Geant4 Hadronic Physics: Modeling and model verification.

J.P. Wellisch
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What you can learn/have

- What are the implementation frameworks for hadronic shower simulation in geant4, and how to use them to build a physics list
- What are the activities and implementations existing
- How do we validate/verify the physics
- A show of slides of verification/validation.

Part-II

The implementation frameworks and their use in the physics lists

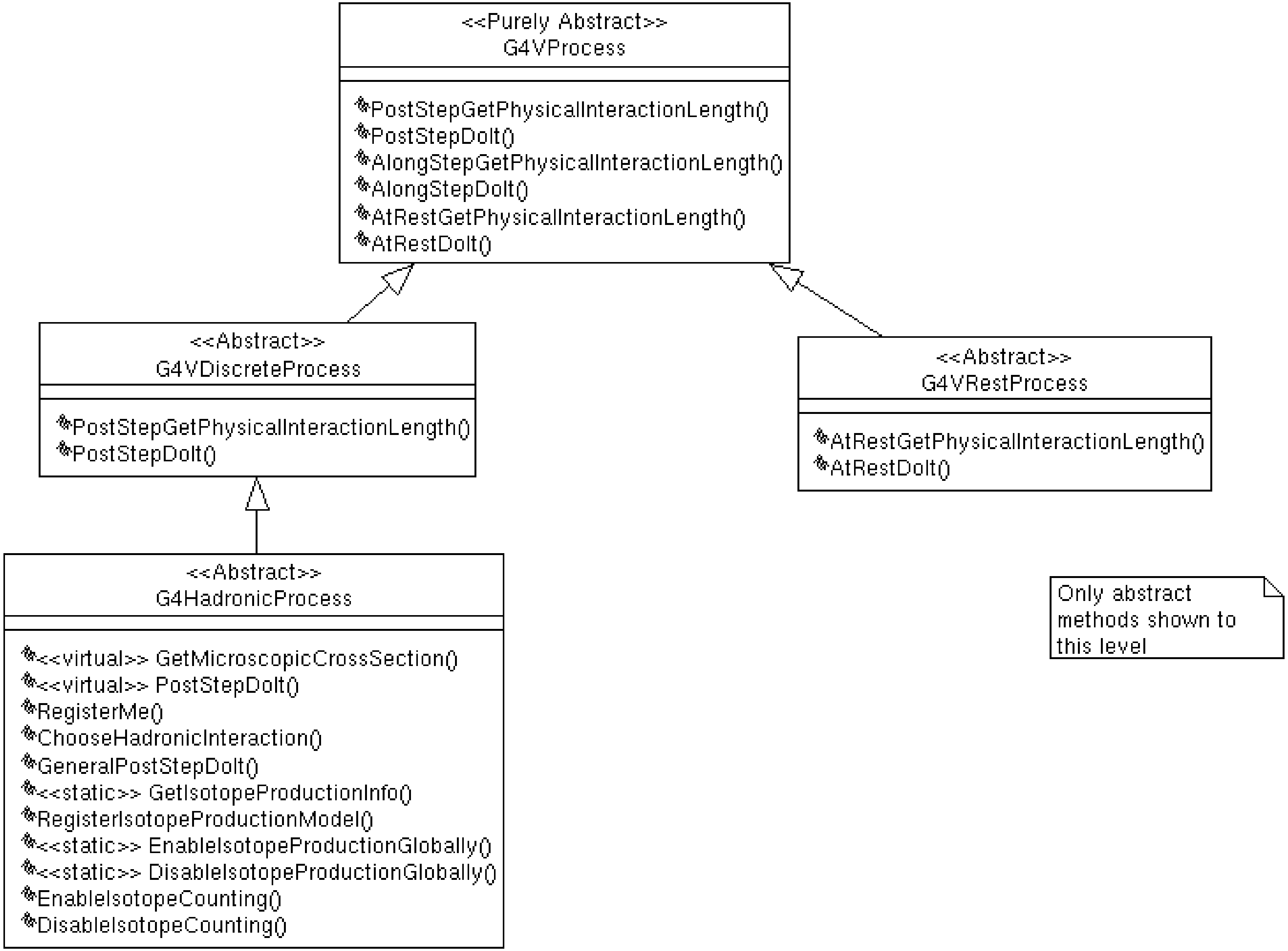
Principal considerations:

- Framework functional requirements are obtained through use-case analysis
- Framework components are found by grouping use-cases into independent bundels (cohesion)
- Complex problems require structured solutions
  - Keep abstractions general and implement in framework interfaces
  - Address more specific use-cases in specialized frame-works, that are implementing the interfaces of the more general frameworks
  - Repeat the pattern until all use-cases are covered

==> The ***Russian dolls*** approach to framework design

Level 1 framework requirement

- Provide the flexibility to allow for calculation of cross-sections and final states for particles in flight and at rest in a medium.



<<Purely Abstract>>
G4VProcess
PostStepGetPhysicalInteractionLength()
PostStepDoIt()
AlongStepGetPhysicalInteractionLength()
AlongStepDoIt()
AtRestGetPhysicalInteractionLength()
AtRestDoIt()
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G4VDiscreteProcess
PostStepGetPhysicalInteractionLength()
PostStepDoIt()
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G4VRestProcess
AtRestGetPhysicalInteractionLength()
AtRestDoIt()
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G4HadronicProcess
<<virtual>> GetMicroscopicCrossSection()
<<virtual>> PostStepDoIt()
RegisterMe()
ChooseHadronicInteraction()
GeneralPostStepDoIt()
<<static>> GetIsotopeProductionInfo()
RegisterIsotopeProductionModel()
<<static>> EnableIsotopeProductionGlobally()
<<static>> DisableIsotopeProductionGlobally()
EnableIsotopeCounting()
DisableIsotopeCounting()
Only abstract methods shown to this level

Implementation

- Inelastic process classes are available for α, anti Λ, anti n, anti Ω, anti p, anti Σ-, anti Σ+, anti Ξ-, anti Ξ0, deuteron, electron, ion, K-, K+, Kl, Ks, Λ, n, Ω, p, γ, π–, π+, e+, Σ–, Σ+, triton, Ξ-, Ξ0.
- There also are process classes for capture of neutral hadrons, fission, and coherent elastic scattering.
  - See geant4/source/processes/hadronic/processes

How to use it in the physics list?

- G4ParticleDefiniton * theNeutron = G4Neutron::NeutronDefinition();
- G4ProcessManager * theMan = theNeutron->GetProcessManager();
- G4NeutronInelasticProcess * thePro = new G4NeutronInelasticProcess("inelast");
- theMan->AddDiscreteProcess(thePro);

level 2 framework requirements

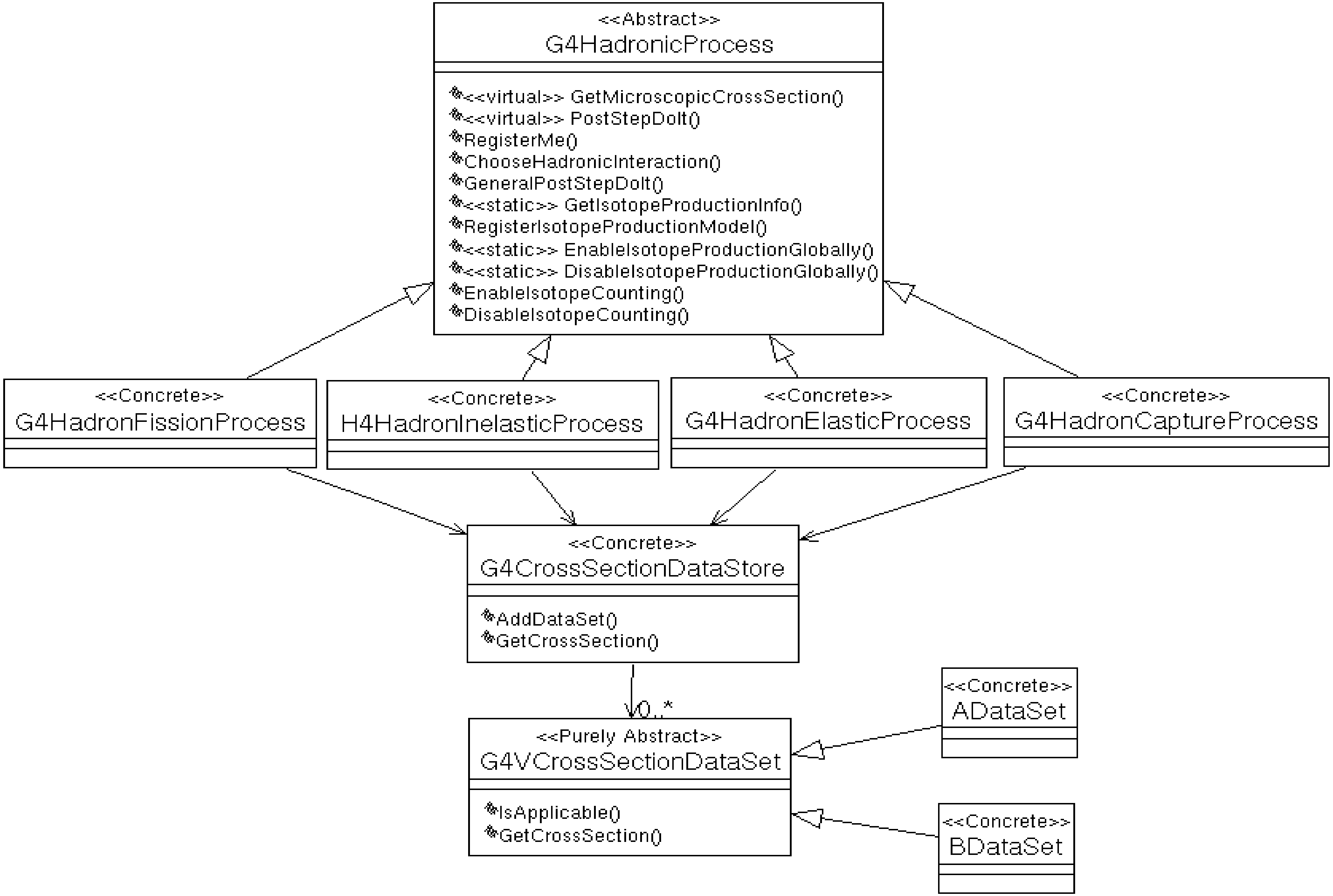
- Flexible choice of inclusive scattering cross-sections
- Possibility to use different data-sets for different parts of the detector
- Run geant4 against user defined cross-section data in a seamless manner
- See geant4/source/processes/hadronic/cross_sections

- Flexible choice of final state production code.
- Ability to use different codes in one run, depending on the conditions at the point of interaction
- Ability to use user-defined models in a seamless manner
- See geant4/source/processes/hadronic/models

level 2 framework requirements

- Flexible choice of isotope production codes, to run parasitically to any kind of transport codes
- Ability to use different codes in one run, depending on the conditions at the point of interaction
- Ability to use user-defined isotope production codes
- See geant4/source/processes/hadronic/models/isotope_production

! This grouping of requirements according to related use-cases results quite naturally in three almost independent framework components at the same level of abstraction.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G4HadronFissionProcess
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H4HadronInelasticProcess
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G4HadronElasticProcess
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G4HadronCaptureProcess
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G4CrossSectionDataStore
AddDataSet()
GetCrossSection()
0..*
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G4VCrossSectionDataSet
IsApplicable()
GetCrossSection()
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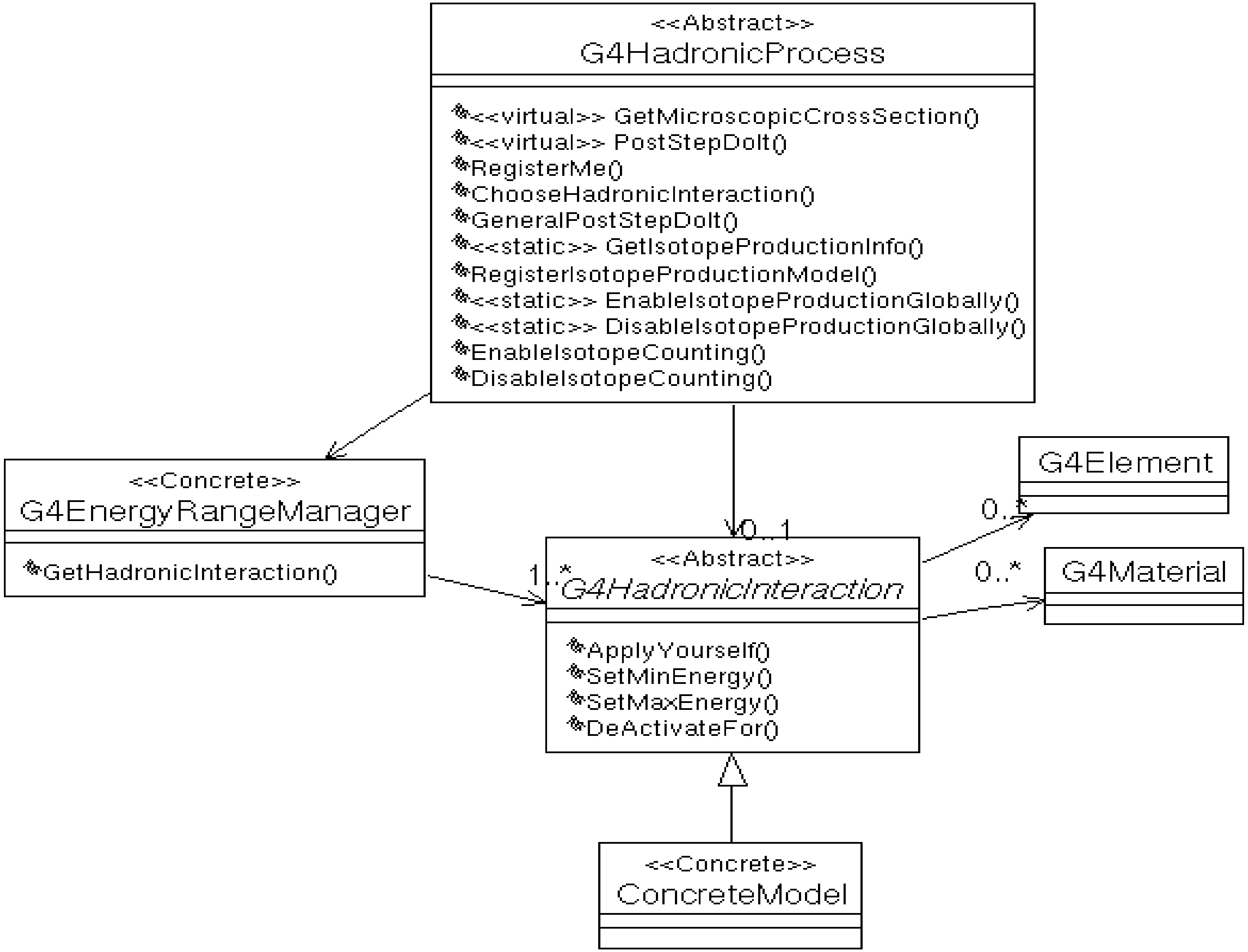
ADataSet
<<Concrete>>
BDataSet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G4EnergyRangeManager
GetHadronicInteraction()
0..1
1..*
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G4HadronicInteraction
ApplyYourself()
SetMinEnergy()
SetMaxEnergy()
DeActivateFor()
G4Element
0..*
G4Material
0..*
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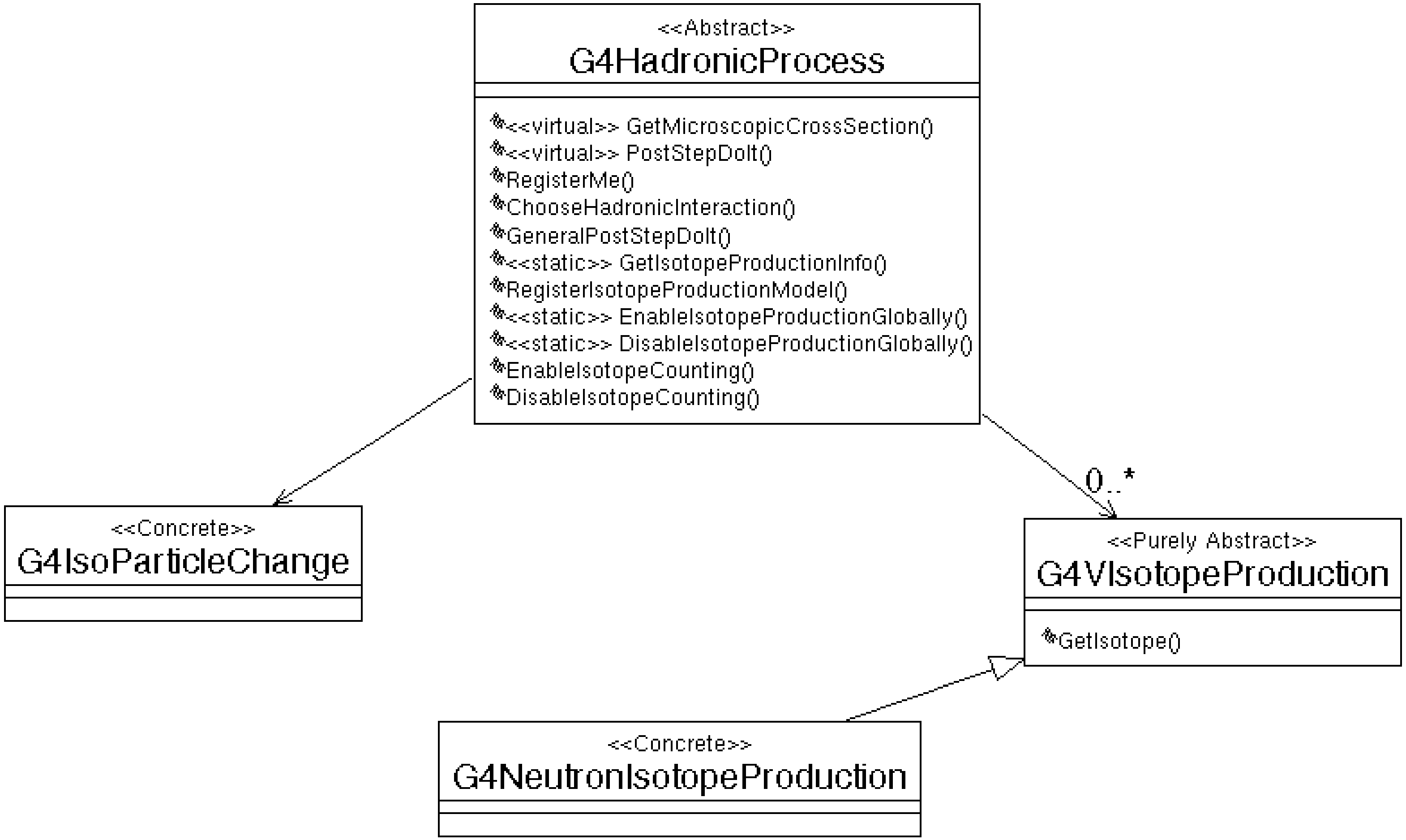
ConcreteModel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DisableIsotopeCounting()
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G4IsoParticleChange
0..*
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G4VIsotopeProduction
GetIsotope()
<<Concrete>>
G4NeutronIsotopeProduction

