Simulation of the production of radionuclides using Geant4

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on behalf of the Geant4 collaboration

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Outline

Geant4

- Brief overview of hadronic processes of Geant4

Results for production of radionuclides

- Validation against measurement of radioactive products induced in copper by high-energy heavy ions

Testing performance of multi-threaded application

Summary

What is Geant4

A ***toolkit*** for the simulation of the passage of particles through matter.

Widely used in detector simulation of various kind of physics experiments from scale of LHC to desktop

Also used in space sciences, medical applications, reactor kinematics and many other fields

We have participated in the ”Inter-comparison Problems of Neutron Attenuation” organized by the task force on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF), and has proven its capability in the area since 2006

Geant4 10.01

The latest version of Geant4 is 10.01

- Patch Geant4.10.01.p01 was released the end of Mar 2015.
- All validation plots are calculated on this version.

Multi-threading

- This release includes support for multi-threaded Geant4 applications.
- Parallelism is achieved at the event level, with events dispatched to different threads.
- The default build of Geant4 is still sequential.

Hadronic Processes, Models and Cross Sections

In Geant4 physics is assigned to a particle through processes

Each process may be implemented

- directly, as part of the process, or
- in terms of a model class

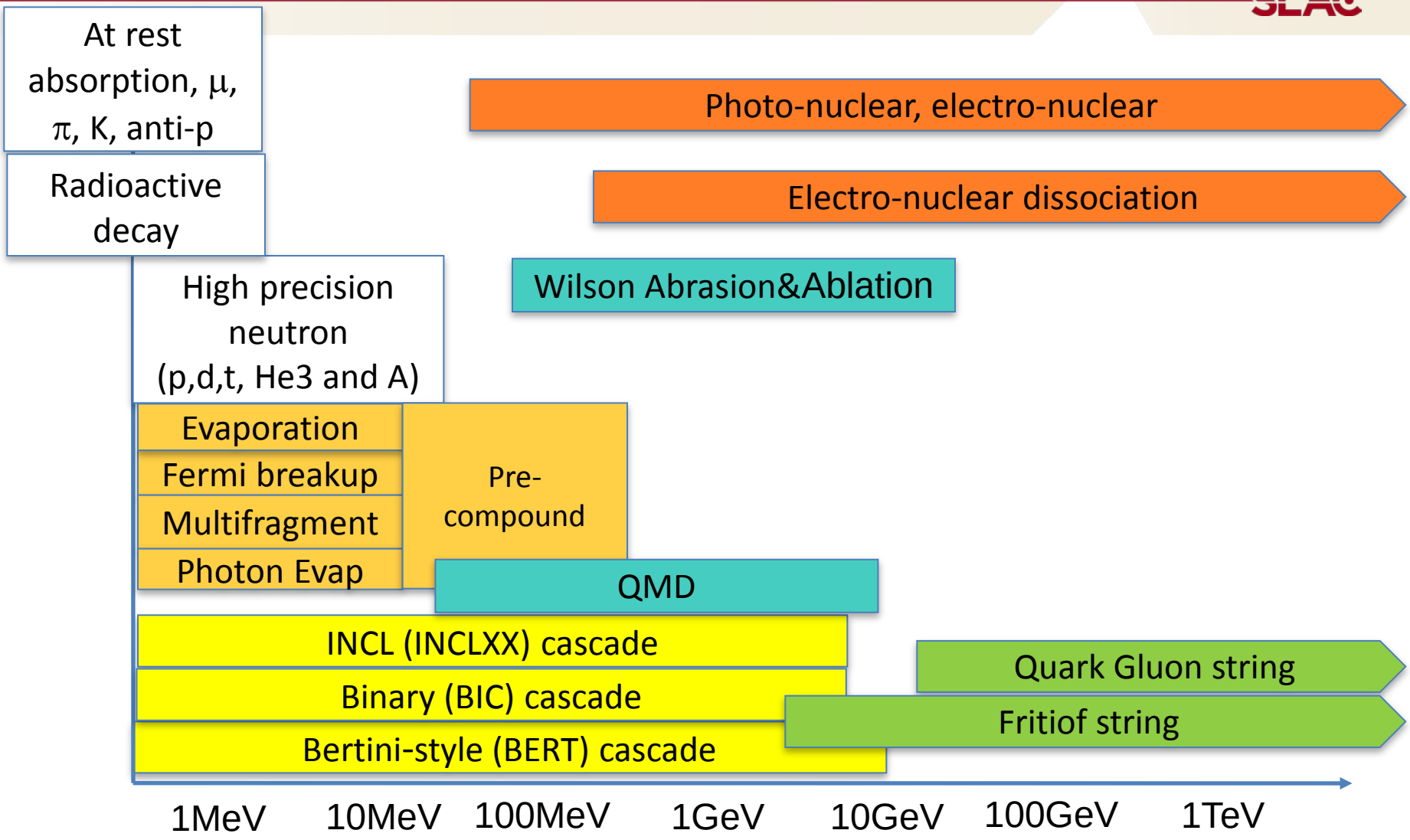
Geant4 often provides several models for a given process

