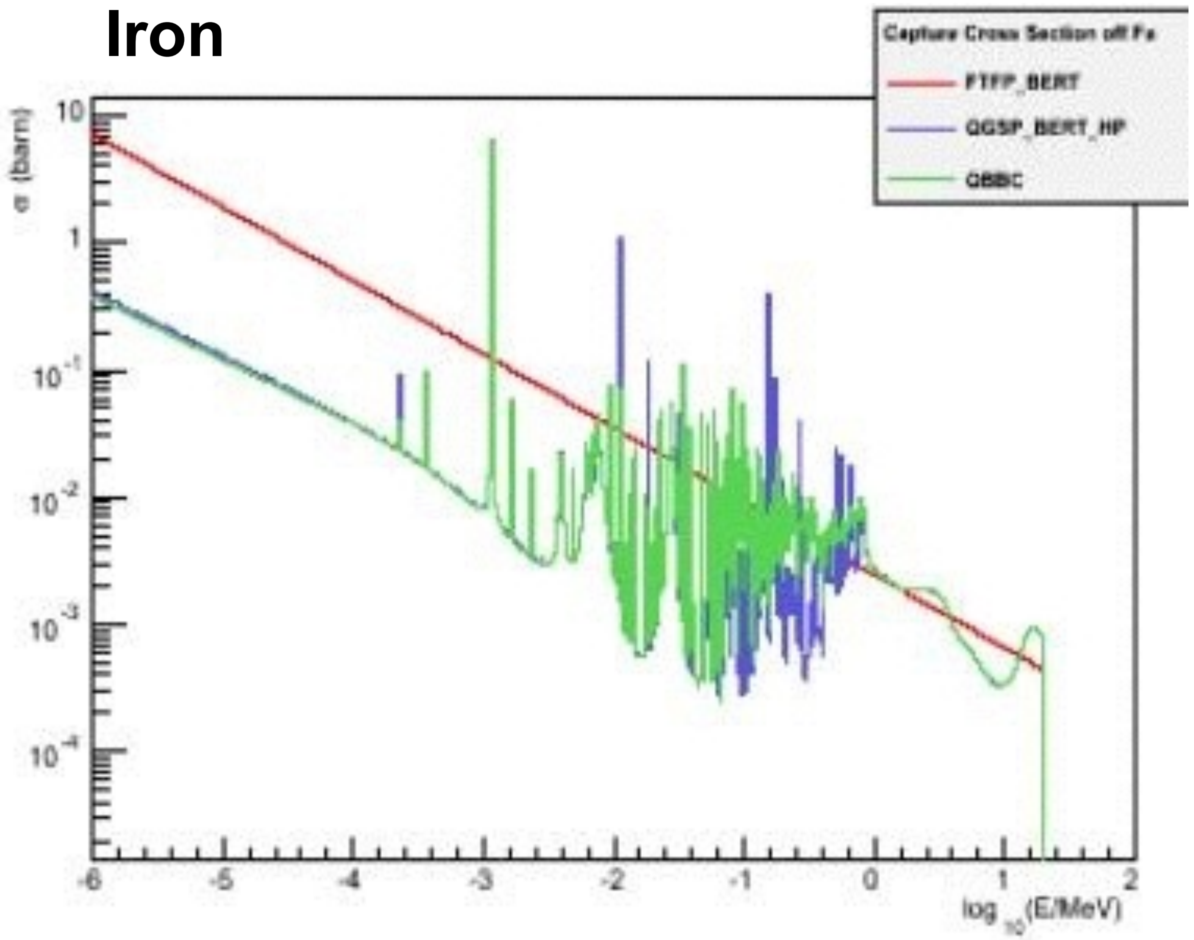
Low Energy: neutron interactions

- **New low energy neutron** cross section sets: G4NeutronInelasticXS, G4NeutronCaptureXS
  - Intended as a faster alternative to NeutronHP models
  - Data from NeutronHP cross sections (G4NDL) are simplified and smoothed over resonance region to increase speed
  - Available for all natural elements, and isotope-wise for 23 most common elements (H, Li, B, C, O, Al, … W, Pb)

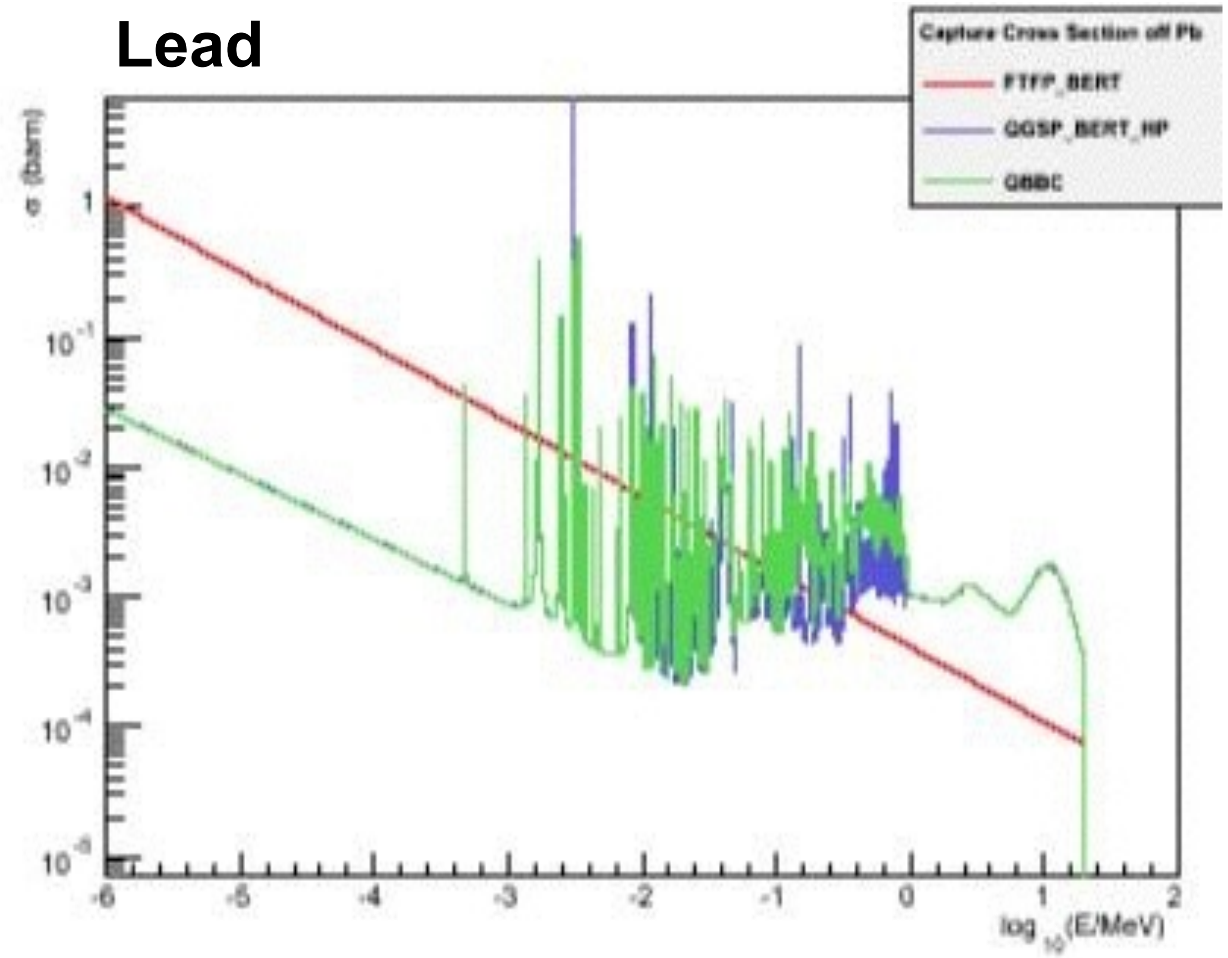
- Now included in all non-HP physics lists
  - new data set required – G4NEUTRONXSDATA