Example: The neutron transport models

- Simulate the cross-sections and interactions of neutrons with kinetic energies below 20 MeV down to thermal energies .
- The upper limit is set only by the evaluated data libraries the code is based on.
- We consider elastic scattering, fission, capture and inelastic scattering as separate models
- Neutron_hp sampling codes for the ENDF/B-VI derived data formats are completely generic (not including general R-matrix for the time being)
- Note that for fission there is a quite competitive theory driven alternative model, G4ParaFissionModel.

Relevant classes

- For cross-sections:
  - G4NeutronHPElasticData
  - G4NeutronHPInelasticData
  - G4NeutronHPCapureData
  - G4NeutronHPFissionData
- Final state production:
  - G4NeutronHPCapture
  - G4NeutronHPElastic
  - G4NeutronHPFission
  - G4NeutronHPInelastic

  - See geant4/source/processes/hadronic/models/neutron_hp

How to register in the physics list?

- Cross-sections:
  - G4NeutronInelasticProcess aProcess;
  - G4NeutronHPInelasticData theData;
  - aProcess.GetCrossSectionDataStore()->AddDataSet(&theData);
  - FILO stack of cross-sections!
- Final state production:
  - G4NeutronHPInelastic theModel;
  - aProcess.RegisterMe(&theModel);
  - Change energy range and/or validity for individual and all materials and elements as you deem right for your case.

The data - G4NDL

- Based on evaluated data libraries
  - ENDF, Jef, EFF, JENDL, FENDL, CENDL, ENSDF, Brond, and MENDL.
  - We use the UNIX file-system to ensure granular and transparent access/usage of data sets, as well as tailoring by the user.
- Two variants exist:
  - G4NDL3.7 - includes thermal resonances.
  - G4NDL0.2 - excludes thermal resonances.
  - Tailoring these data is easy, but requires expertise.
- Not to forget:
  - setenv NeutronHPCrossSections environmental variable to point to your copy of G4NDL.

No details on the mathematics...

- For the mathematics, in this particular contest, the ENDF/B data formats documentation is an excellent source of information...
- Important note: Doppler broadening is done on the fly, so there is no need for pre-processing the 0K data.

Isotope production models

- Aimed at activation studies.
- Cover primary neutron energies from the spallation energy range down to thermal energies.
- Cover the scattering of neutrons and protons off nuclei.
- Run in parasitic mode to any combination of hadronic shower models in geant4, in any set-up.

Detailed requirements

- ISO-01: There shall be detailed isotope production for incident neutrons and protons
- ISO-02: There shall be information available on which model produced the isotope
- ISO-03: There shall be information available on what was the target
- ISO-04: There shall be information available on energy and direction of the projectile
- ISO-05: There shall be information available on time and location of production

How to register?

- Isotope production models:
  - G4NeutronInelasticProcess aProcess;
  - G4NeutronIsotopeProduction thePro;
  - aProcess.RegisterIsotopeProductionModel(&thePro);
  - Enable/disable for individual processes or globally, as you deem good for your application.

Data: G4NDL0.2, 3.7

- Are granular selections of data from (alphabetic)
  - Brond 2.1
  - CENDL 2.2
  - EFF-3
  - ENDF/B (VI.0, VI.1, VI.5)
  - ENSDF
  - FENDL/E2.0
  - JEF 2.2
  - JENDL (3.1, 3.2, FF)
  - MENDL-2(P)
- Large parts of the selection is guided by the FENDL-2 selection

“High energy” cross-sections

- Data for total neutron interaction cross-sections supplemented with parameterization of reaction cross-sections above 20 MeV kinetic energy.
- Energy dependence of total neutron nuclear scattering cross-section assumed to be the same as that of the neutron nuclear reaction cross-section.

$$\sigma_{reac} = F(E_n)\pi p_1^2 \ln(N)[1 + A^{1/3} - p_2(1 - 1/A^{1/3})]$$

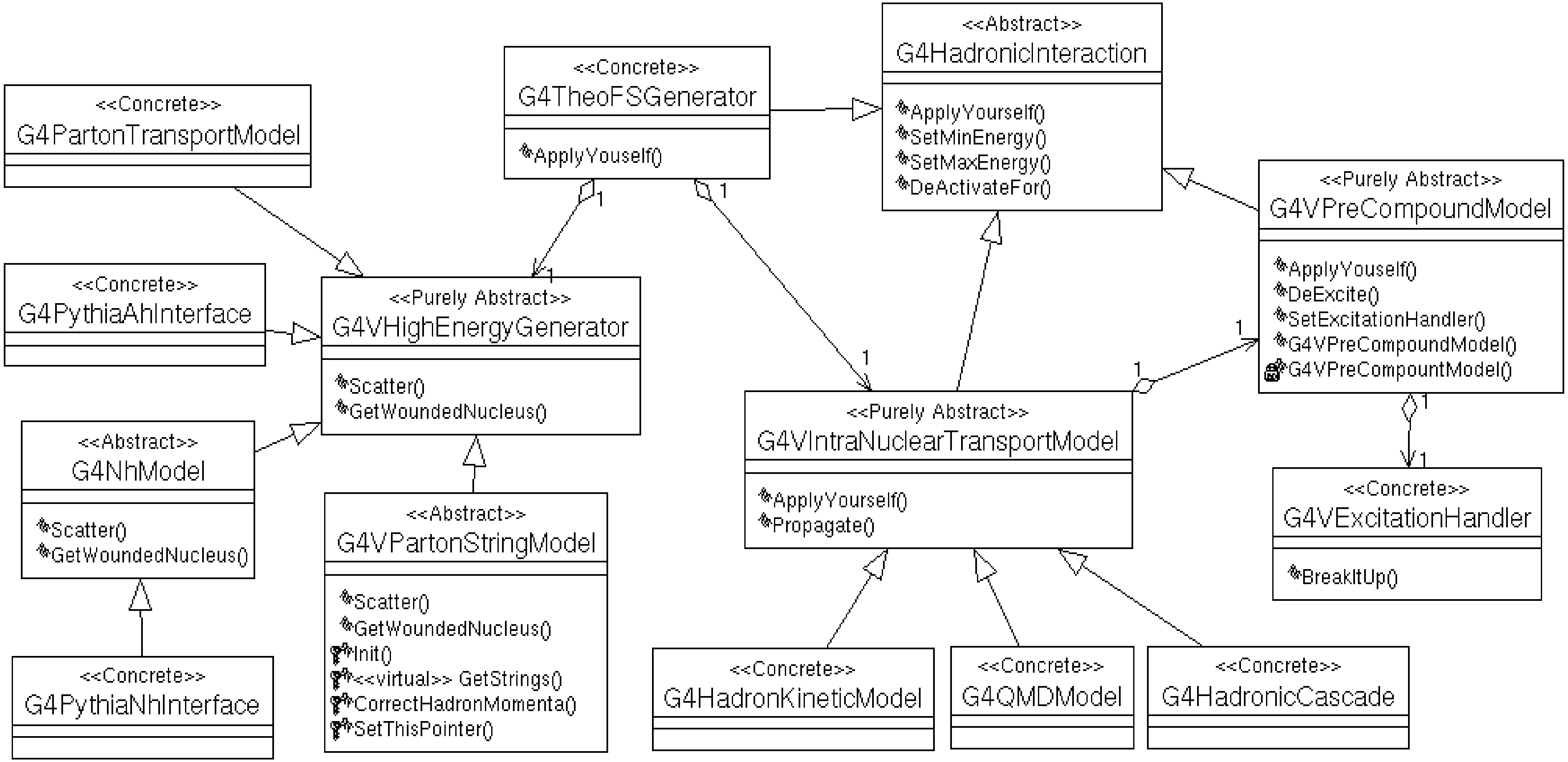
- Please see G4NeutronInelasticCrossSection (and G4ProtonInelasticCrossSection) class

3rd level framework requirements

- For data driven models
  - Possibility to change the data used by the models in a seamless manner.
- For theory driven models
  - Allow to use any string-parton or parton-cascade model
  - Allow to use event generators for final state generation
  - Allow for combination with any intra-nuclear transport
  - Allow stand-alone use of any intra-nuclear transport
  - Allow for combination with any pre-compound model
  - Allow stand-alone use of any pre-compound model
  - Allow for use of any evaporation code

Level 3 framework design

- The requirement on data driven models is fulfilled by using standard data formats



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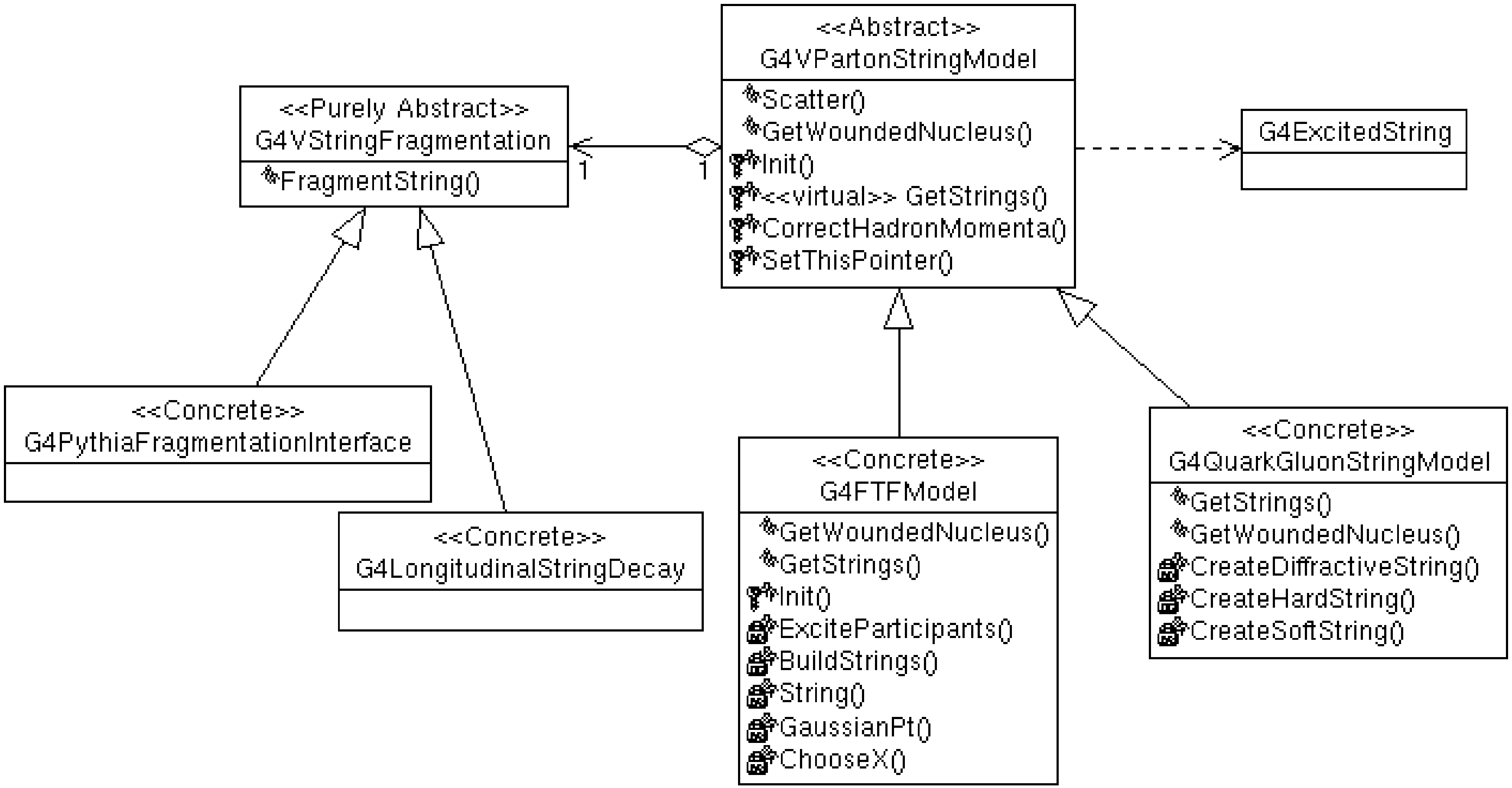
4th level framework requirements

- For string-parton models
  - Be able to choose string decay algorithm, and string excitation
  - Be able to use user-defined string excitation and decay
- For Intra-nuclear cascades
  - Be able to use user-defined models for a nucleus
  - Be able to use user-defined final state and cross-sections data for the intra-nuclear scattering