- user must choose
- can, and sometimes must, have more than one per process

A process must also have cross sections assigned

- here too, there are options

Partial Hadronic Model Inventory



High Energy
QCD String Models

Fritiof (FTF) valid for

- p, n, pi, K, Lambda, Sigma, Omega from 3 GeV to ~TeV
- anti-proton, anti-neutron, anti-hyperons at all energies
- anti-d, anti-t, anti-3He, anti-a with momenta between 150 MeV/nucleon and 2 GeV/nucleon

Quark-Gluon String (QGS) valid for

- p, n, p, K from 15 GeV to ~TeV

Both models handle:

- building 3-D model of nucleus from individual nucleons
- splitting nucleons into quarks and di-quarks
- formation and excitation of QCD strings
- string fragmentation and hadronization

Cascade models in Geant4

Bertini-like (BERT)

- Shell structure in target potential

Binary cascade (BIC)

- Optical potential for target and projectile (in light ion cascade)

INCL (INCLXX)

- True potential is not used for projectile nucleus, but binding energy is taken into account
- True potential is used for target

QMD

- Self generate potentials for both target and projectile
- Dynamic in entire stage of reaction

PreCompound and DeExcitation models in Geant4

G4PreCompound model which can work as standalone model in Geant4,

- Also used as post-model for highly excited nucleus produced by high energy and cascade models

DeExcitation models

- G4DeExcitation up to Alpha
- G4GEM (Generalized Evaporation Model) up to Mg

Most cascade model also has own internal PreCompound and DeExcitation model

Specialized models for Low Energy (below 20MeV) Particles

High Precision Neutron (NeutronHP) model and cross section

- Data driven model based on ENDF library
- G4NDL4.5 data library which is equivalent to ENDF/B-VII.1 is distributed from Geant4 web page up to Uranium
- Data from other data libraries (JENDL, JEFF,,,) can be download from IAEA web page in G4NDL format

Thermal Scattering S(alpha,beta) model is also available

ParticleHP

- An enhancement of NeutronHP
- Handling charged particles (p,d,He3 and A) inelastic interactions below 20MeV based on ENDF and/or TENDL library

Low Energy Nuclear Data model and cross section

- New data format and API for generalized description of low energy nuclear reactions.
- ENDL99 and ENDF/B-VII.0 data in the format is available from LLNL web page

Ion interaction

Binary Light Ion Cascade

- Up to carbon either projectile or target

INCL++

- Up to carbon (oxygen?)

QMD

- All combination of projectile and carbon

WilsonAbrasion WilsonAblation EM-Dissociation models

- Based on the NUCFRG2 model (NASA TP 3533)

Interface for external reaction model

- DPMJET (will be dropped soon)

Radioactive decay model in Geant4

Process to simulate radioactive decay of nuclei

- α, β+, β-, γ decay and electron capture (EC) implemented
- Both in flight and at rest decays are supported