G4NeutronXS Capture Cross Section

Iron



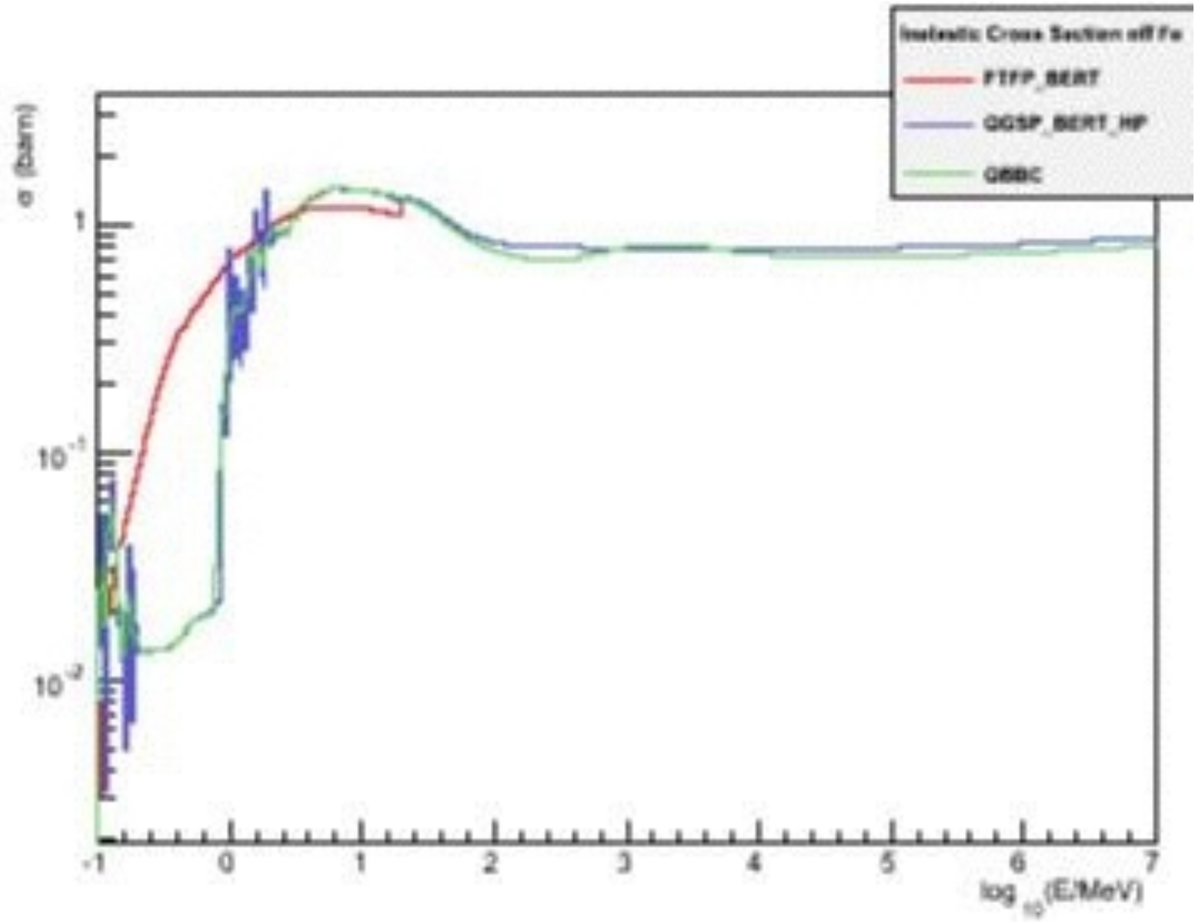
Lead



- Similar results to HP
- Without CPU penalty

G4NeutronXS Inelastic Cross Section

Iron



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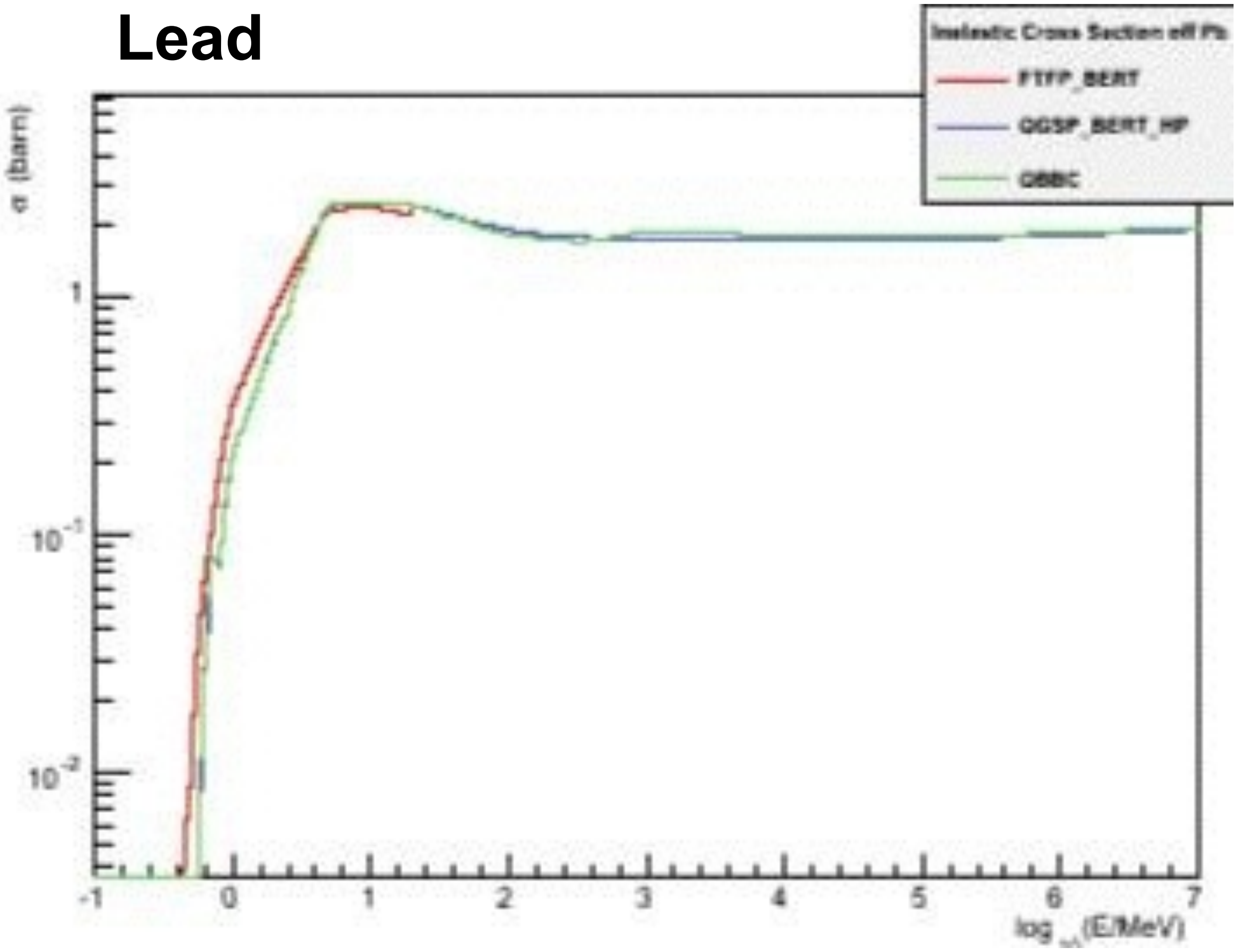
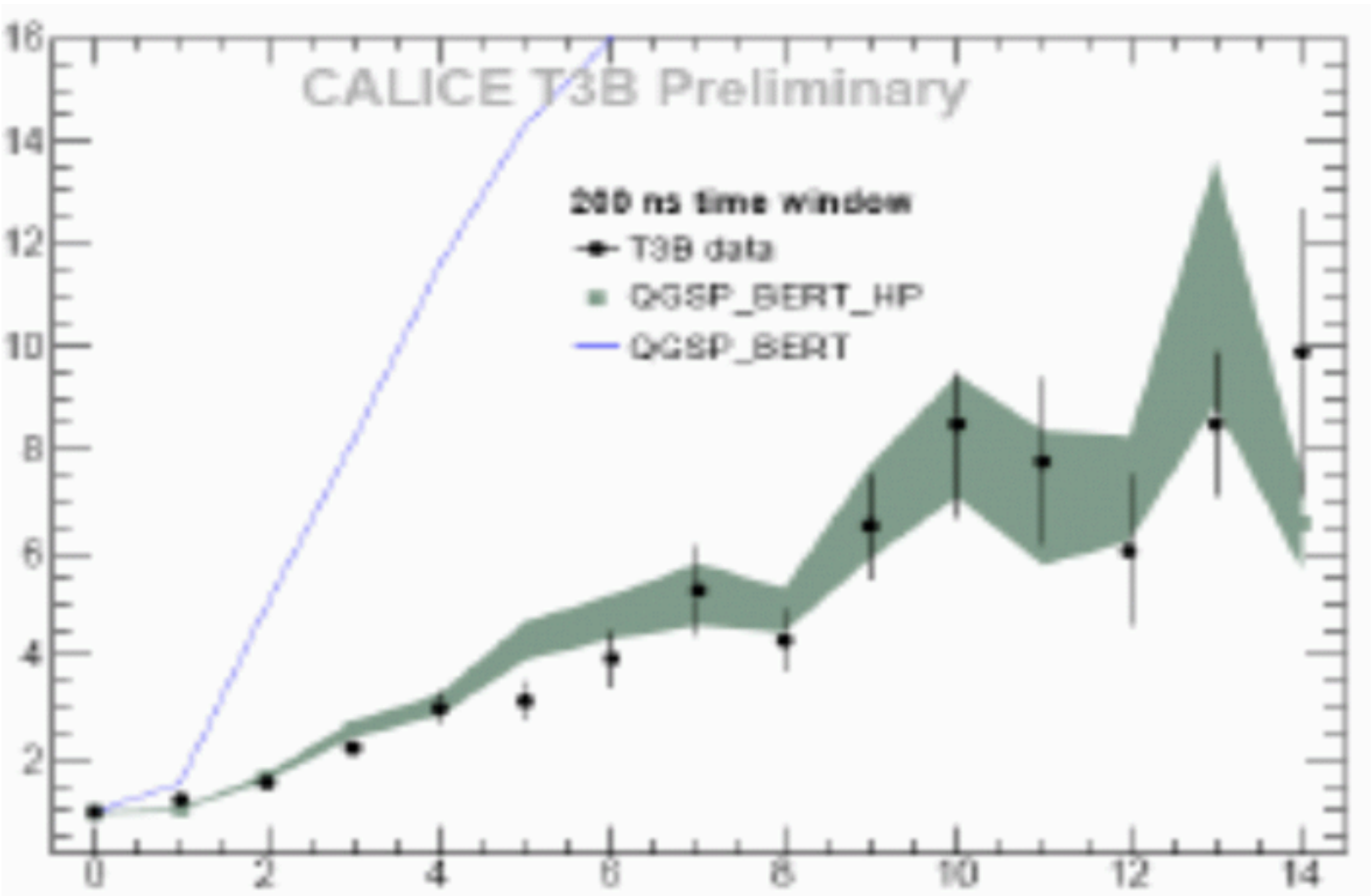


- Similar results to HP
- Without CPU penalty

Validation required

Does this change when using new Cross Section?



Technical Updates

Event Level Parallelism

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- **Version 10 supports (optional) event-level parallelism**
  - Can now take advantage of the full CPU power of your machine which likely has more than 1 core
  - You may still opt for a sequential (non-multi-threaded) build (e.g. if you rely on non thread-safe external code)

- Installation
  - No new dependencies, see the Geant4 Installation Guide accessible from the Geant4 web page (User Support -> Documentation -> Installation Guide)
  - Turn on MT via cmake switch
  - See also latest developments and performance at http://twiki.cern.ch/twiki/bin/view/Geant4/MultiThreadingTaskForce

CPU / Memory performances

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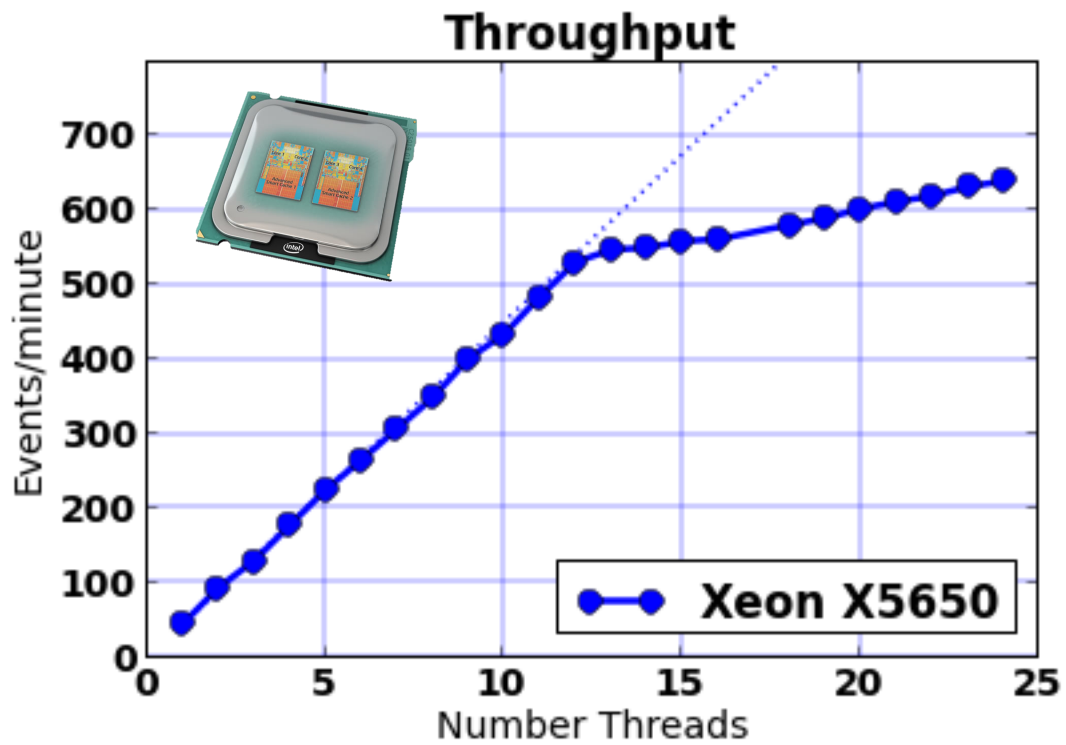
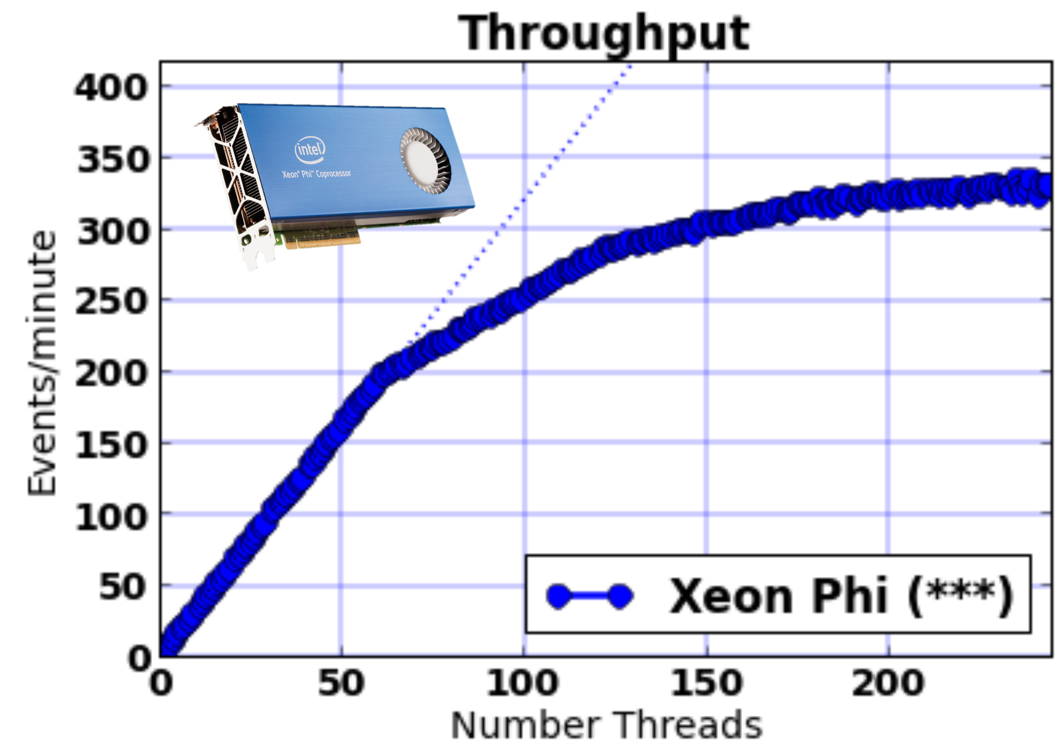
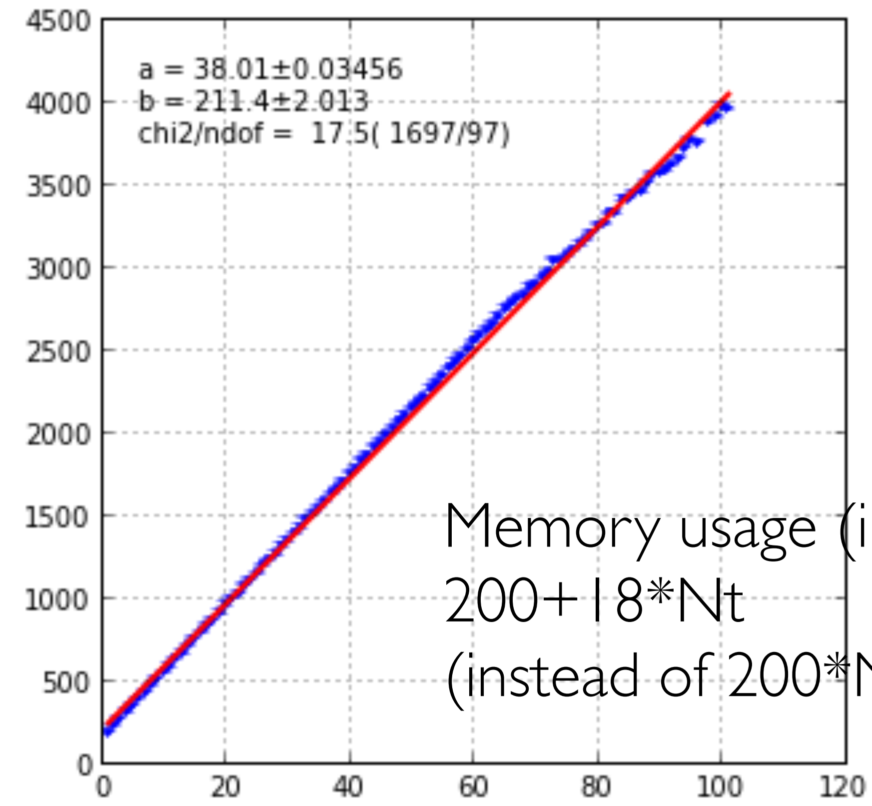