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G4VPartonStringModel
Scatter()
GetWoundedNucleus()
Init()
<<virtual>> GetStrings()
CorrectHadronMomenta()
SetThisPointer()
<<Purely Abstract>>
G4VStringFragmentation
FragmentString()
1
1
G4ExcitedString
<<Concrete>>
G4PythiaFragmentationInterface
<<Concrete>>
G4LongitudinalStringDecay
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G4FTFModel
GetWoundedNucleus()
GetStrings()
Init()
ExciteParticipants()
BuildStrings()
String()
GaussianPt()
ChooseX()
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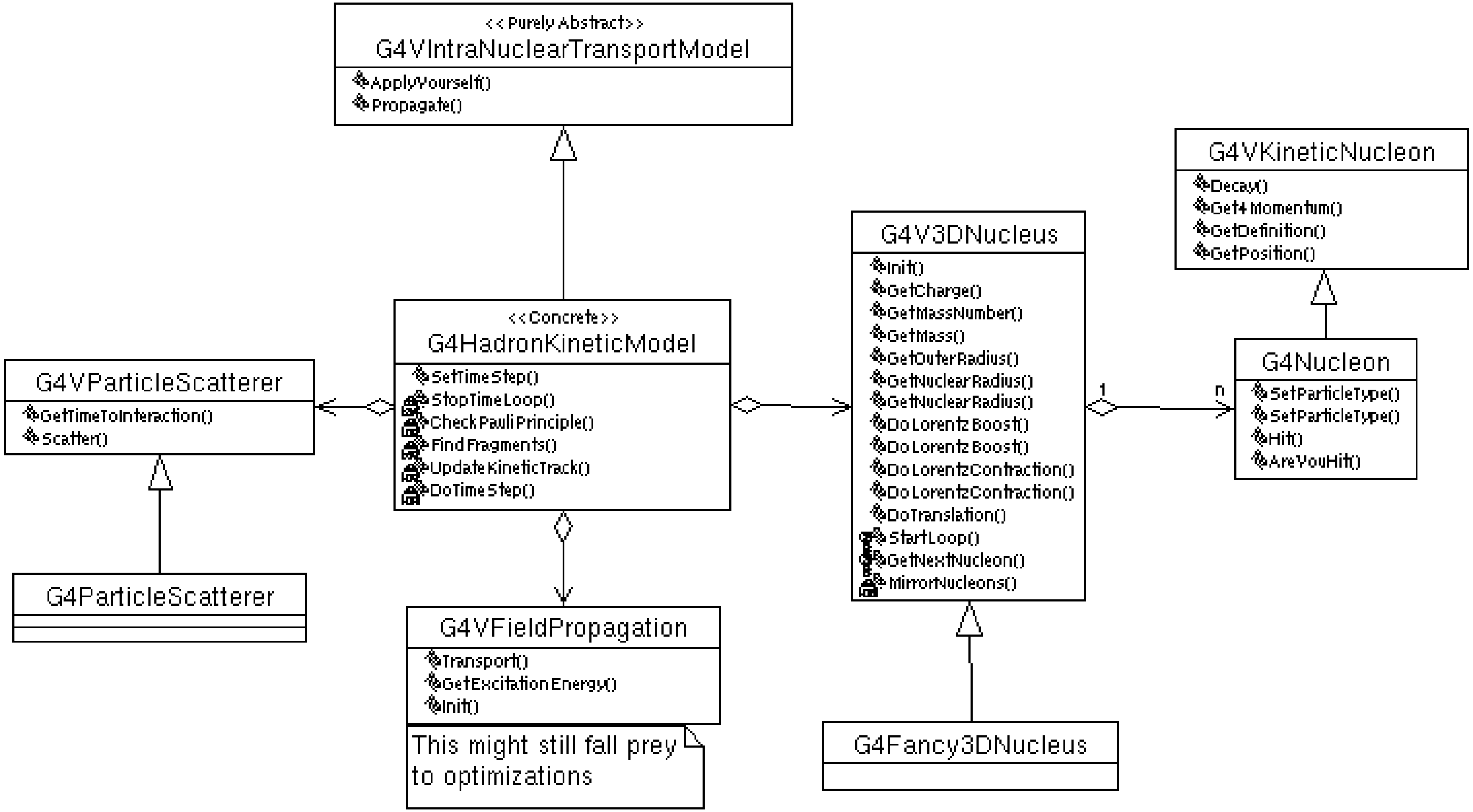
G4QuarkGluonStringModel
GetStrings()
GetWoundedNucleus()
CreateDiffractiveString()
CreateHardString()
CreateSoftString()



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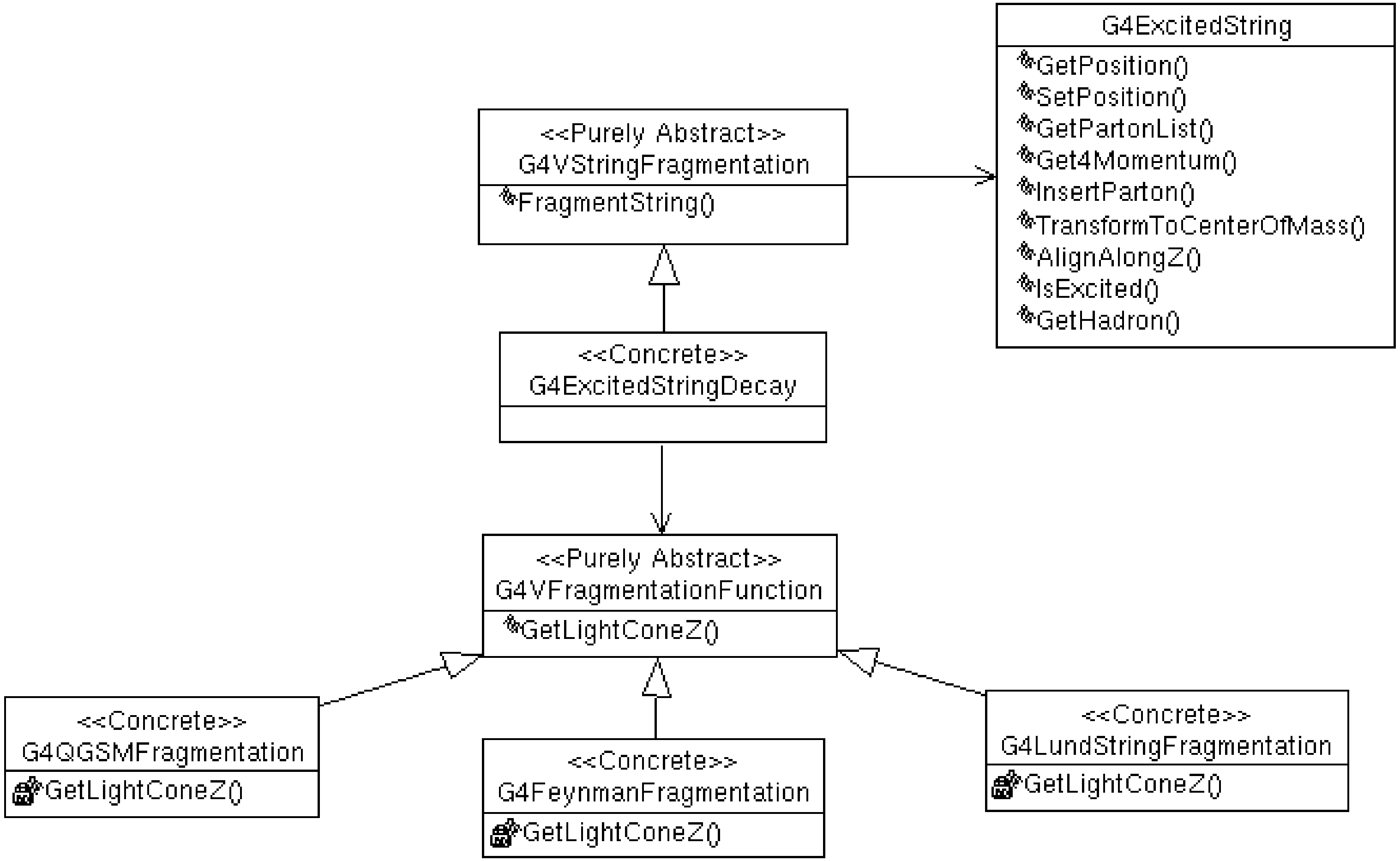
5th level requirements

- For string decay
  - Allow to change the fragmentation function
  - …more under study…

! At this level, the framework approach has essentially exhausted the complexity of the topic, but note that ***concrete implementations are possible at any level of the Russian doll***. Each doll could be the last.


G4ExcitedString
GetPosition()
SetPosition()
GetPartonList()
Get4Momentum()
InsertParton()
TransformToCenterOfMass()
AlignAlongZ()
IsExcited()
GetHadron()
<<Purely Abstract>>
G4VStringFragmentation
FragmentString()
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G4ExcitedStringDecay
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G4VFragmentationFunction
GetLightConeZ()
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G4QGSMFragmentation
GetLightConeZ()
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G4FeynmanFragmentation
GetLightConeZ()
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G4LundStringFragmentation
GetLightConeZ()

Part -III

Activities and implementations

Activities and implementations

- Particles at rest:
  - One complete set of processes 'a'la Geant3'
  - Alternative process implementations for stopping pi-, K-, mu-
  - Upgrade program for anti-protons, including chips
  - Upgrade to include the electromagnetic transitions of the exotic atom prior to capture, and effects of atomic binding for muon capture
- Radio-active decay

Activities and implementations

- Inclusive cross-sections:
  - Complete set of cross-section classes ‘a la’ Geant3.21
  - Specialized data-sets for neutron and proton induced reactions below 20 GeV
  - Data-sets for electro and gamma nuclear reactions
  - Data-sets for ion nuclear reactions
  - Data set for ion reactions on hydrogen
  - Data sets for neutron induced reactions, elastic scattering, capture and fission of neutrons for energies below 20 MeV.
  - Upgrade for strange particle induced reactions underway.
  - Review of the reaction cross-sections on the way.

Data libraries

- Systematic collection and evaluation of experimental data from many sources worldwide
- Databases
  - ENDF/B, JENDL, FENDL, CENDL, ENSDF, JEF, BROND, EFF, MENDL, SAID, EPDL, etc.
- Distribution centres
  - NEA, LANL, LLNL, BNL, KEK, IAEA, IHEP, TRIUMF, FNAL, Helsinki, Durham, etc.
- The use of evaluated data is important for the validation of physics results

Activities and implementations

- In flight
  - Coherent elastic scattering
    - One set 'ala' Geant3.21, I.e. 2 slopes parametrized as a function of target mass
    - Reggee theory based alternative implementation for incoming pi, K, nucleon in preparation
    - Data driven specialized models for low energy nucleon scattering off Hydrogen was released.
    - Alternative data driven model for low energy (<20 MeV) neutron coherent elastic scattering with possibility to run against any formatted data library (ENDF/B, FENDL, JENDL, G4NDL, etc..)

Activities and implementations

- Capture of neutral particles
  - One set ‘ala’ Geant3
  - Alternative data driven model for low energy (<20 MeV) neutron capture with possibility to run against any formatted data library (ENDF/B, FENDL, JENDL, G4NDL, etc..)
  - Gamma absorption (CHIPS)

Activities and implementations

- In flight
  - Fission
    - One model ‘ala’ Geant3
    - Alternative data driven model for low energy (<20 MeV) neutron induced Fission (1st, 2nd, 3rd and 4th chance) with possibility to run against any formatted data library (ENDF/B, FENDL, JENDL, G4NDL, etc..)
    - Alternative theory driven model, with special focus on fragment yields.

Activities and implementations

- In flight
  - Inelastic scattering
    - Two models ‘ala’ Geant3
    - Alternative data driven model for low energy (<20 MeV) inelastic neutron nuclear scattering (36 exclusive final states are considered) with possibility to run against any formatted data library (ENDF/B, FENDL, JENDL, G4NDL, etc..)
    - Alternative theory driven models, see next slides

Activities and implementations

- In flight, inelastic scattering
  - Theory driven models
    - One parton transport model (concept)
    - Two alternative string model (released)
    - Two types of string fragmentation (released)
    - One quantum molecular dynamics model (release expected 2003)
    - Three alternative intra-nuclear cascades (1 time-driven, 2 space-driven; release imminent for two)
    - One chiral invariant phase-space decay model (released)
    - Re-write of fully biased MARS (<5GeV, released).
    - Three alternative nuclear descriptions (2 released)
    - Two alternative pre-equilibrium decay models (1 released)
    - Three alternative evaporation implementations (released)
      - Fermi break-up, Weisskopf-Ewing, Bondorf multifragmentation, Photo-evaporation.
      - Internal conversion is coming (release imminent)
    - Etc..

Apologies

- My apologies for this flat list of activities without citations or making reference to the people doing/having done the work.
- This is solely for the sake of briefness.
- Many of the concrete implementations were done by others, and much help was provided in several areas by theorists that have invented the models employed.

Part-IV

Validation and verification

Model validation

- Four tier strategy
  - Author validation plots for the individual models
    - Precondition for model to be a candidate for inclusion.
  - Independent validation on thin target data with regression suites by the working groups
    - Verified before every release
  - Independent validation on benchmarks, where these are available
    - Verified before every release, where possible
  - Validation on full simulation programs
- geant4 takes model validation much more seriously than it was in the times of geant3.

GHAD Validation&Verification

- Our validation strategy is deployed since spring 1999. It was submitted as paper to CHEP2001.
- It was subsequently presented again in CMS and ATLAS, at the LHC-geant4 validation meeting, the SLAC users workshop, and the ACAT2002 conference in Moscow.

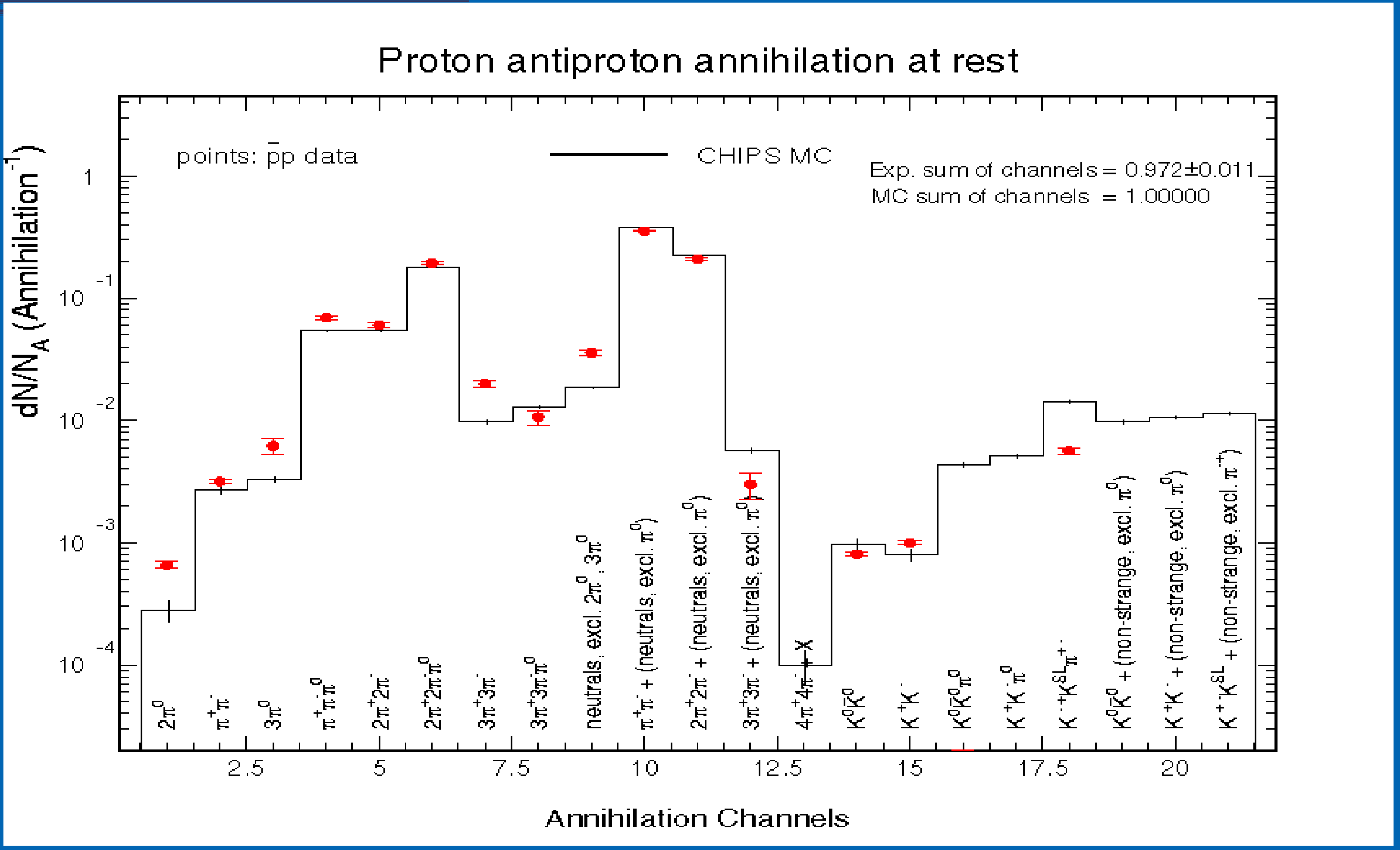
Author validation

- Author validation
  - Comparisons, typically with measurements from thin target data; I.e. event generator like application.
  - Looking at cross-sections, particle yields and distribution, eta and pt distributions, invariant cross-sections, x_f distributions, particle ratios, etc..
  - Requested by the working group when mayor changes to a model occur.
  - Owned by the author, like the test-beam result of an experimental group

Working group validation

- Working group validation suites
  - For eta, pt, xf, mult, $d3\sigma/d3p$, $d\sigma/dT$, n_prong, charge ratios, $d2\sigma/d\Omega dE$, etc. in place for the various energy regimes. Is already quite satisfactory.
  - Trivial quantities now also are checked.
  - Note that this can be done only with the consent of the author.
  - This level of validation was never performed in any depth for geant3.

Anti proton annihilation



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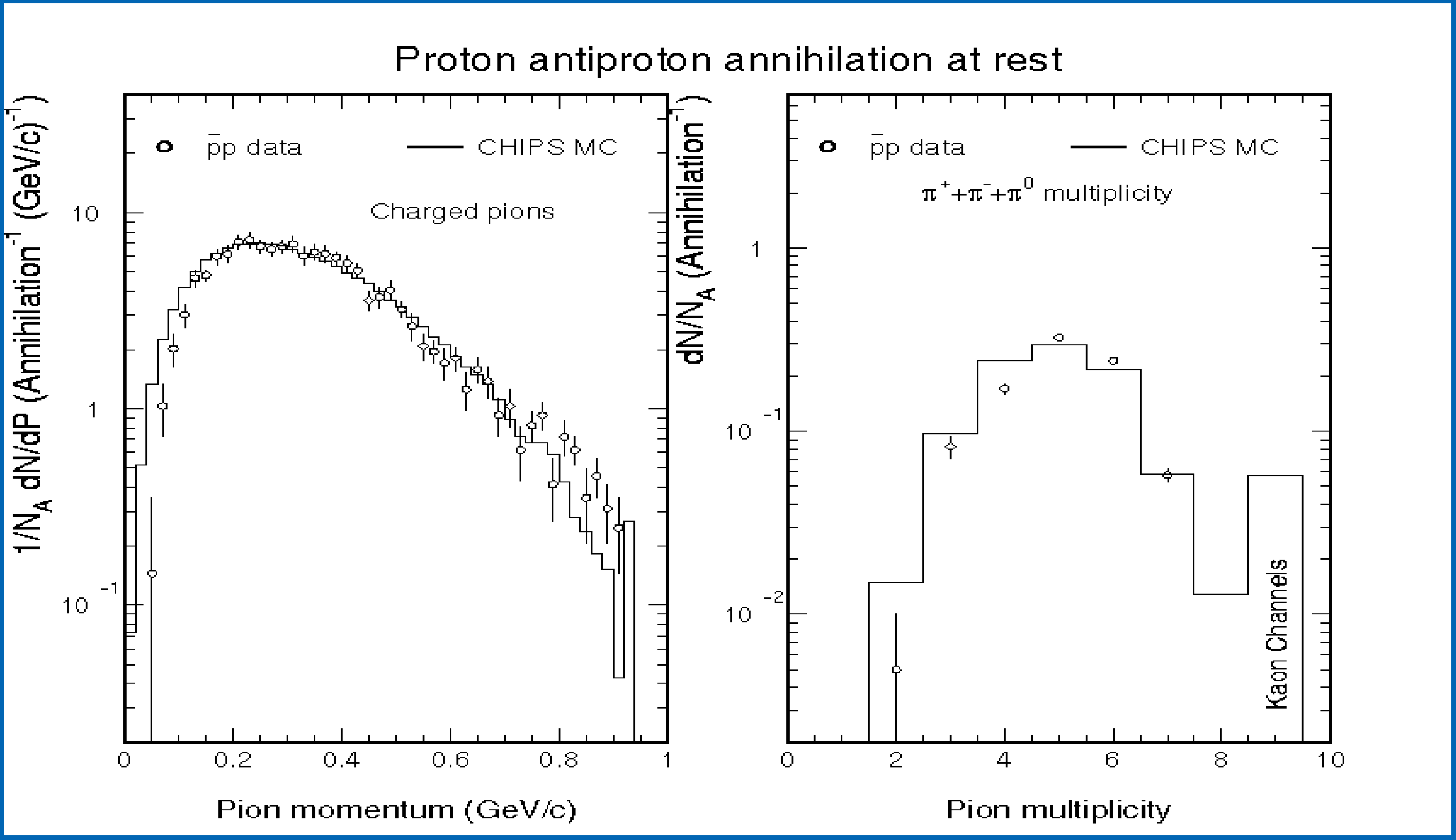
Anti proton annihilation



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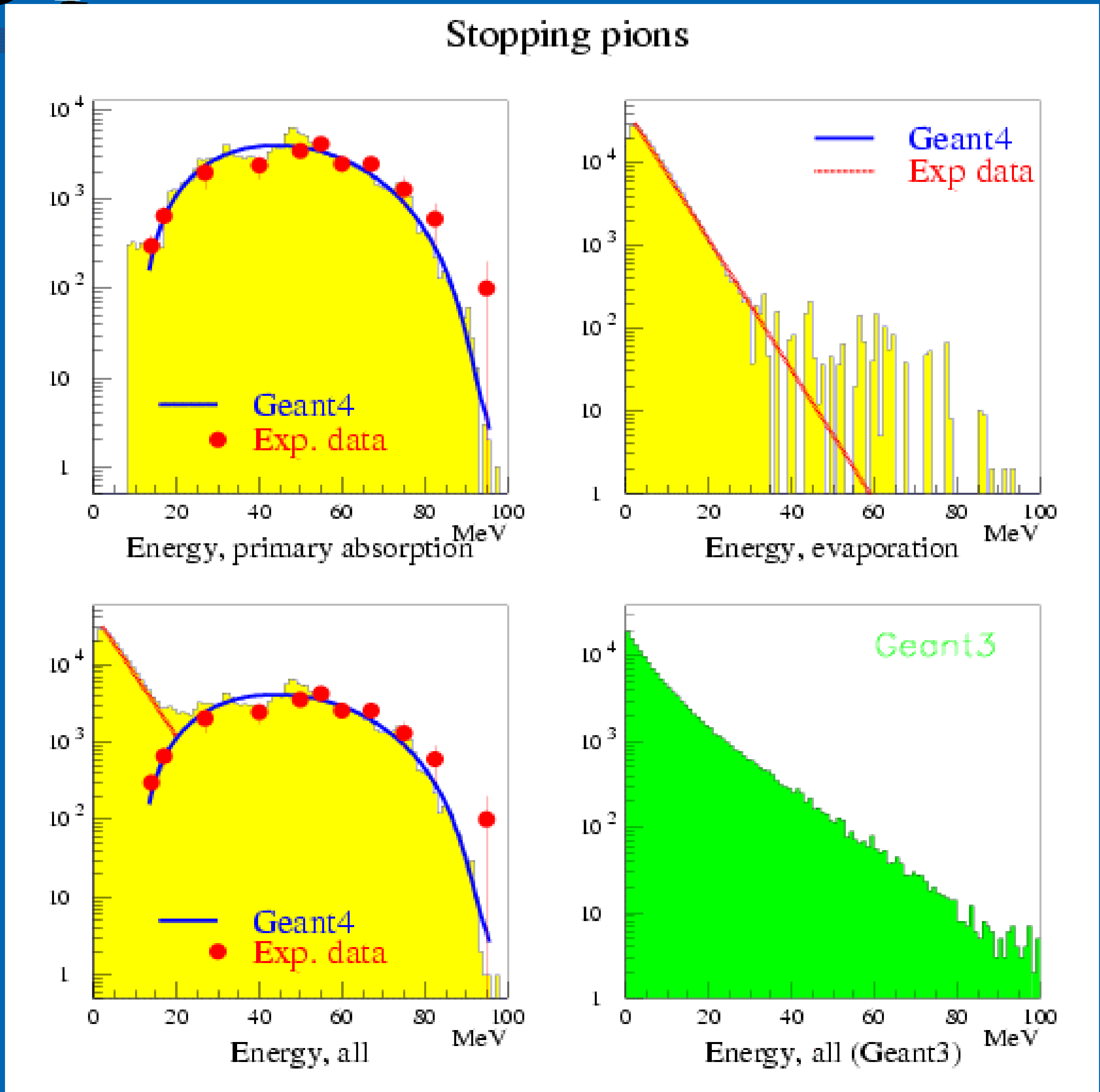
Stopping pion minus



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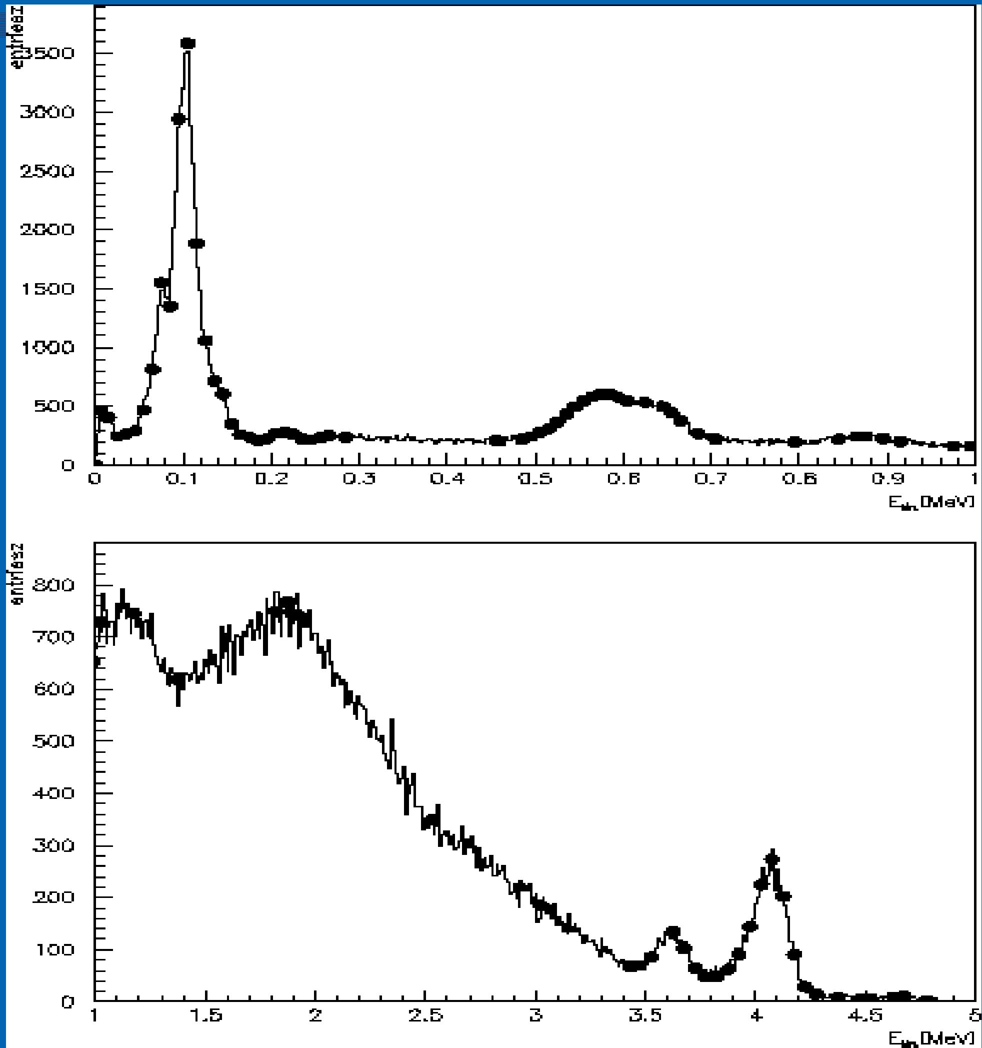
Low energy neutron capture



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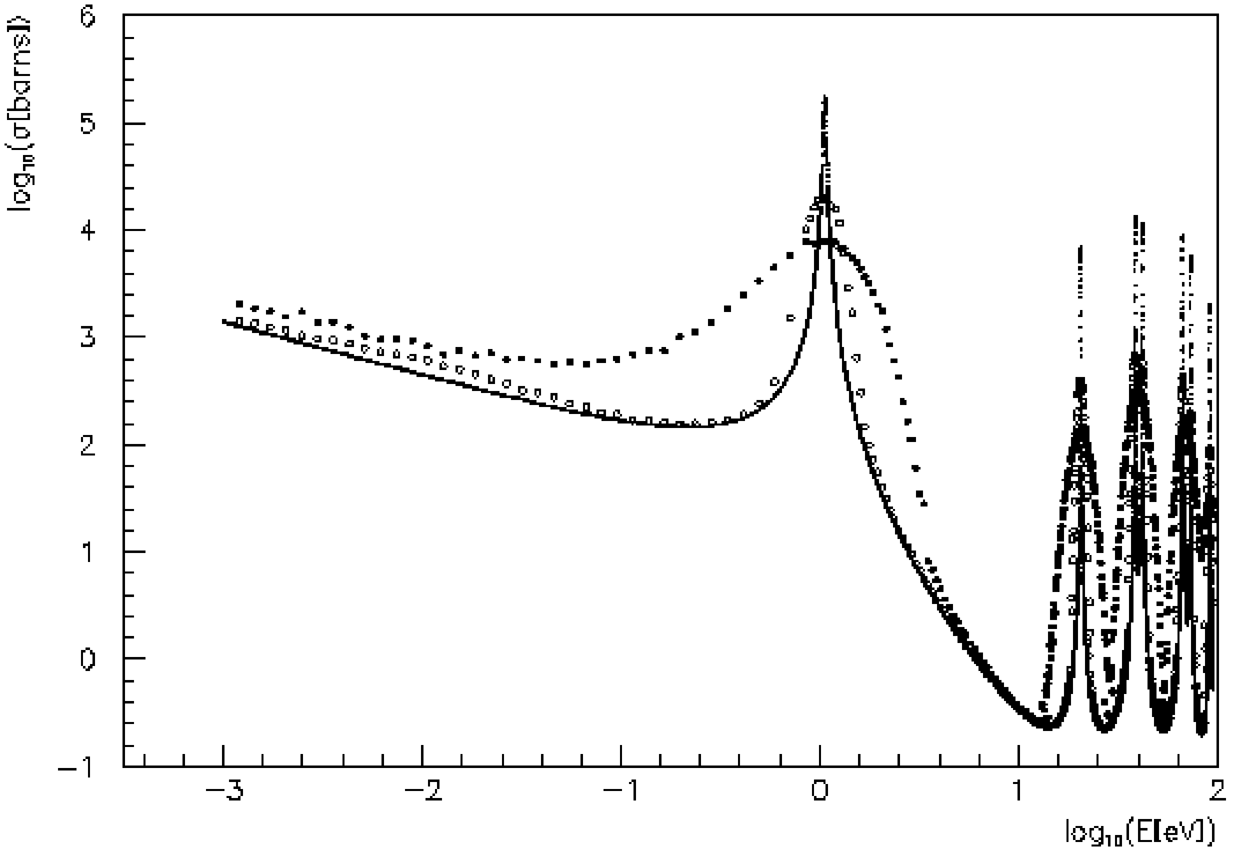
Doppler broadening