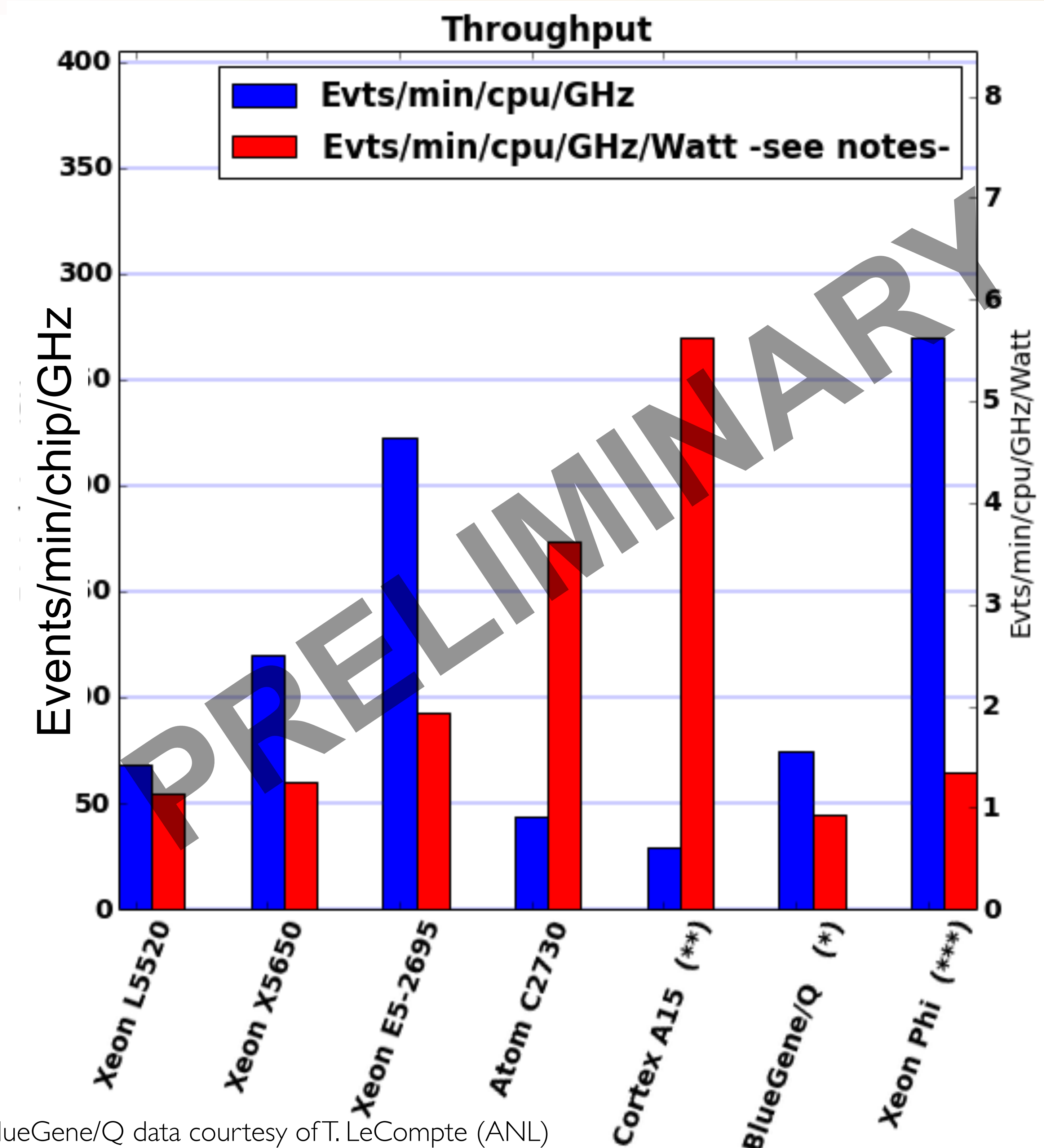




Memory usage (in MB)
200+18*Nt
(instead of 200*Np)

Obtained with "CMS-style" geometry

Different Architectures



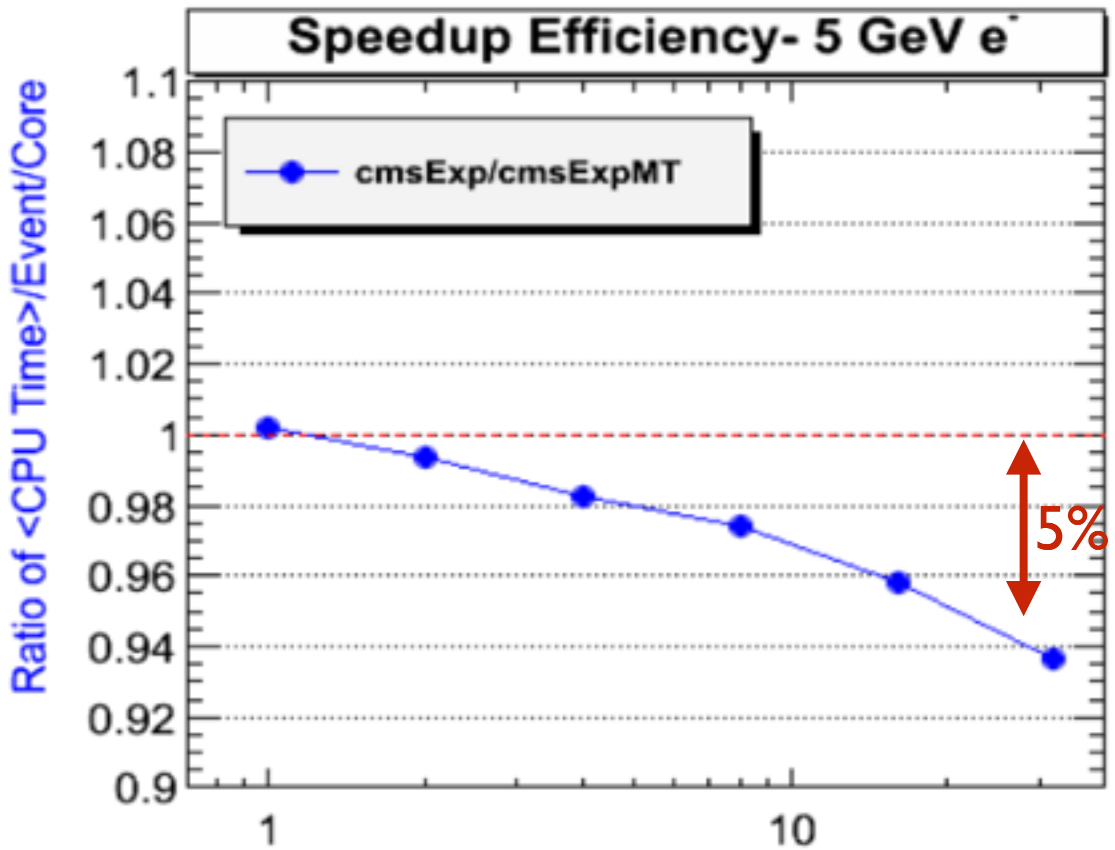
Geant4 has been run with success on a variety of hardware architectures:

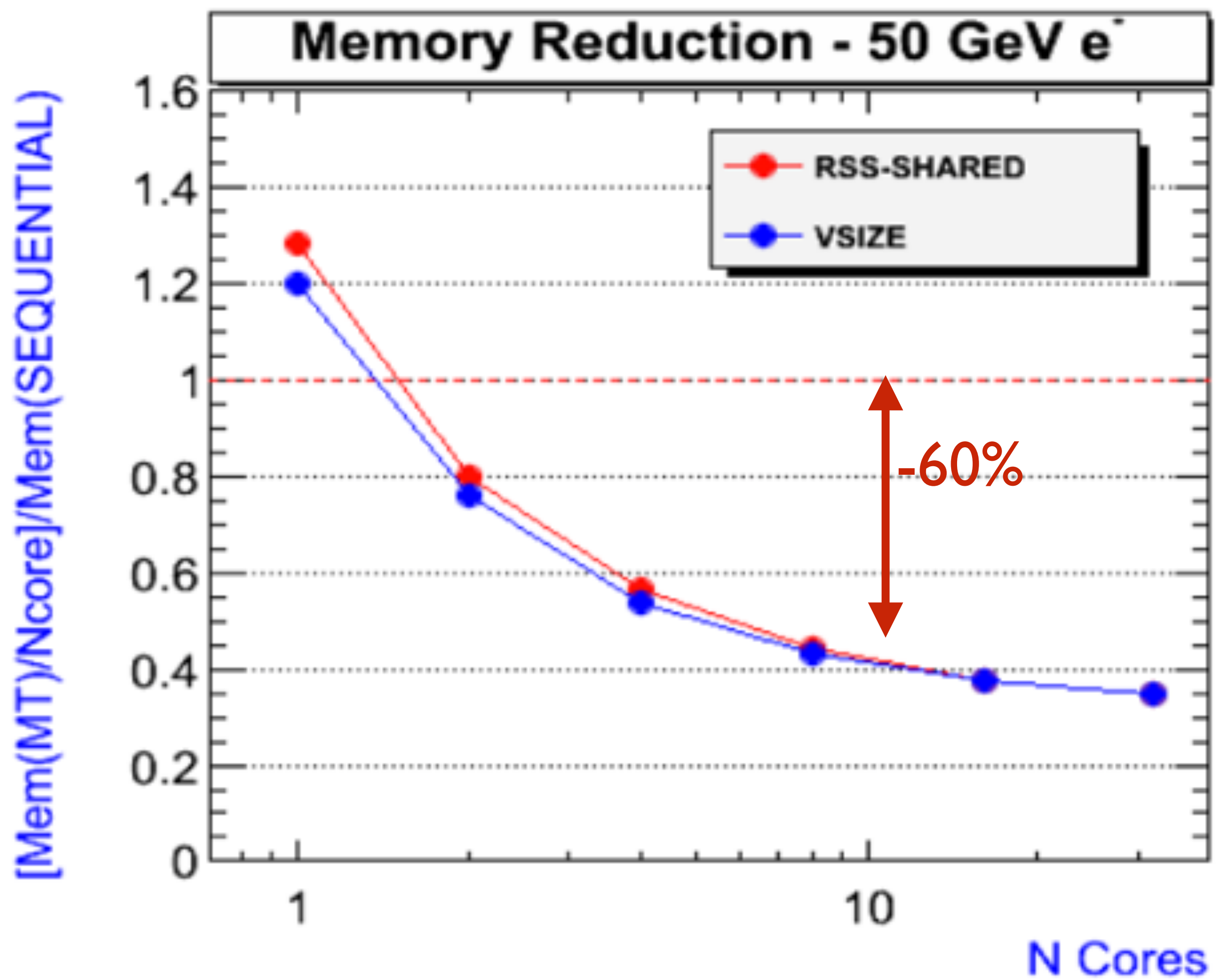
- Intel / AMD
- MIC
- PowerPC (BG/Q)
- ARM / Intel Atom

BlueGene/Q data courtesy of T. LeCompte (ANL)
ARM tests in collaboration with P.Elmer (Princeton;CMS)
Hardware courtesy of OpenLab (CERN)

Obtained with "CMS-style" geometry

Comparison with Sequential



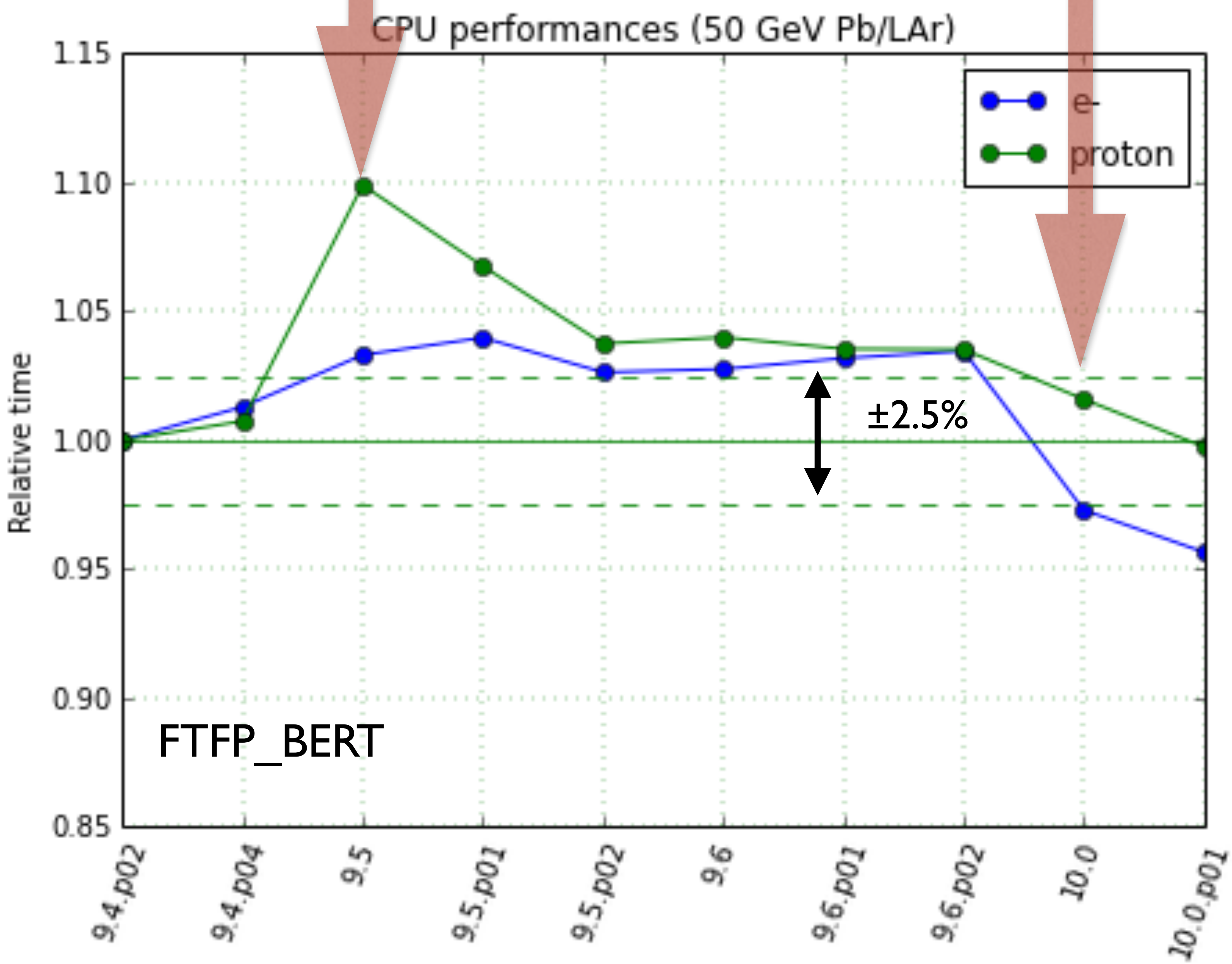


Obtained with "CMS-style" geometry

Absolute throughput (sequential)

Heavy developments: FTF becomes competitive with QGS

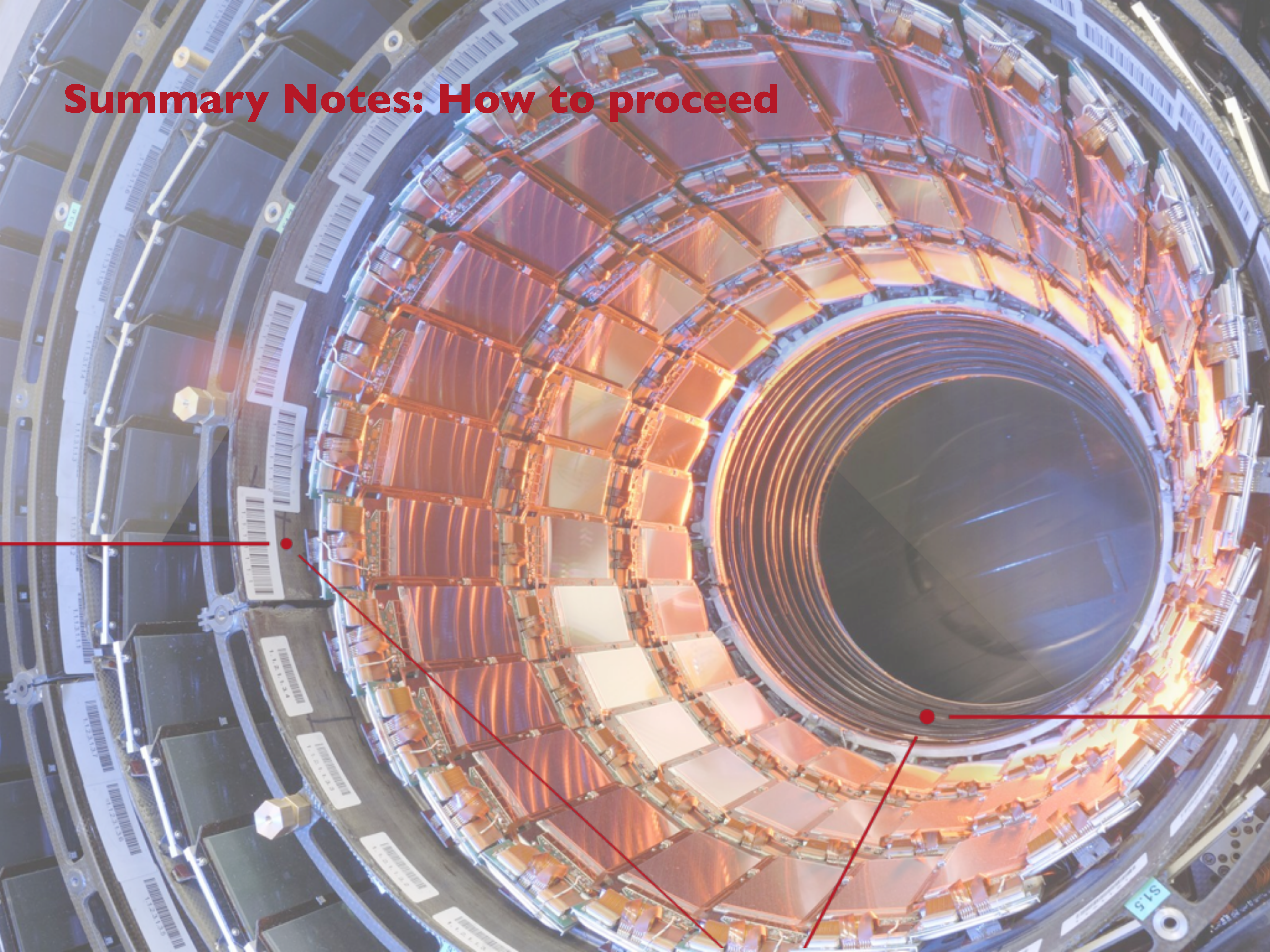
Fast Log/Pow mathematics



Improvements for MT also bring benefits to sequential

We have substantially improved physics (extended HAD theory driven processes, more precise EM tables, new processes) and at the same time improved CPU performances.
We believe there are more opportunities for optimizations in our code and we are actively working on them

Summary Notes: How to proceed



Some requests

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- Very good experience with LHC experiments during the *pre-beam era*
  - LHC experiments providing fast feedback to G4 developers
  - **Running development versions of G4 on test-beam simulation**
- Official "LCG Physics Validation Project" at CERN
- Could it be possible to have something like this?
  - With which time scale? 2/y?
- **We have a "simplified calorimeter" application that mimics a simple setup (using published data)**
  - We want to use this to simulate CALICE test-beam but…
  - … manpower
  - … not accurate enough for "full-scale" validation, CALICE is more precise than LHC. Still need fast feedback from you
- Some CALICE peculiarities: shower shape, W-based calorimeters
  - These cannot be studied anywhere else

Conclusions

Summary

- **Improvements of Hadronics Physics in all sectors**, driven by new developments and new tunings
  - New FTF tuning, improved BERT internals, new n-Capture model
  - Removal of old models (poor physics or technical performances, not possible to maintain)
- **Further "fine" tuning of EM physics models**
  - Mainly related to MultipleScattering: more and more stable, only one option is now default for HEP
  - Only HEP-specific developments discussed here
- Major development: **event-level parallelism** via multi-threading
- Even if physics is more precise, we managed to make G4 faster
  - Focus on software quality is becoming more and more important

LPCC Workshop Conclusions (still preliminary!)

SLAC

A. Ribon's preliminary summary

Status of G4 EM physics

- Geant4 electromagnetic physics looks in "*pleine forme*"
  - As an healthy 20-year old guy is expected to be!
- Of course, the LHC data we got up to know is only the tip of the iceberg, so we have to be prepared for much tougher validation tests in coming years!
- We are continuing with our "normal" development work:
  - Reviewing and consolidating the EM processes
  - Extending the set of validation tests
  - Using regularly these tests, and striving to improve the agreement between simulation and data
- Important progress in recent years has been made on bremsstrahlung, gamma conversion, and multiple scattering
  - Feedback from the experiments has been essential
  - Monitor sensitive observables: Z->ee line-shape, shower shape

12

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LPCC Workshop Conclusions (still preliminary!)

SLAC

A. Ribon's preliminary summary

Status of G4 hadronic physics

- General satisfaction has been expressed in this Workshop
- Of course, this is not because discrepancies are absent, but because of following two, independent reasons
  - In collider-data, it is difficult to distinguish between Geant4 aspects, event-generator effects, and experiment-specific issues (materials, digitization, pile-up)
  - For cleaner test-beam data, excellent agreement is not expected given the well-known complexity of hadronic physics!
- Since the last workshop, we have improved
  - Fritiof (FTF)
  - Bertini-like (BERT) model
  - Inelastic cross sections
  - Low-energy neutron treatment, in particular capture

The main effects on hadronic showers has been on lateral shower shapes

24

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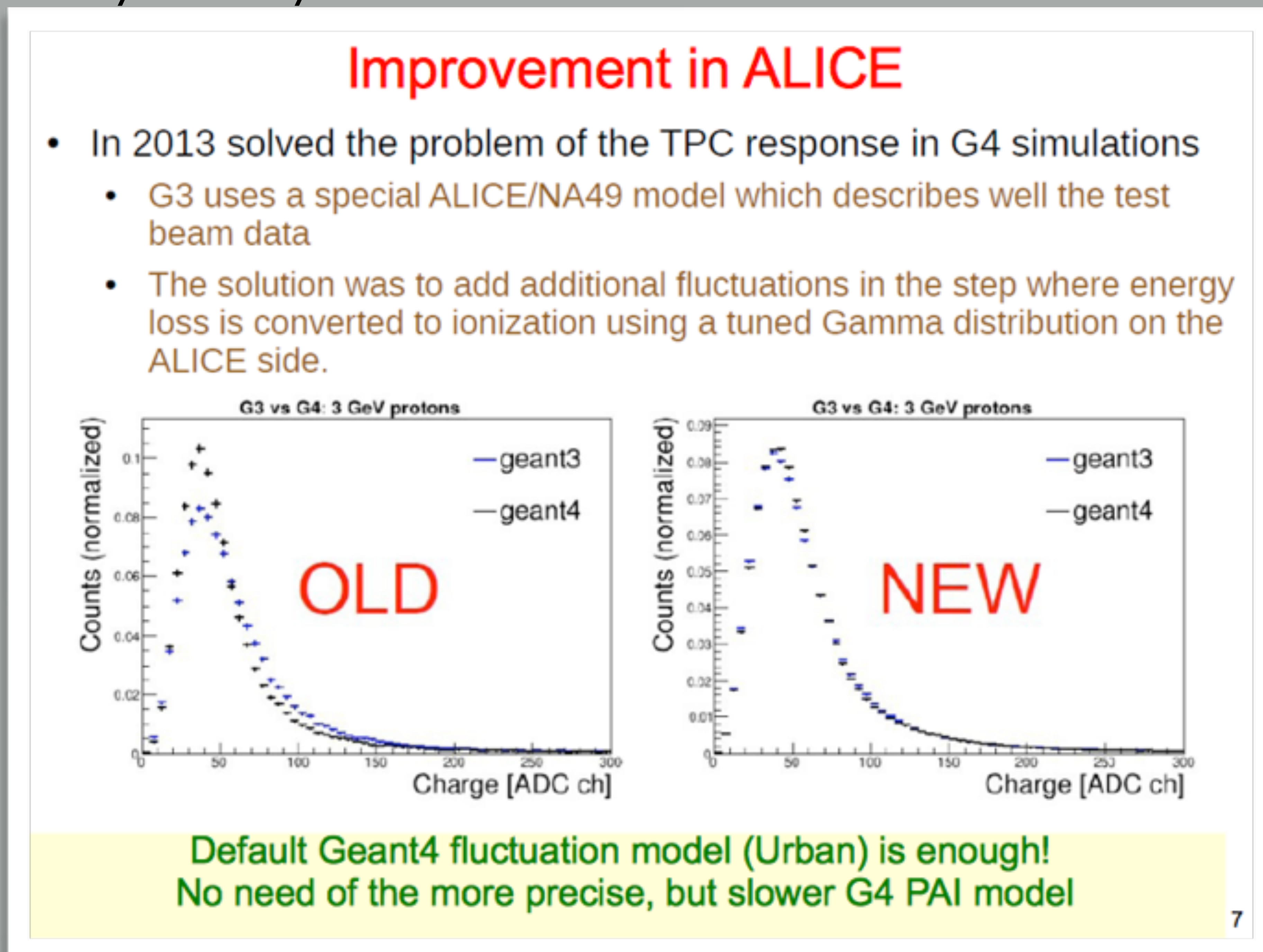
Backup

More Slides from LPCC workshop

A. Ribon's preliminary summary



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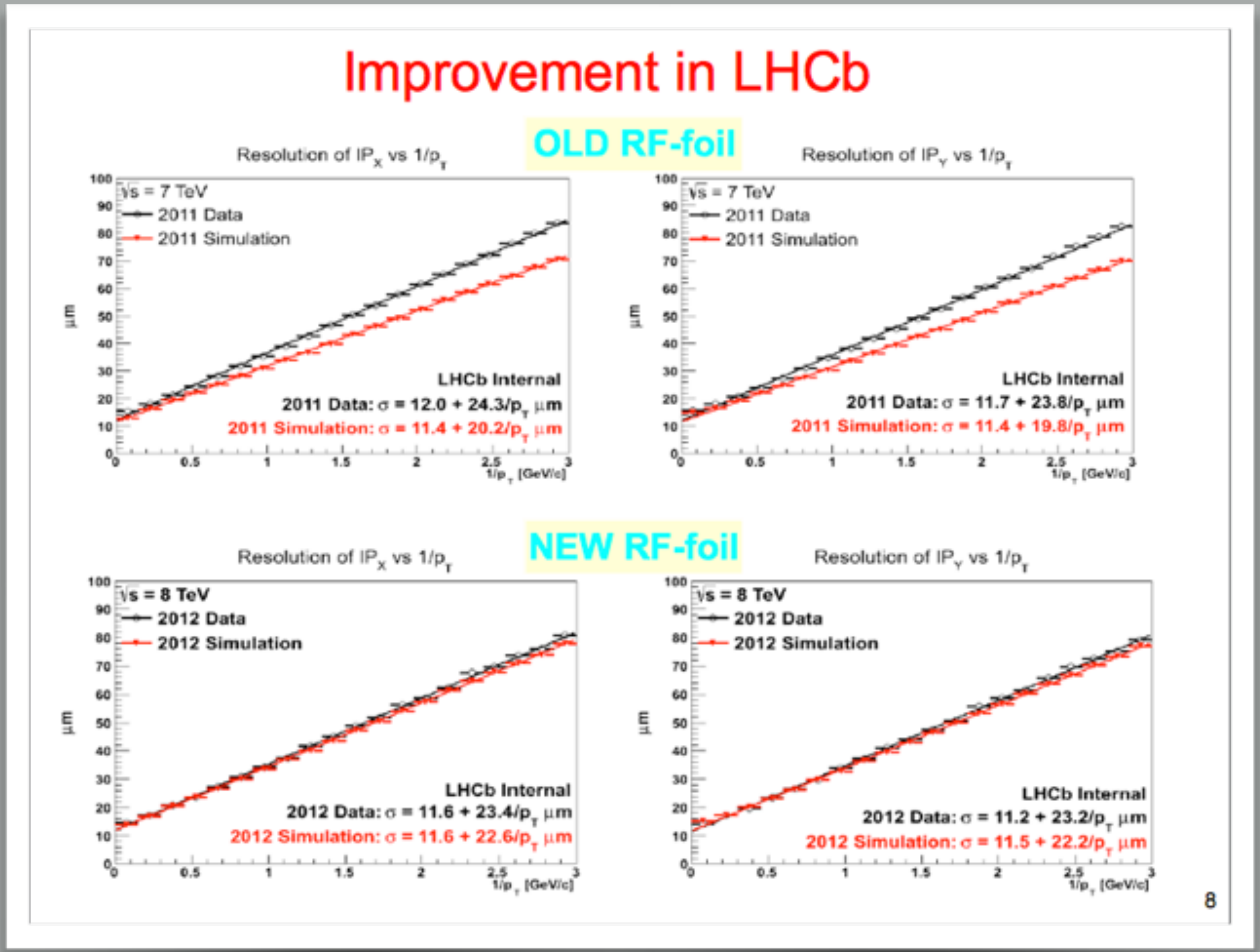

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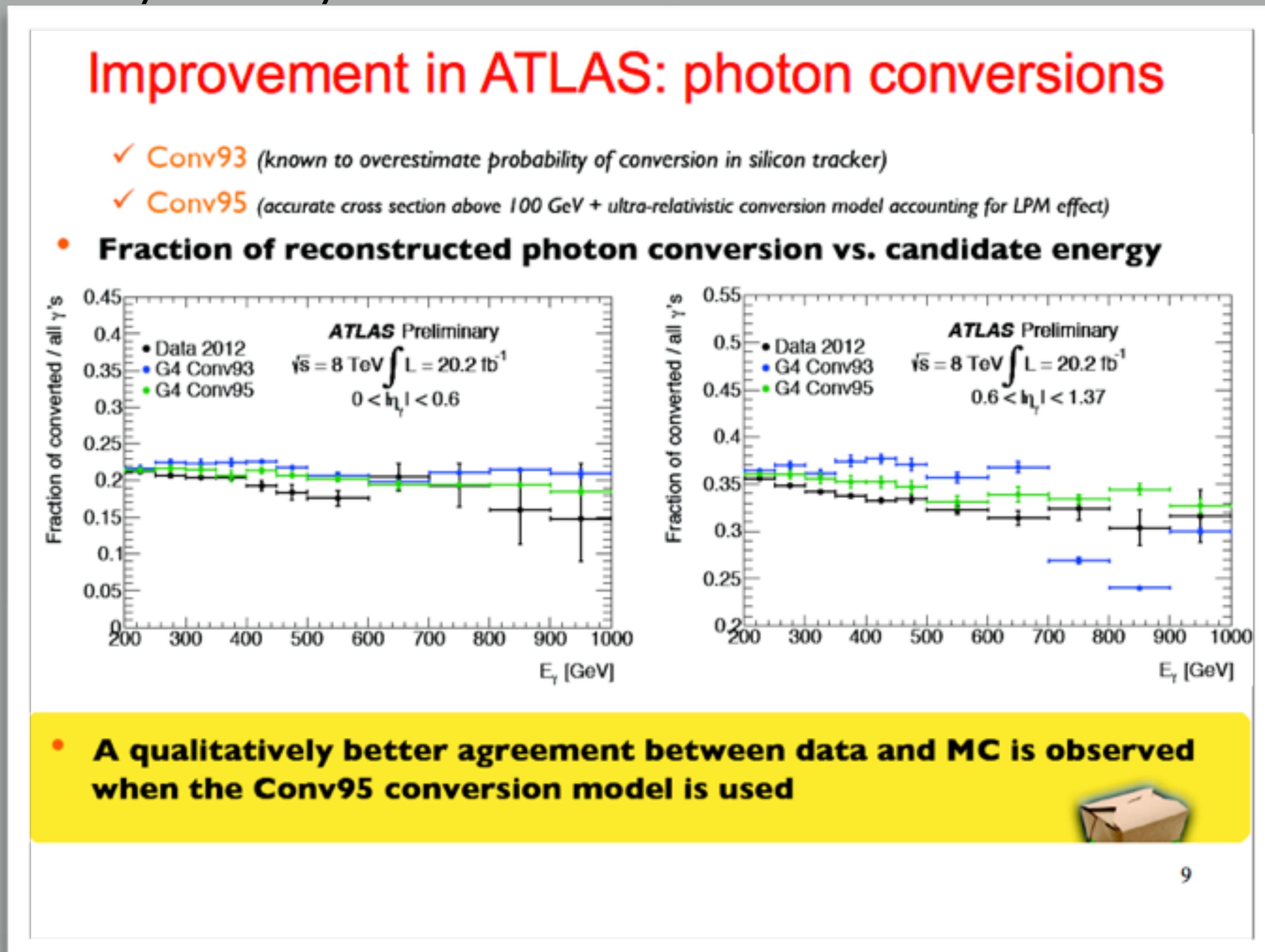