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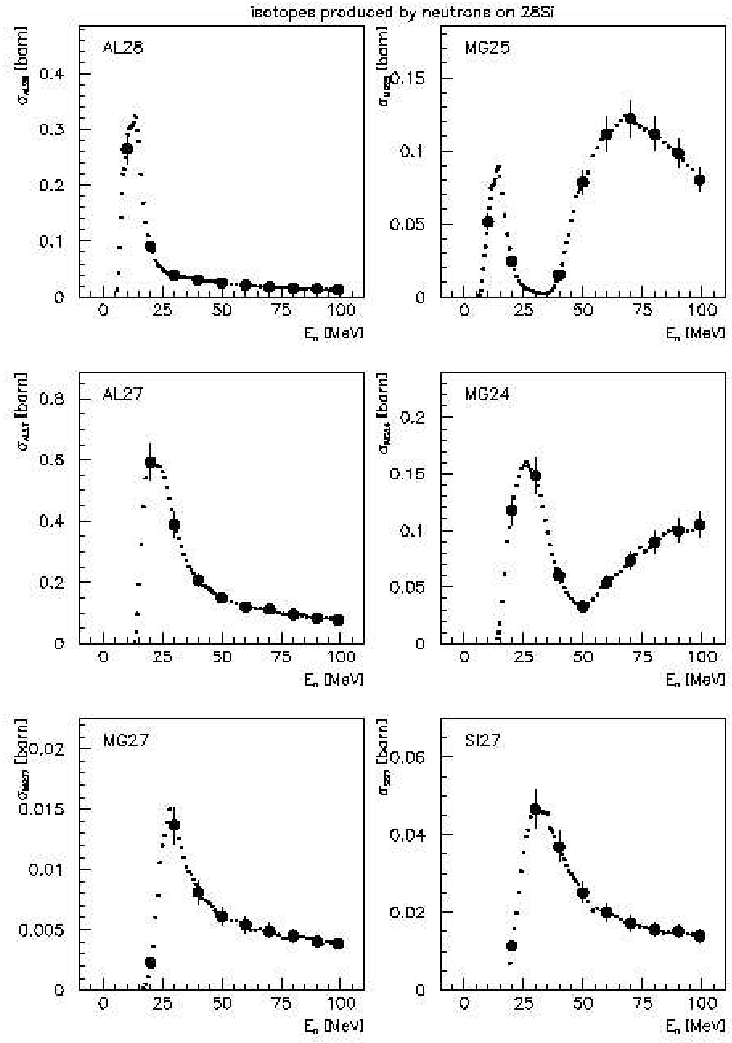
Neutron induced isotope production



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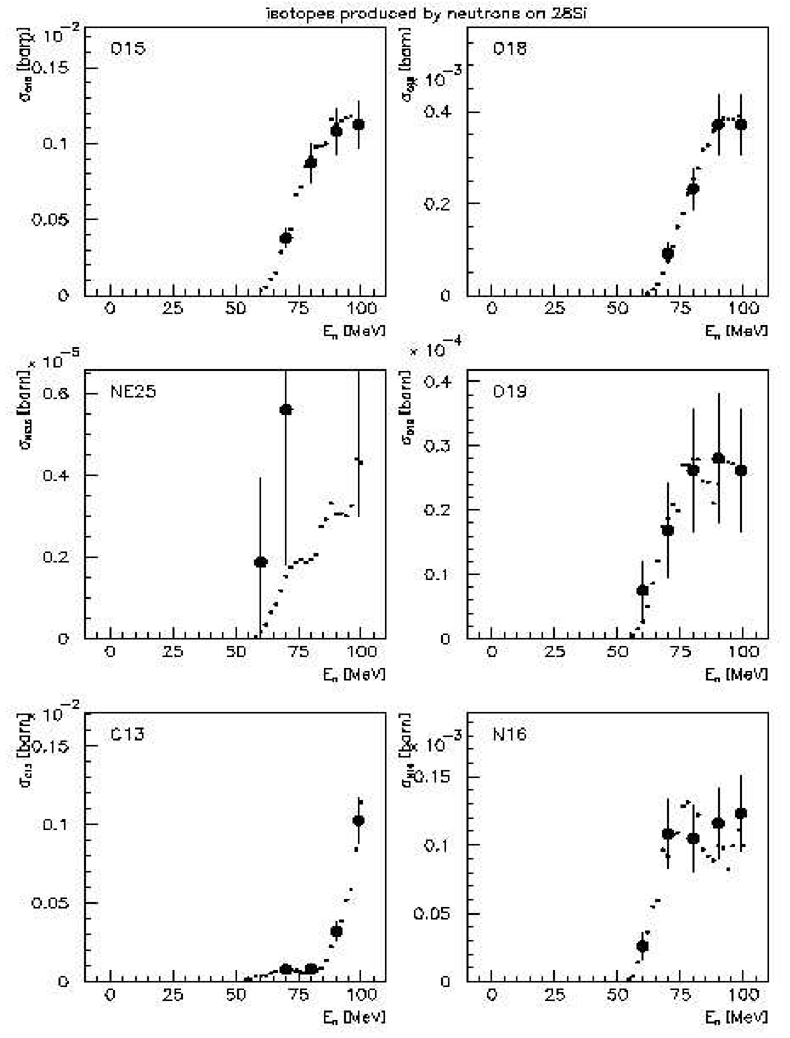
Isotope production



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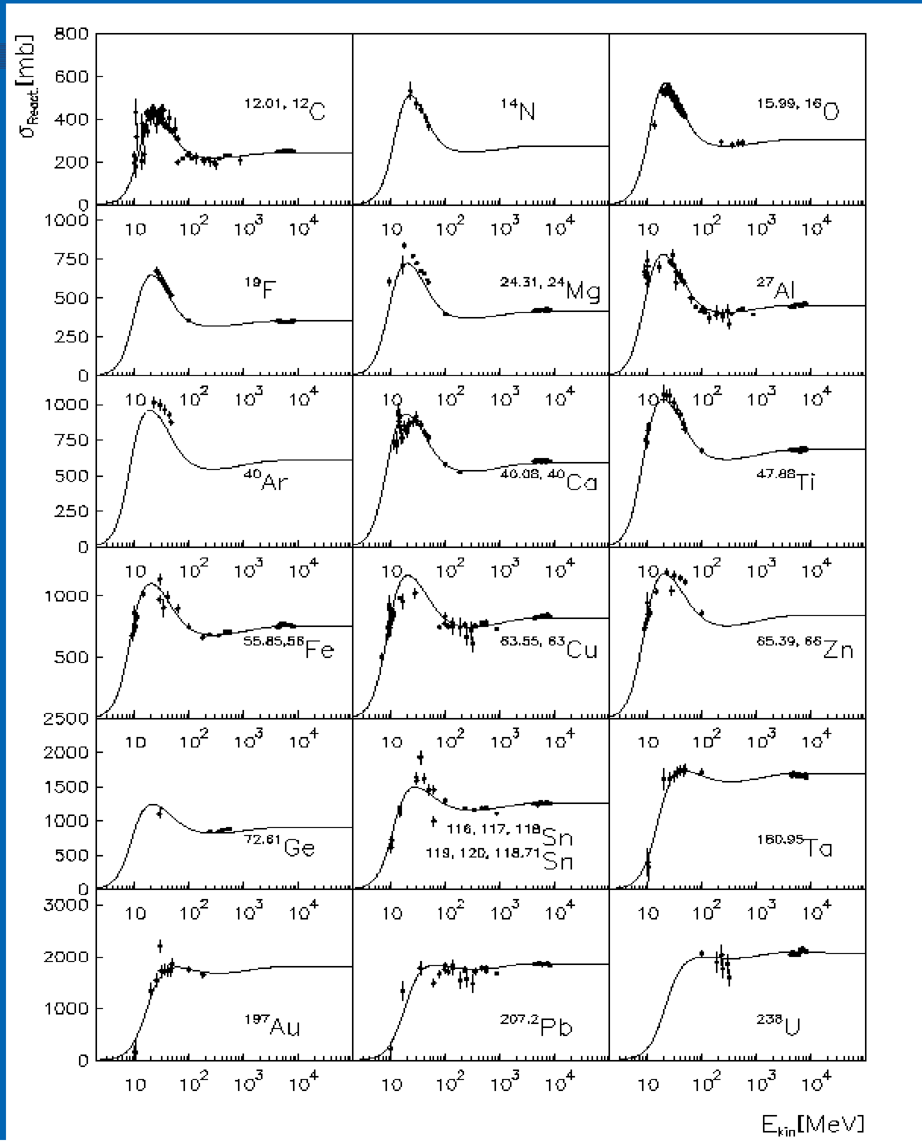
Proton induced reactions



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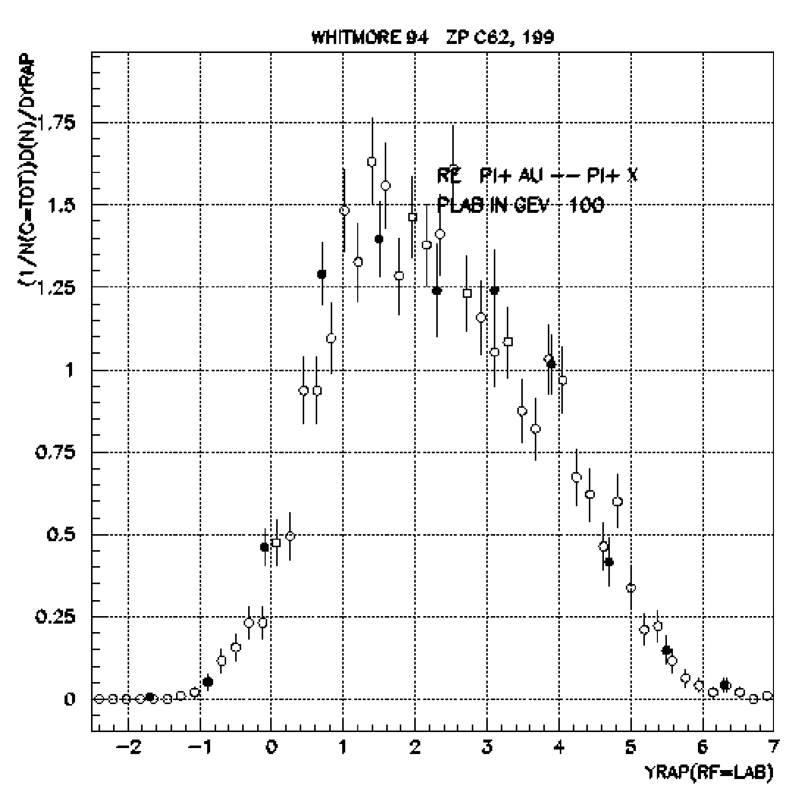
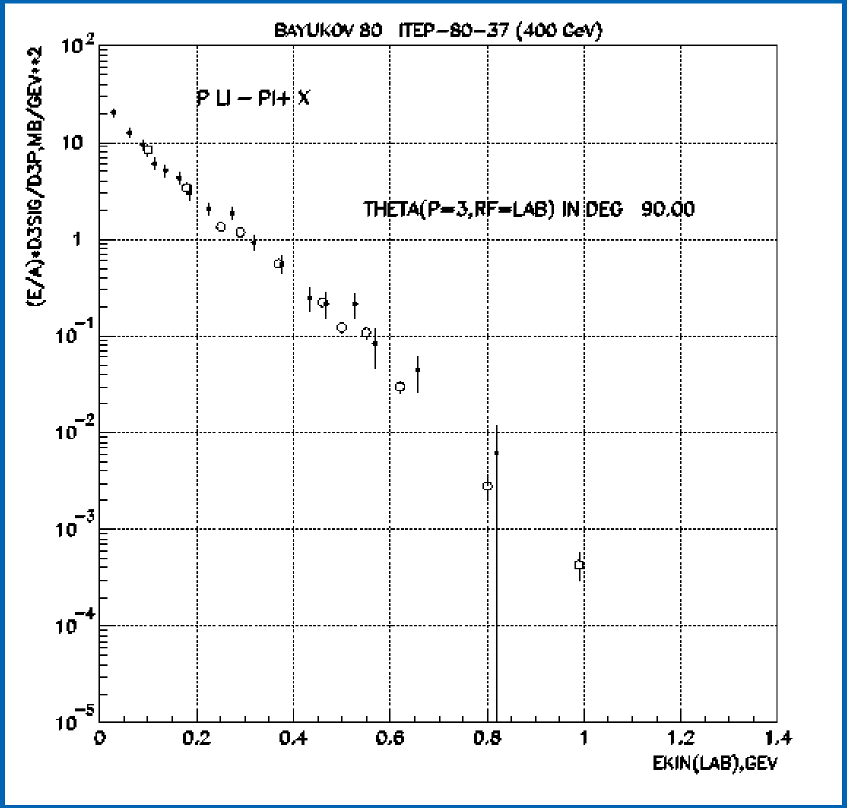
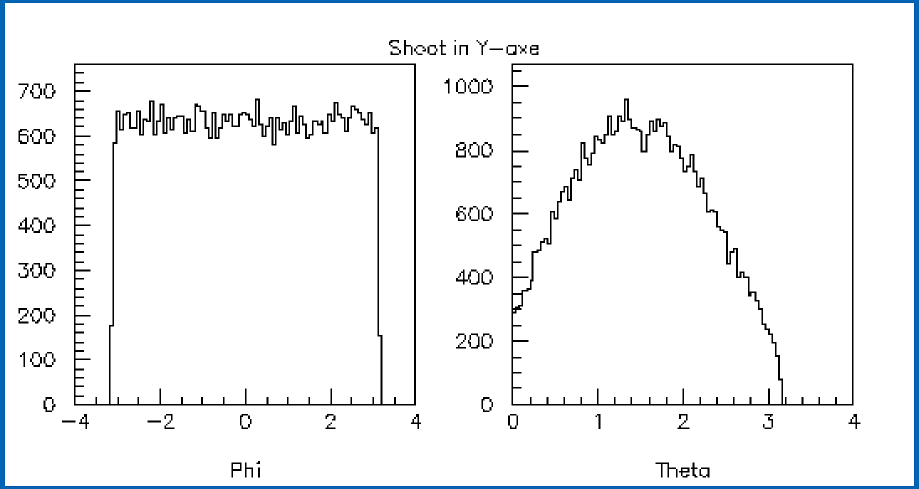
Example WG test results







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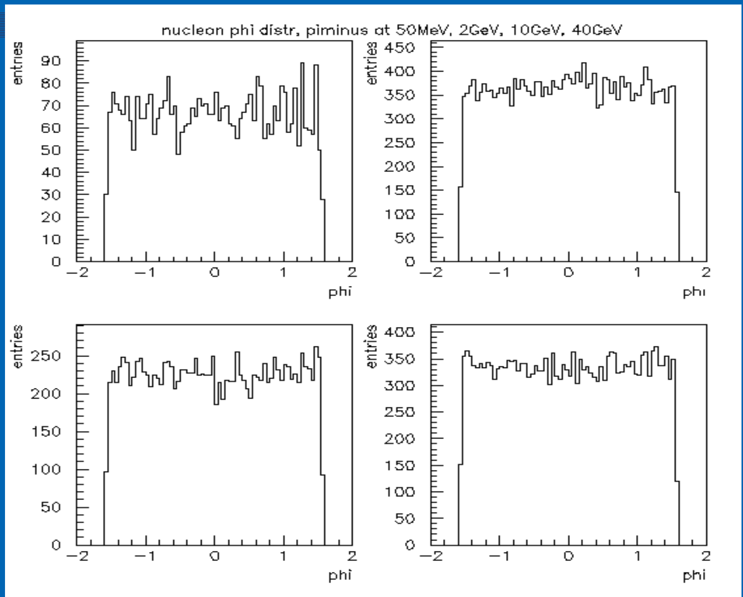
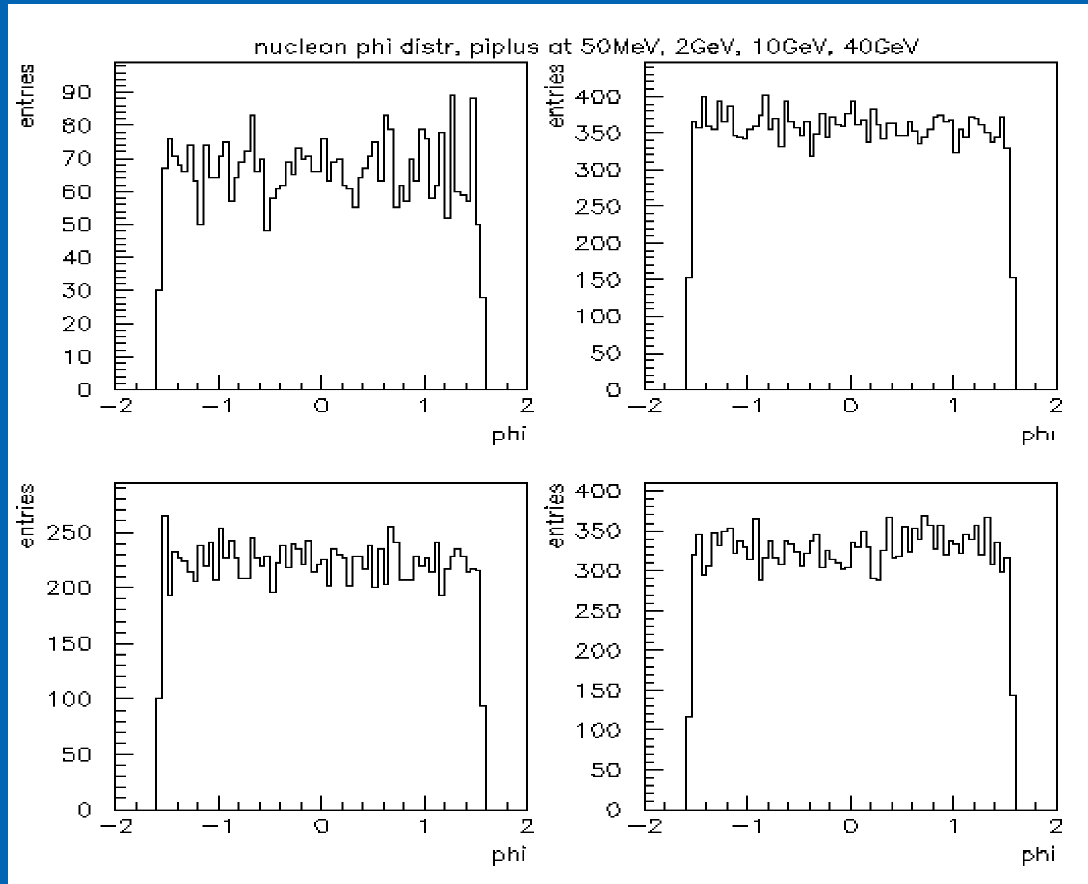
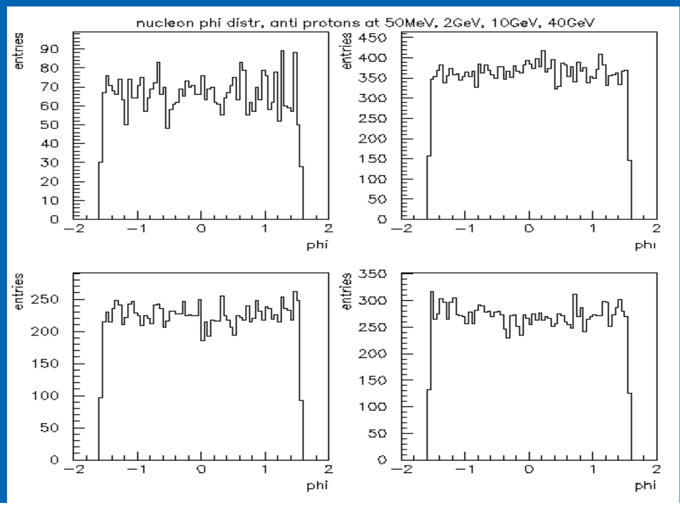
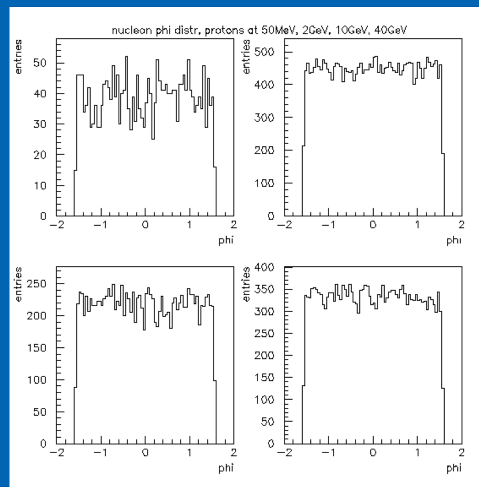
'phi' plots (in Pb)





Nucleon phi distributions
For incident π+, π-,p-bar,p
At energies 50MeV-40GeV





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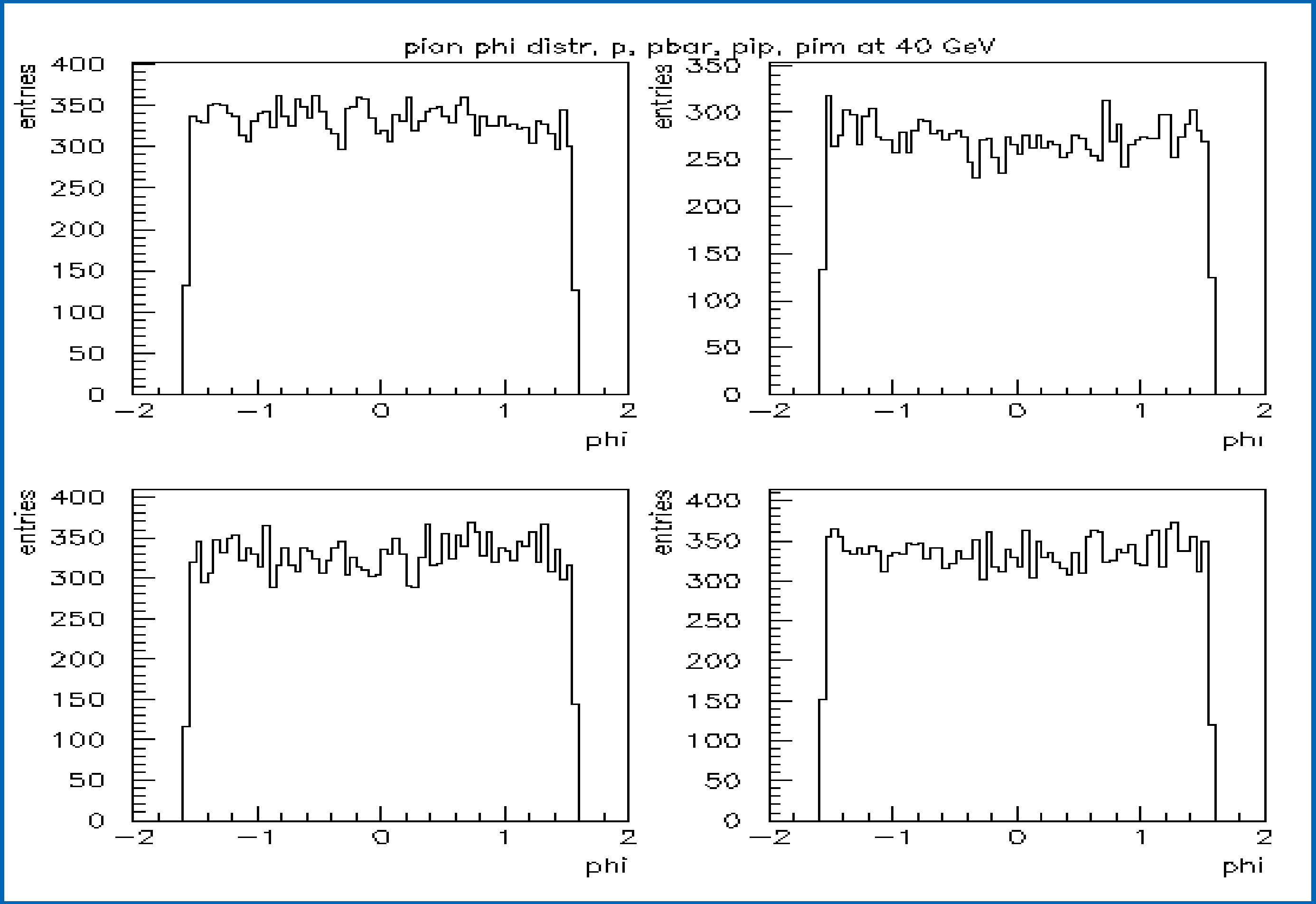
More 'phi' distributions (in lead)



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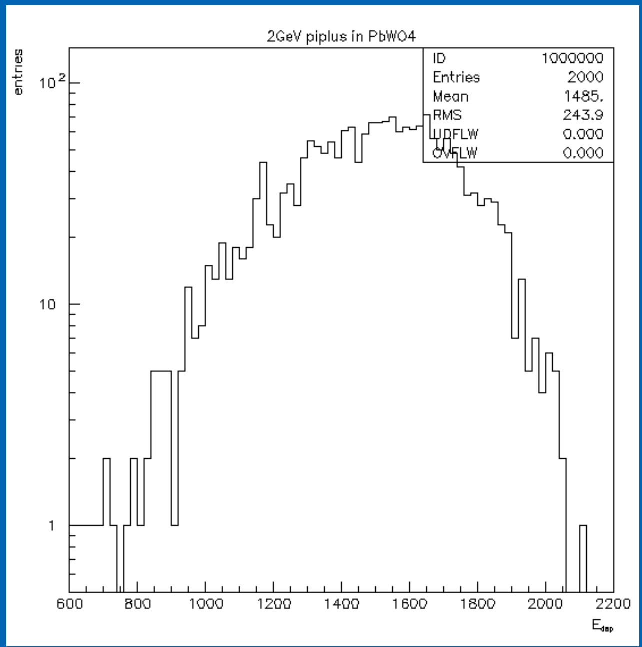
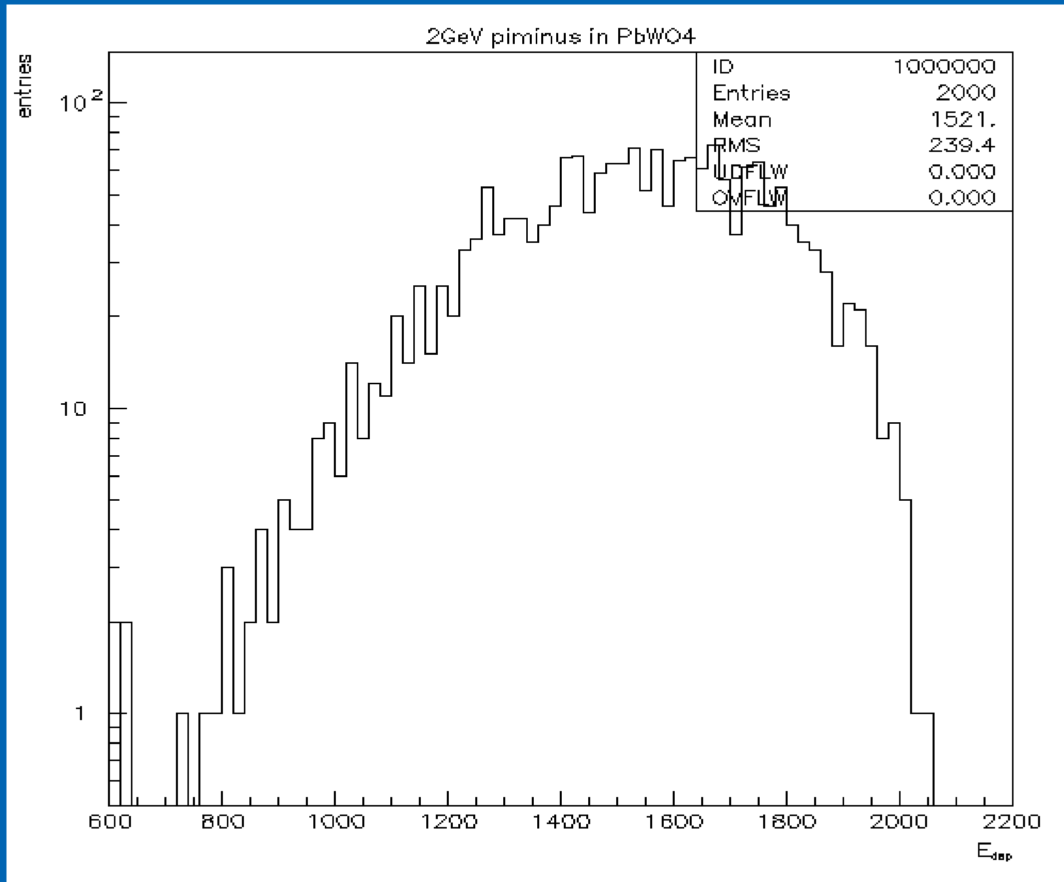
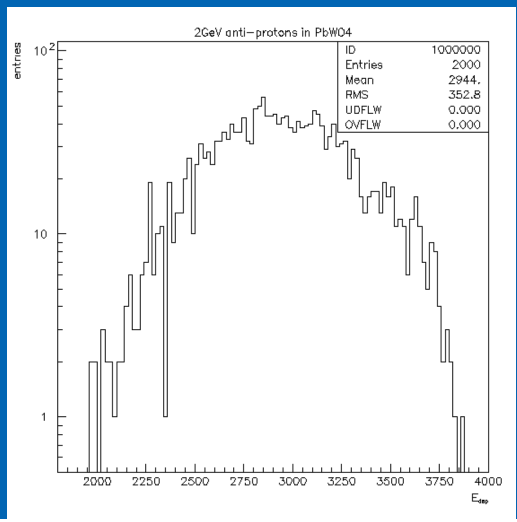
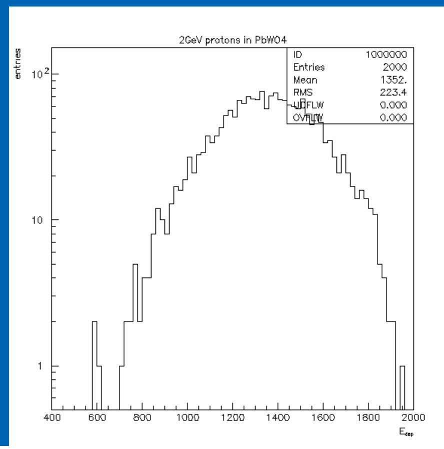
'Trivial' plots energy deposition