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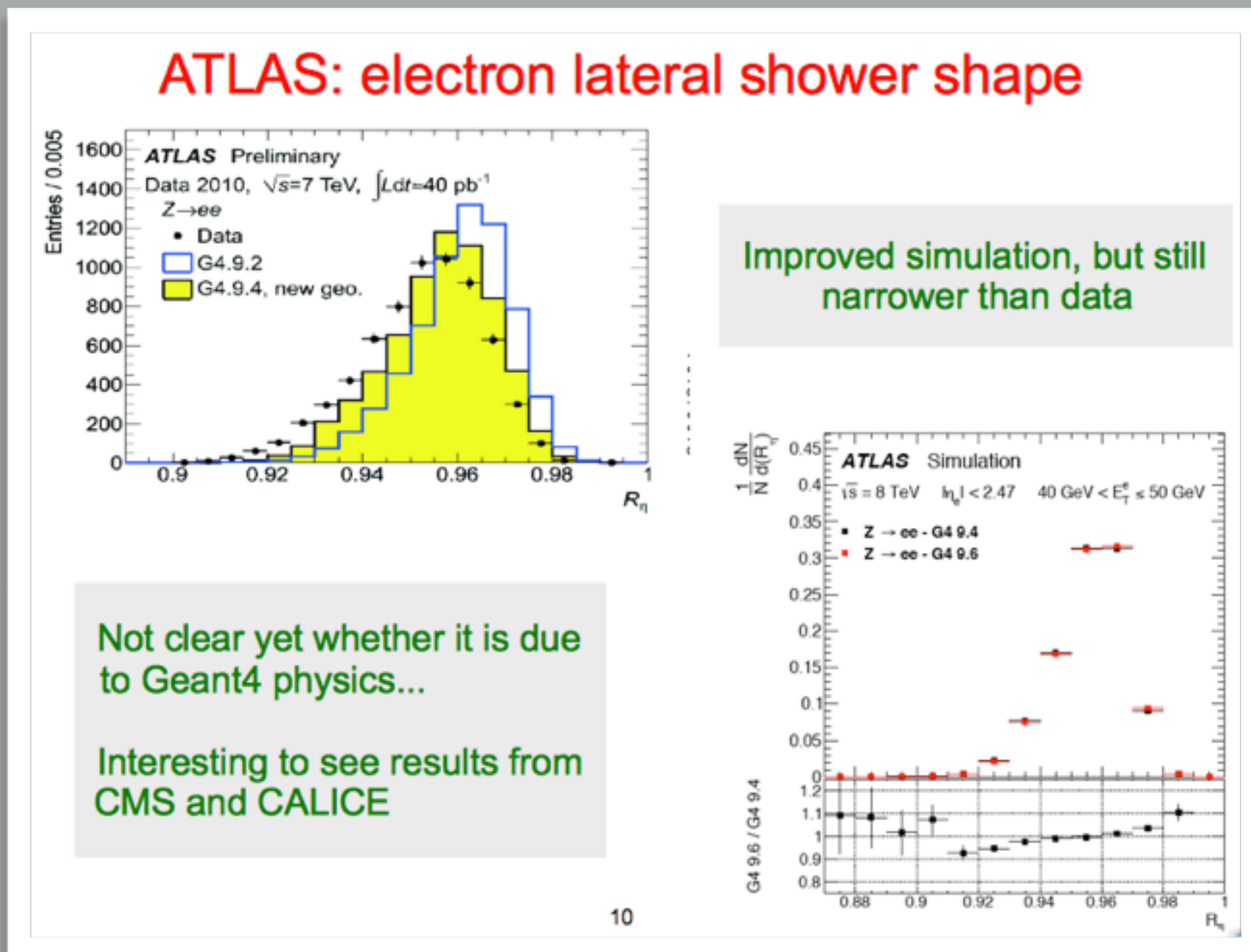

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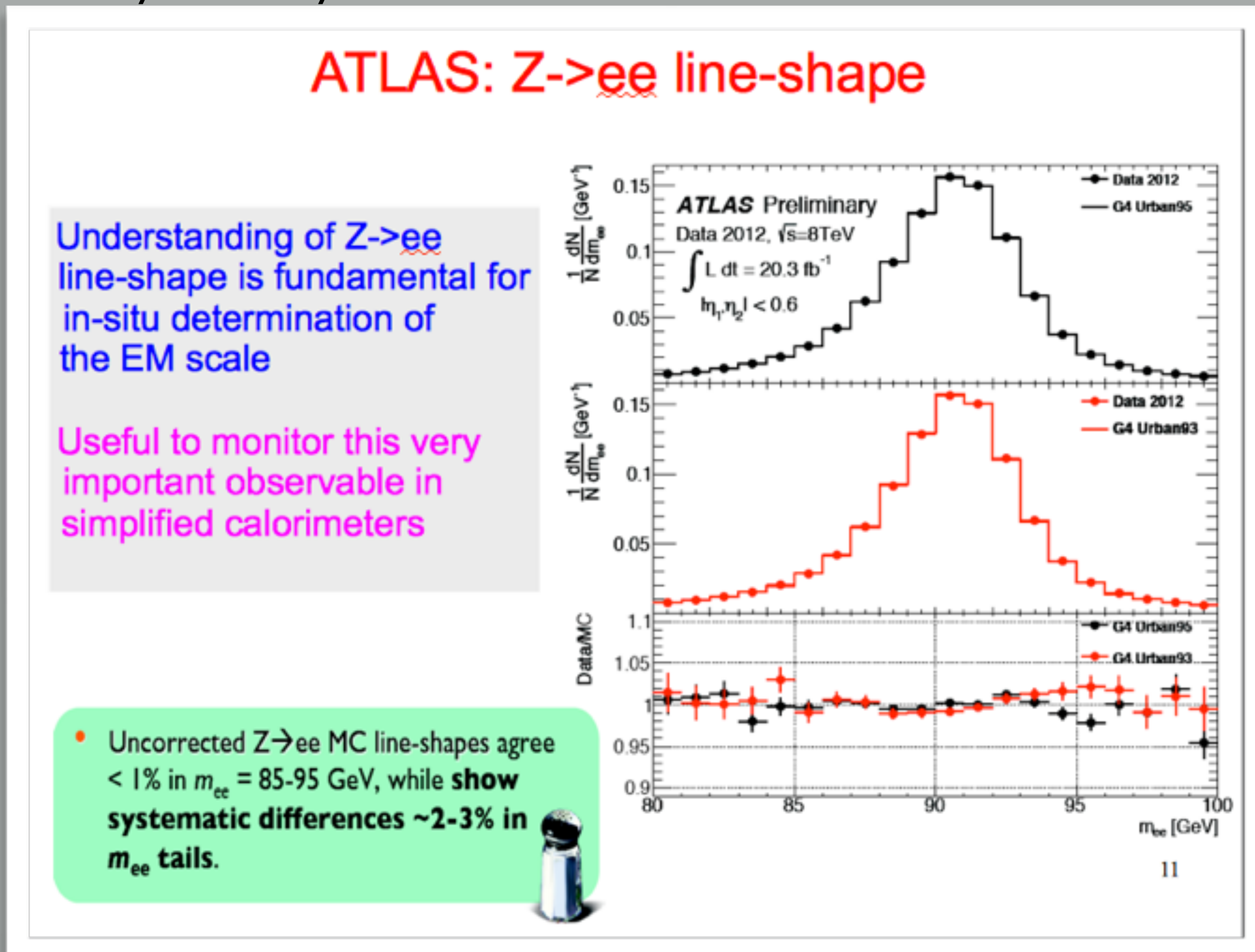

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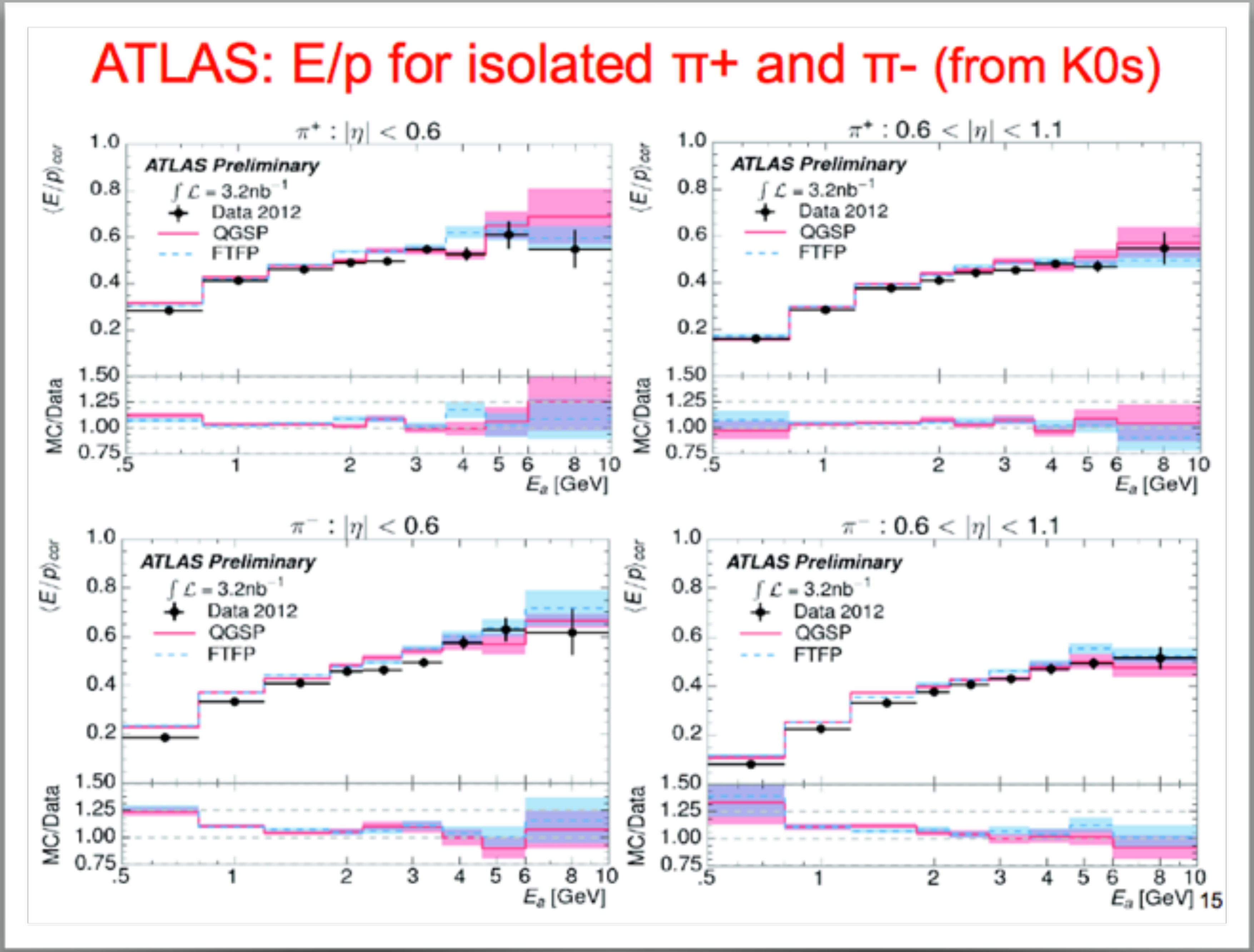