BTEV: All distributions are in the expected energy range





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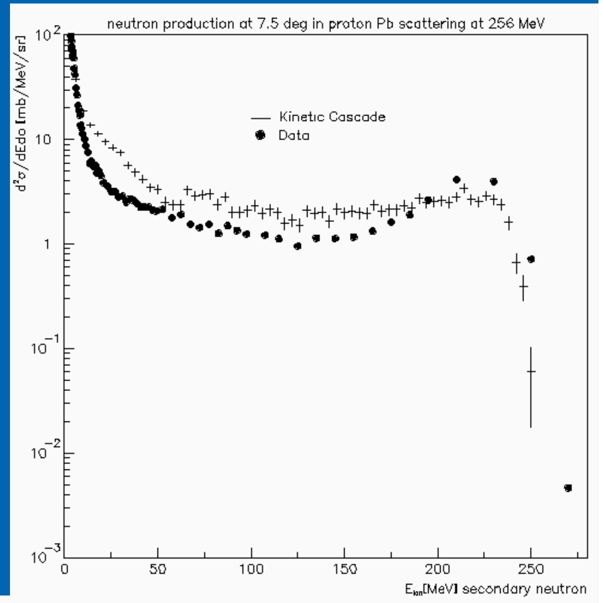
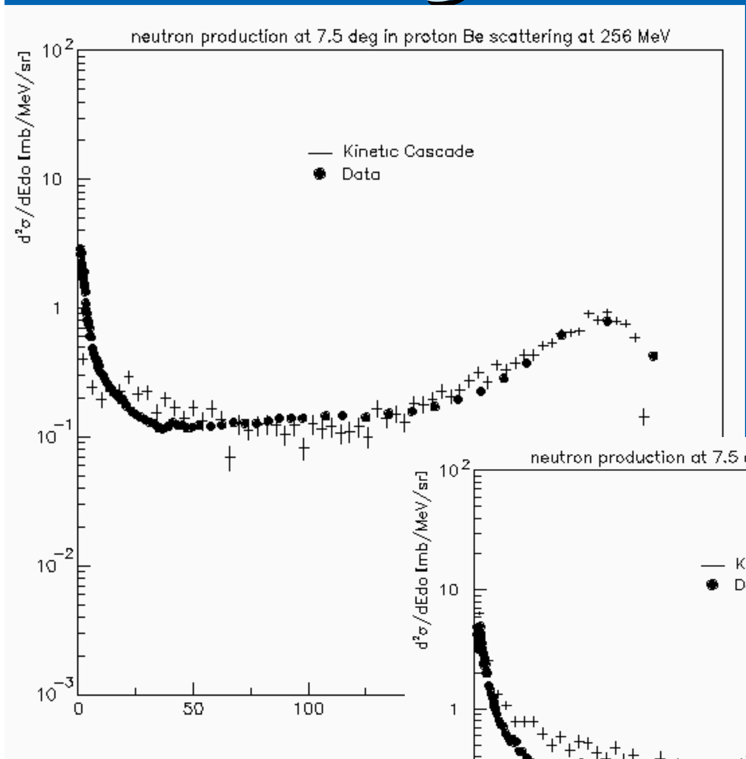
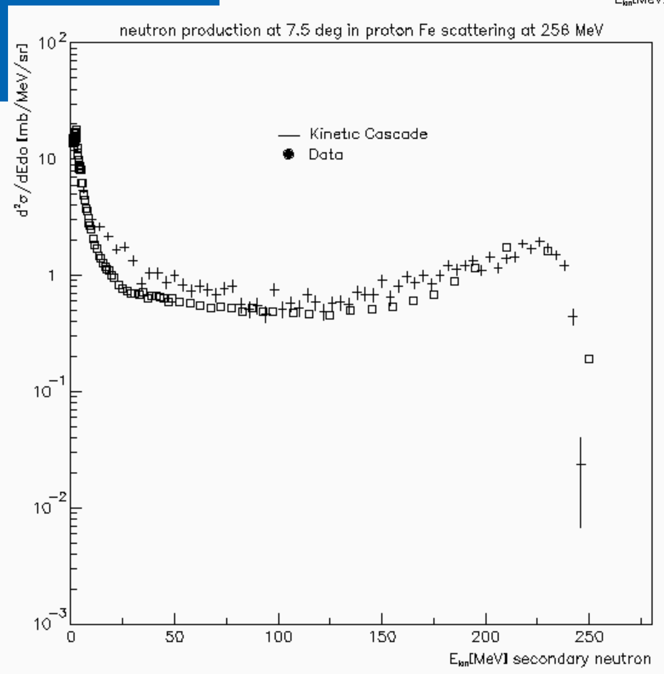
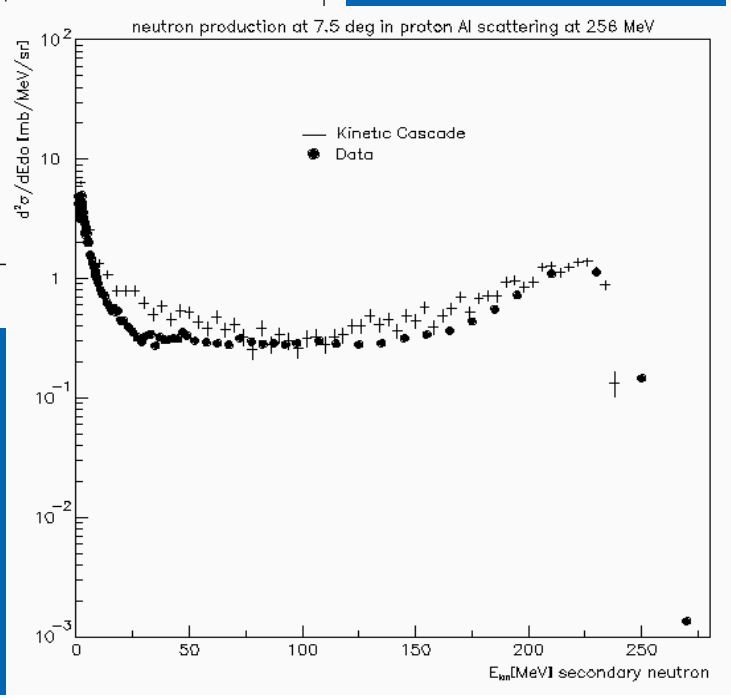
Quasi-elastic peaks in proton scattering









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Validation in complete applications

- Independent validation on benchmarks, where these are available
  - Verified before every release.
- Validation on full simulation programs
  - The validation projects

Benchmark comparisons

- Validation on benchmarks
  - Test-beam simulations
    - Two test-beam simulations in regression
    - Both run prior to each release, to verify model performance.
  - Radiation benchmarks
    - Currently considering two radiation benchmarks
      - Tiara,
      - SATIF-6 and NEA 'standard' benchmark comparisons
  - Experiencing a continued influx of manpower to extend and standardize this further.

Radiation benchmarks – example

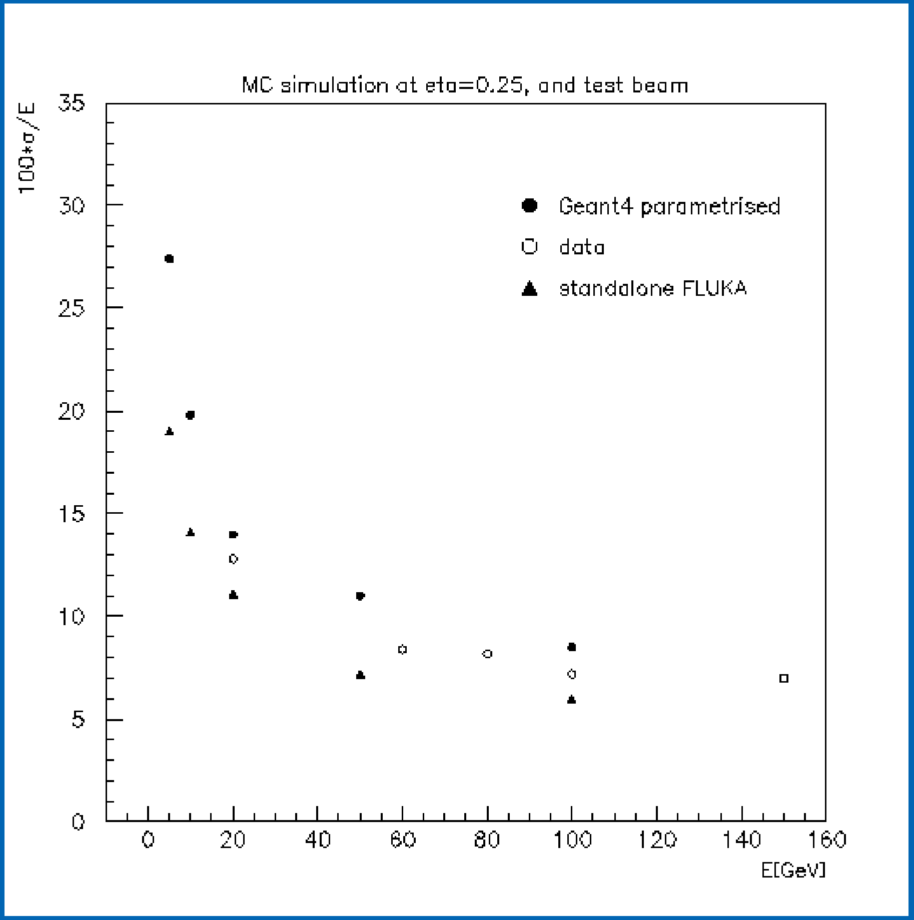
- Tiara - low energy neutron penetration schielding.
  - 43 or 68 MeV (peak) neutron source
  - Use 25cm or 50cm of concrete shielding, or 20 cm or 40 cm of iron shielding
  - Measure neutron flux at beam-axis, and 20cm or 40 cm off beam axis.
- Skipping this is favor of test-beam comparison.

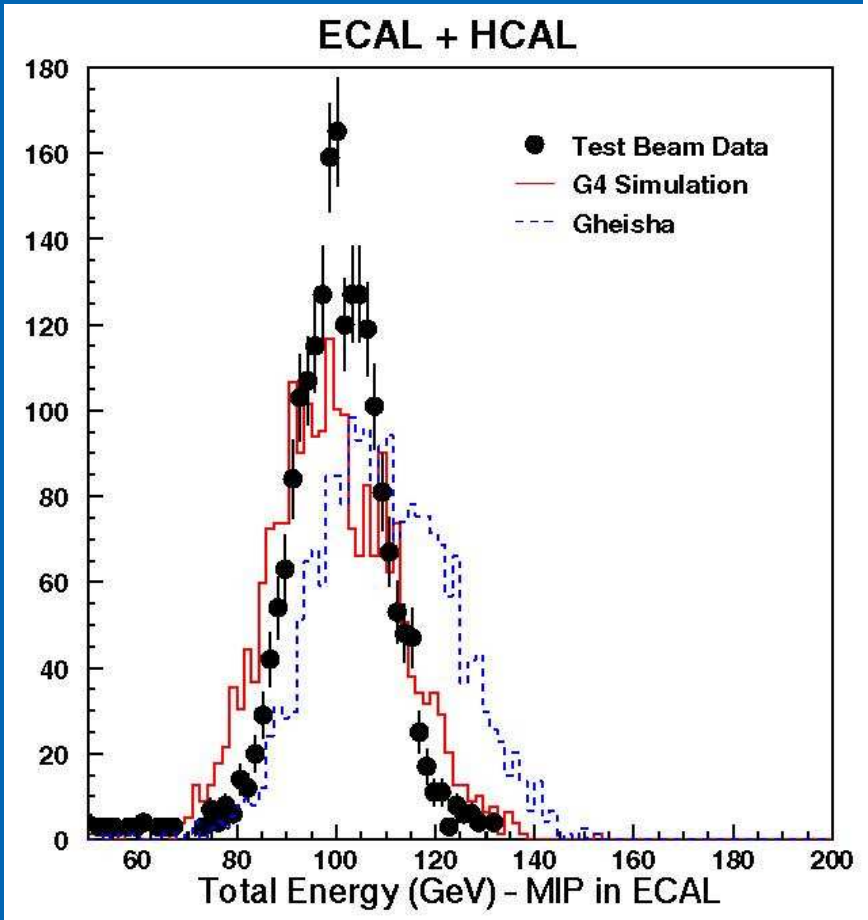
Test-beams

- Hadronic test-beam comparisons come from collaboration of experiments’ detector groups with ‘core’ geant4 personnel.
  - ATLAS Tile test-beam
  - CMS Tile test-beam
  - ATLAS HEC test-beam
  - ATLAS FCAL test-beam
  - BTEV crystal test-beam
  - CMS combined test-beam
  - CsI test-beam benchmark
  - GLAST (starting) test-beam

  - Plots being solicited as courtesy of the experimental groups.

Test-beam sample result





Courtesy of ATLAS TILE prelim.

Courtesy of CMS prelim.

A test beams study in regression

- ATLAS HEC as a calorimeter benchmark set-up
- Detailed description of the detector
  - Very constructive help from the ATLAS calorimeter community
- Analysis: E=E_front + 2E_back
- Results from the ATLAS test-beam analysis are overlaid , and labeled as 'org.'.
- Data are taken from CALOR 2002 paper

The physics lists studied in test-beam

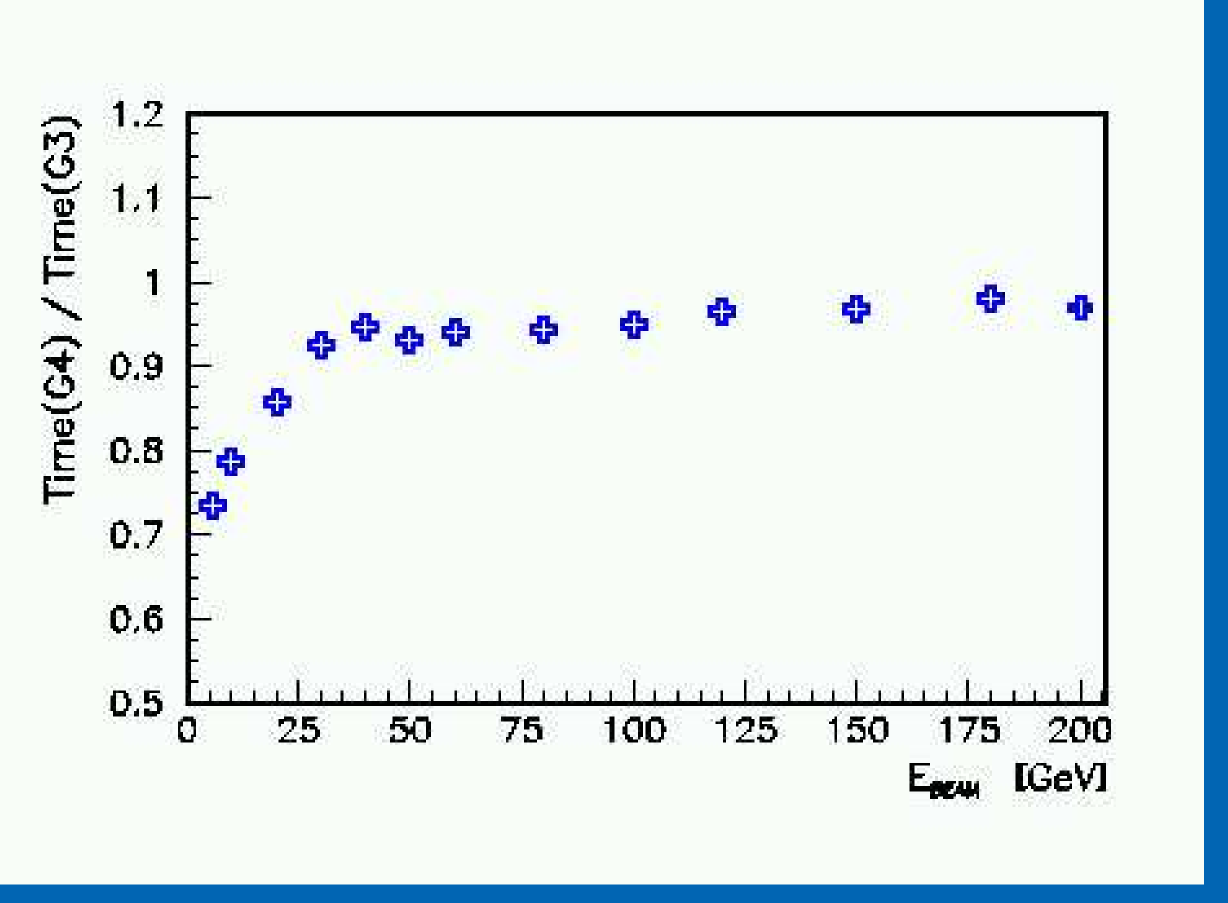
- The physics lists used:
  1. Low energy and high energy parameterized models (LHEP) – check against ATLAS test-beam analysis
  2. Pion inelastic scattering final states simulate with quark gluon string model (first interactions)+chiral invariant phase-space decay (fragmentation) (QGSC)
  3. Pion inelastic scattering final states simulate with quark gluon string model+precompound model (QGSP)
  4. Pion inelastic scattering final states simulate with diffractive string model+precompound model (FTFP)