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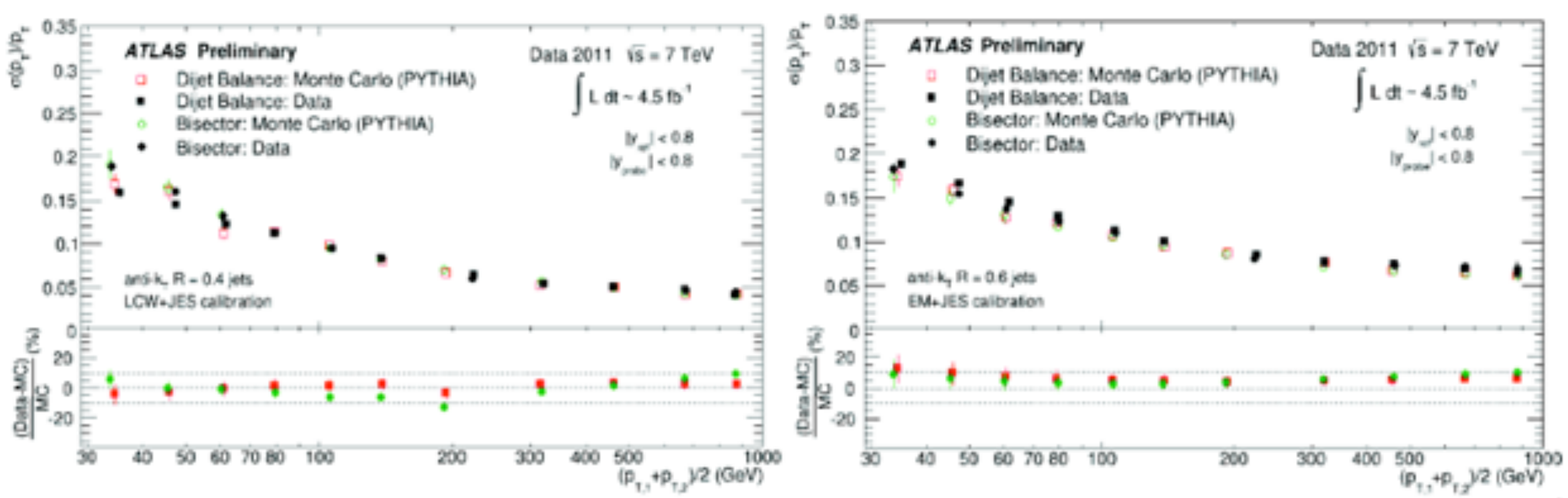
A. Ribon's preliminary summary

ATLAS: jet energy resolution

- Jet resolution looks much better in the full 2011 dataset (bottom) than we had feared at the last workshop
  - This is G4 9.4 with QGSP_BERT; picture might change with 9.6 / FTFP
- This doesn't mean that single particle resolution is a solved problem, of course, but it is not something we'll be able to get at from here
- Will revisit this issue with the full 2012 dataset soon, when we'll have more data to cover an even wider range of momenta



16

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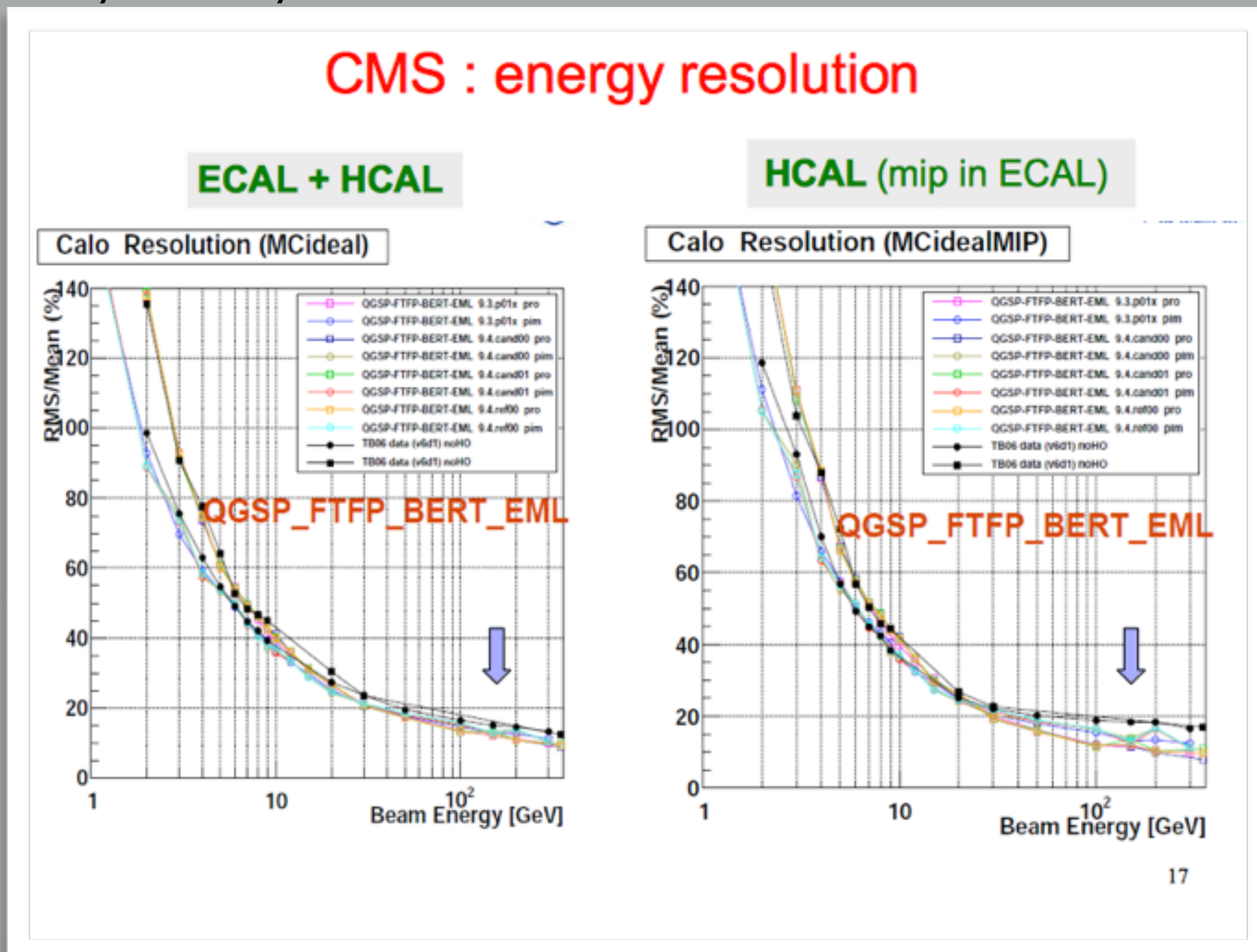

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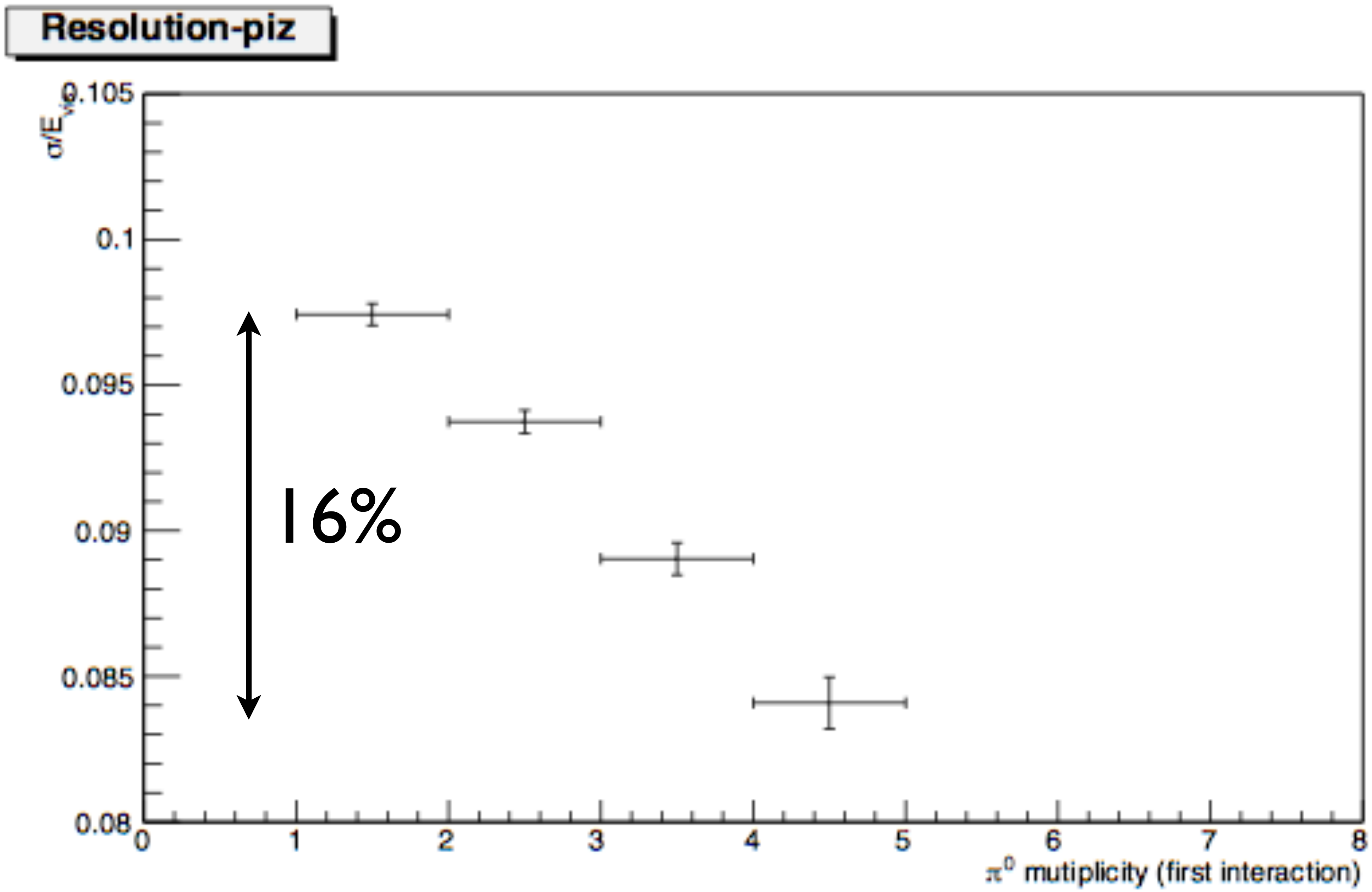
π0 Multiplicity



Low multiplicity:FTF

"Gradient" (resolution improvement per π0): -4%

Hadronic Physics improvements

- Meta-stable isotopes now produced in hadronic interactions
  - Default minimum lifetime is 1 μs
  - User my set smaller value by setting G4ENSDFSTATDATA to point to new (optional) data set
  - Uses new G4ENSDFSTAT-1.0 database (download-able)

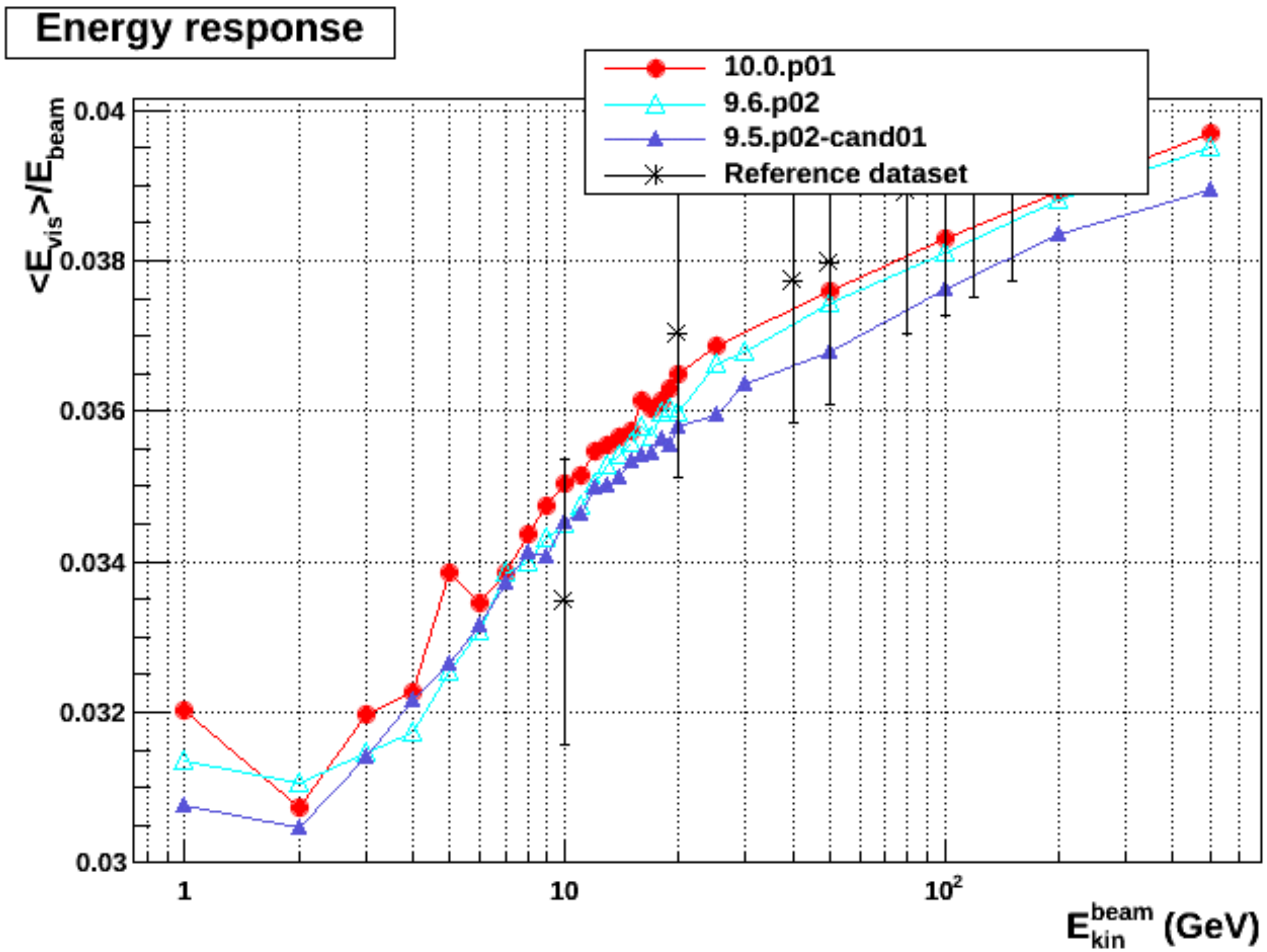
Radioactive Decay

- Process to simulate radioactive decay of nuclei
  - α, β+, β−, γ decay, electron capture (EC), internal conversion (IC), Auger and fluorescence processes implemented
- Many improvements for version 10.0:
  - Now 2792 data files taken from Evaluated Nuclear Structure Data Files (ENSDF)
    - Download-able as RadioactiveDecay4.0
    - Includes all meta-stable states with lifetimes longer than 1 ns
  - All known gamma transitions (regardless of lifetime) for 2071 nuclides
    - Download-able as PhotonEvaporation3.0
  - More consistent treatment of decay chains

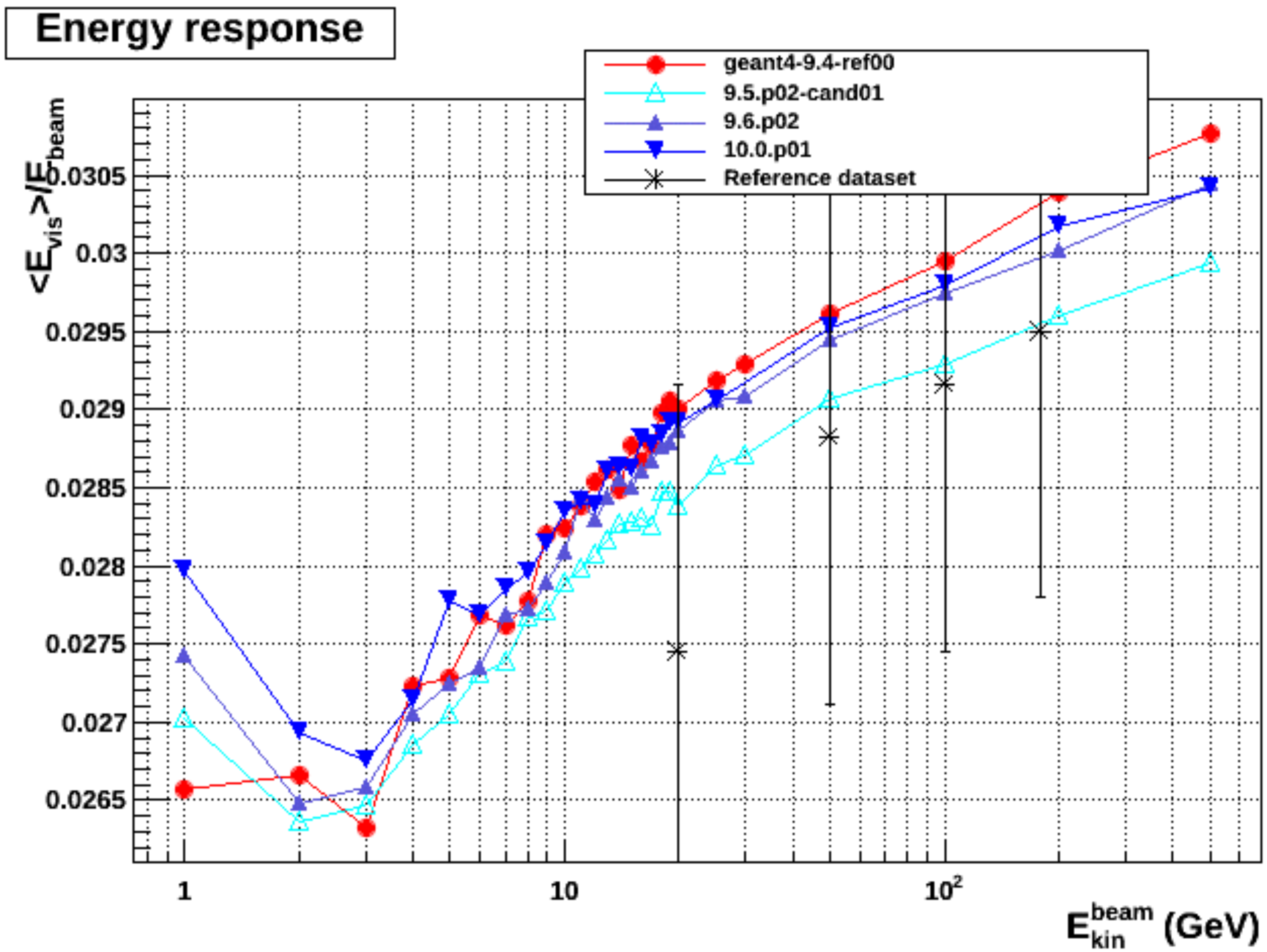
Radioactive Decay Errata

- Events using radioactive decay are not reproducible in multi-threaded mode
  - Random seed at end of series of events not always the same given identical seeds at beginning
  - Completely reproducible in sequential mode
  - Working on this
- Small energy non-conservations (~ keV) still exist for some reactions (α , γ)
  - Working on this, too
- Minor inconsistencies between ground state gamma transitions in RadioactiveDecay4.0 and PhotonEvaporation3.0
  - Fixed in RadioacticeDecay4.1 and PhotonEvaporation3.1

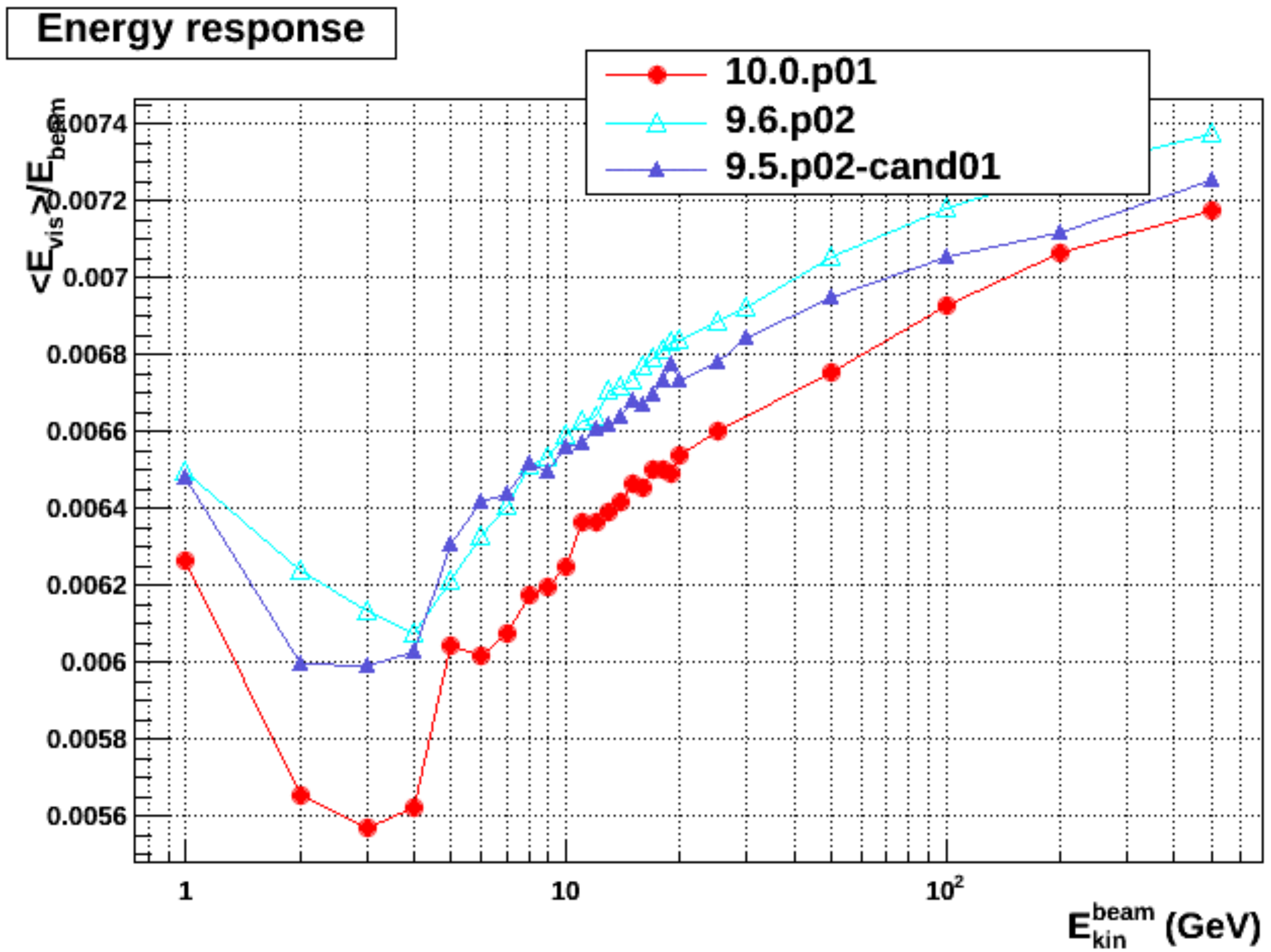
Pions on ATLAS-HEC (Cu/LAr) simplified Calorimeter



Pions on ATLAS-TileCal (Fe/Sci) simplified Calorimeter



Pions on ATLAS-FCAL (W/LAr) simplified Calorimeter



Pions on ATLAS-FCAL (W/LAr) simplified Calorimeter