The overall parameters

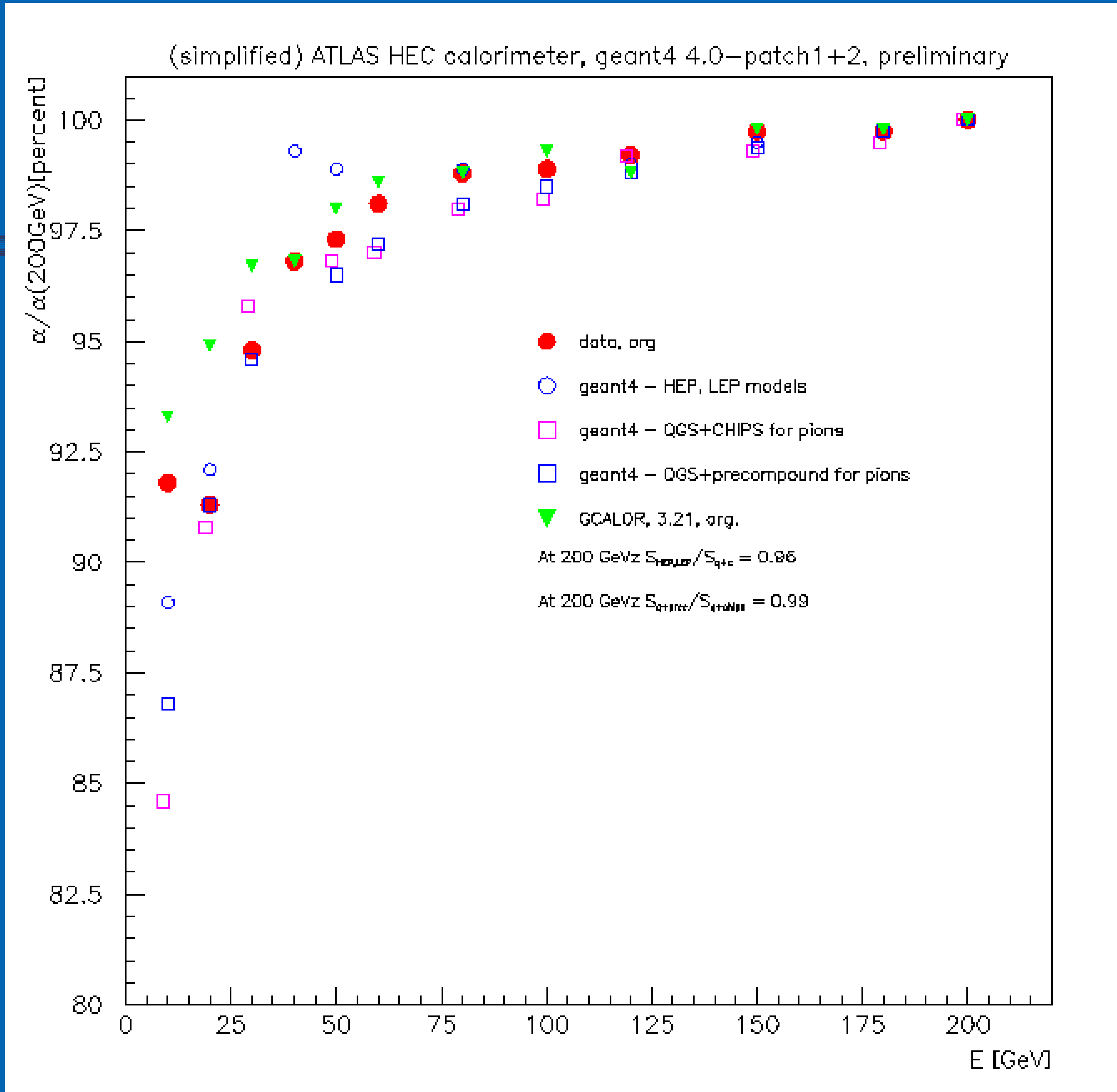
- Geant4 version:
  - geant4 4.0 patch 1+2; no tuning
- Energies:
  - 10, 20, 30, 40, 50, 60, 80, 100, 120, 150, 180, 200 GeV pions and electrons
- 700 microns range cut
- 2000 events per ‘point’

- Looking at performance, linearity, shower shape, energy resolution, and e/pi

Relative timing of geant3 and geant4 for pion test-beam



ATLAS HEC, CALOR 2002



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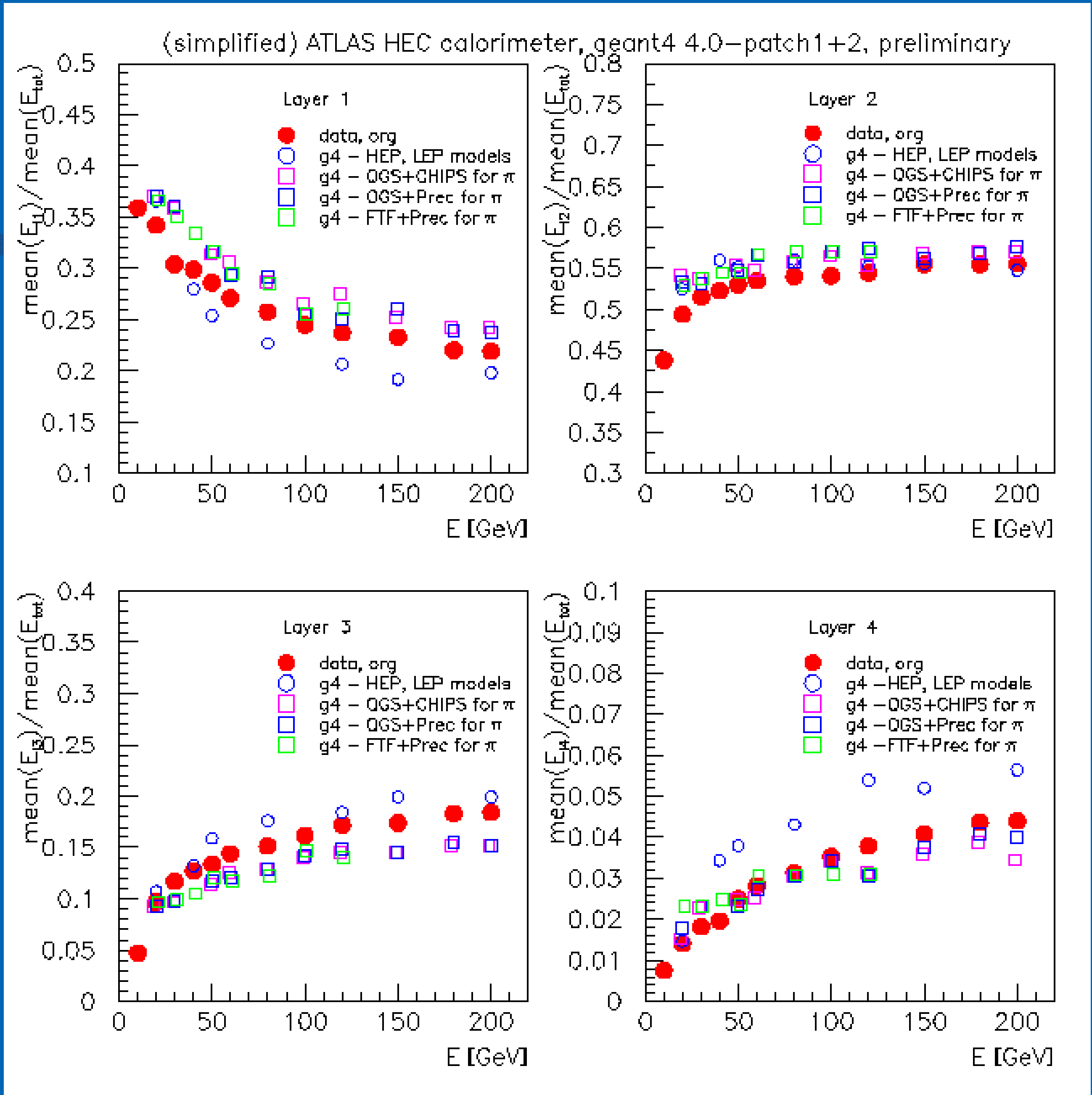

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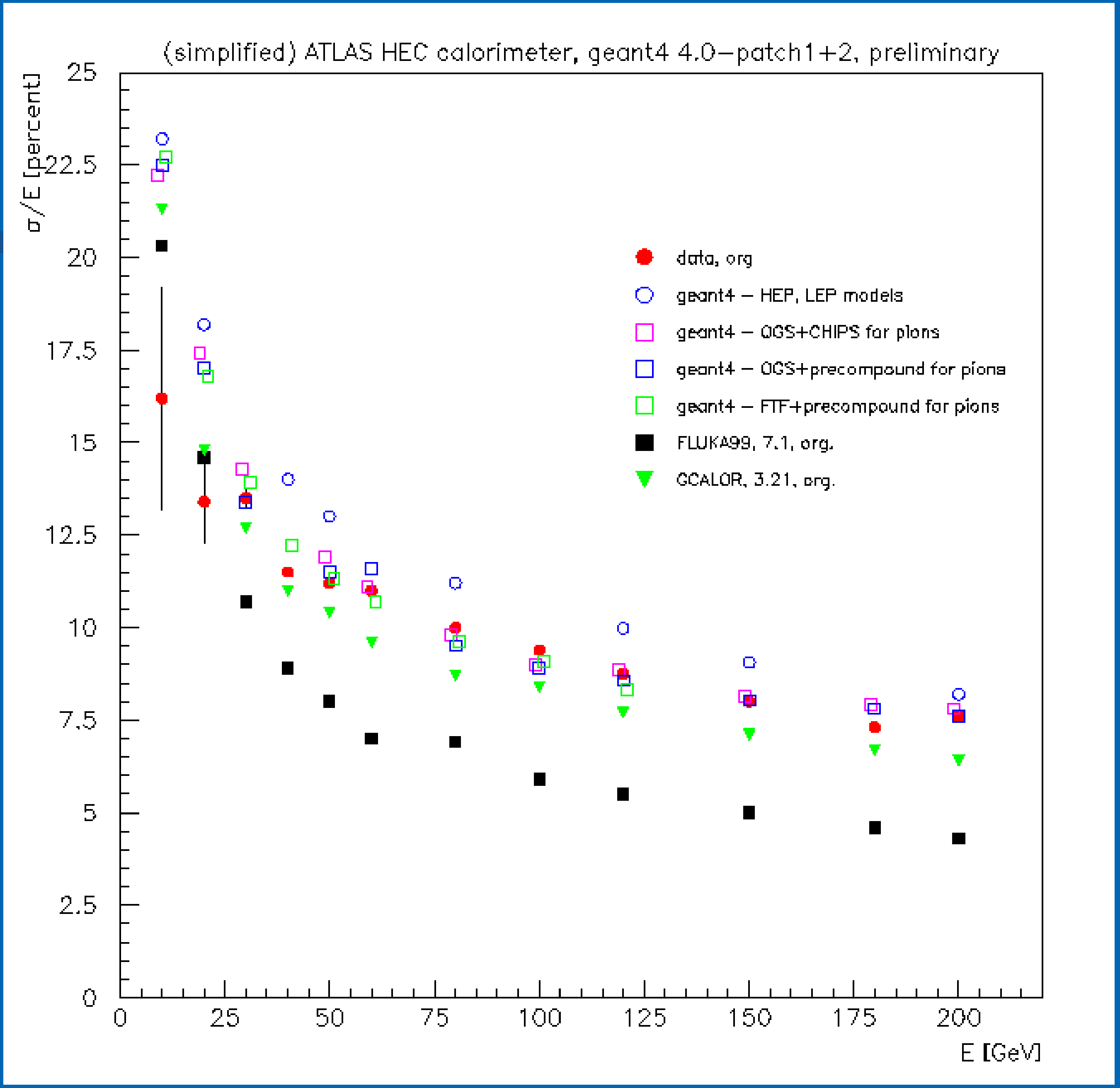

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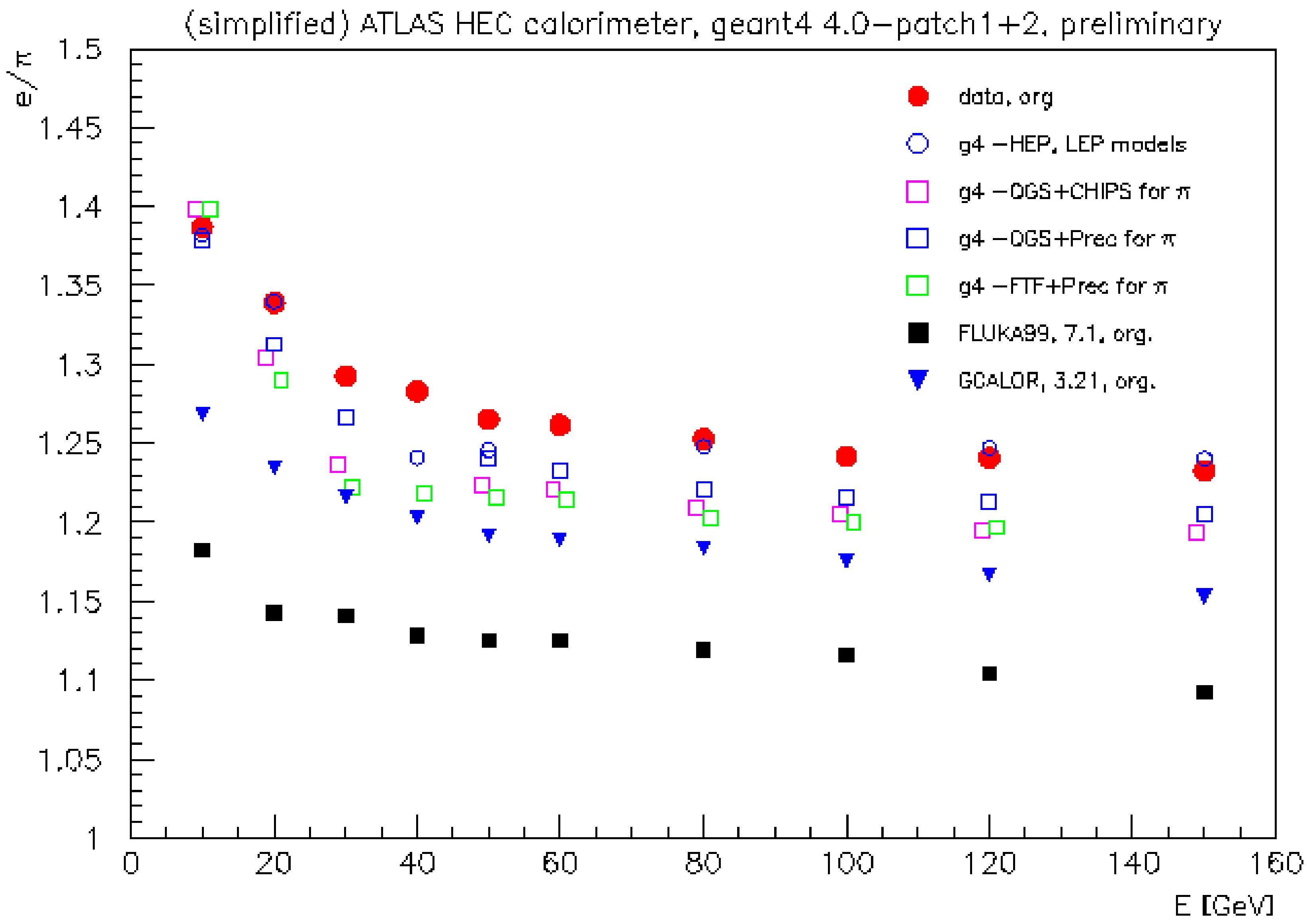

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Other areas of known usage (likely incomplete)

- Tracker performance
  - ATLAS, CMS, BaBar
- Medical
  - Uppsala, TERA, Univ Mass., etc..
- Neutron dosimetry, measurement, beam-lines
  - SNO, Los Alamos, CERN/PS, DoD/Can, etc..
- Radiation schielding, activation, thermalization
  - DYNAMIX, MECO, ALICE?, CMS, ESA, etc..
- Oil search and similar
  - Mitsubishi, General electrics, EXXON, ALCATEL…

Collaboration with 3rd parties
Some of the reasoning:

- Geant3 had used two strategies. There were shower packages released with geant3, and there were interfaces released with geant3; the latter were interfacing to external packages. The first was a working model, for the latter, geant3 was always claimed to be obsolete.
- GISMO: the no physics situation, but only interfacing to external packages. They never really got support for the use of these codes with GISMO.
- MCNPX: Gets it right. They encourage and help 3rd parties to release MCNP interfaces with their 3rd party code. It solves the support question.

Collaboration with 3rd parties

- Basis: We provide a set of well defined, published, and highly stable interfaces that allows interested 3rd parties to release adapters to use their code, or to use geant4 physics implementations within their infrastructure.
- EGS: geant4 chips code for γ-nuclear reactions also in EGS
- HETC: Being re-written to become natively available in G4
- INUCL: Being integrated to become natively available in G4
- UrQMD: In the process of being re-engineered to become natively available in geant4
- MCNP: Discussion on using the geant4 interfaces in MCNP
- G-FLUKA: Interfaced by 'air shower' users for their own use.
- Liege Cascade code: Discussion in progress at the technical level.