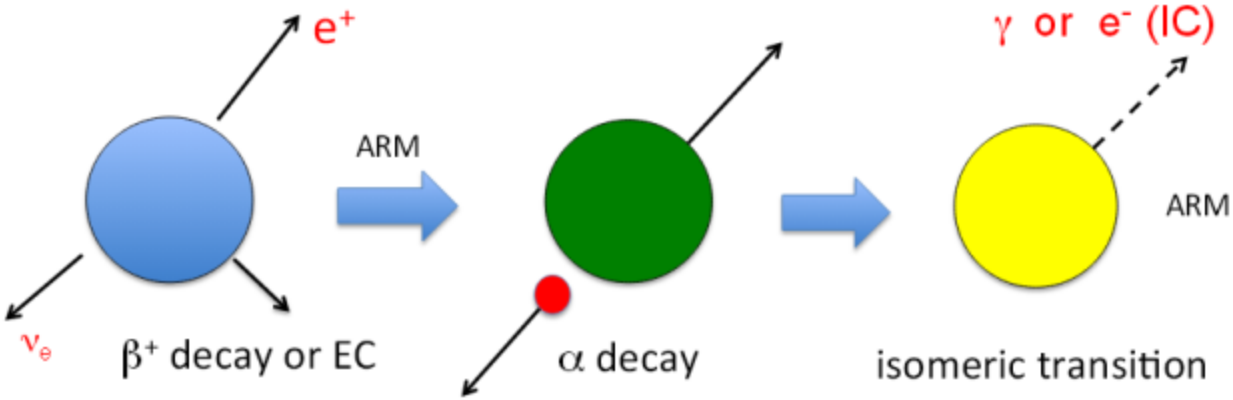
Empirical and data--driven

- Data files taken from Evaluated Nuclear Structure Data Files (ENSDF)
- half lives, nuclear level structure for parent and daughter nuclides, decay branching ratios, energy of decay process
- currently 2792 nuclides, including all meta-stable states with lifetimes > 1nsec for α, β+, β- and EC
  - Does not include γ decay in which smallest time is 1psec

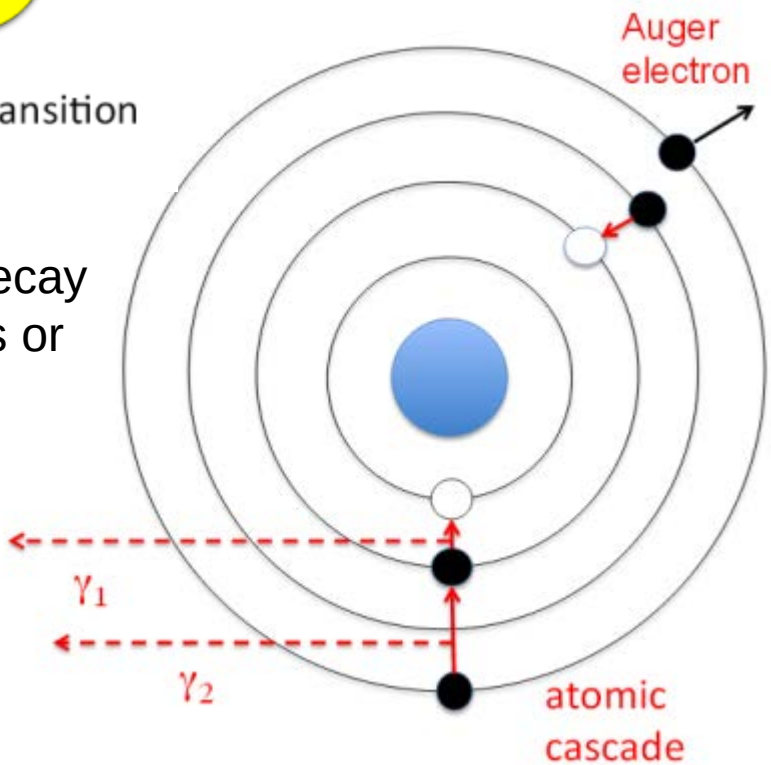
Sampling Radioactive Decay

- Analog (non-biased) sampling is default
- Biased sampling also implemented
  - enhance particular decays within a given time window
  - sample all decay modes with equal probability
  - Split parent nuclide into a user-defined number of copies, letting each decay
  - enhance emission in a given direction

Radioactive decay chain and atomic relaxation model (ARM) in Geant4



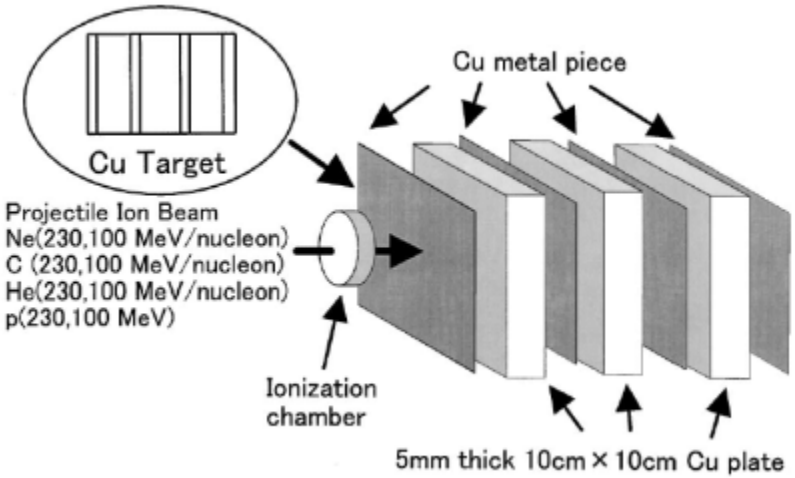
Electron shell configuration may change after decay
inner holes filled by atomic cascade either photons or Auger electrons are emitted
fluorescence option also available



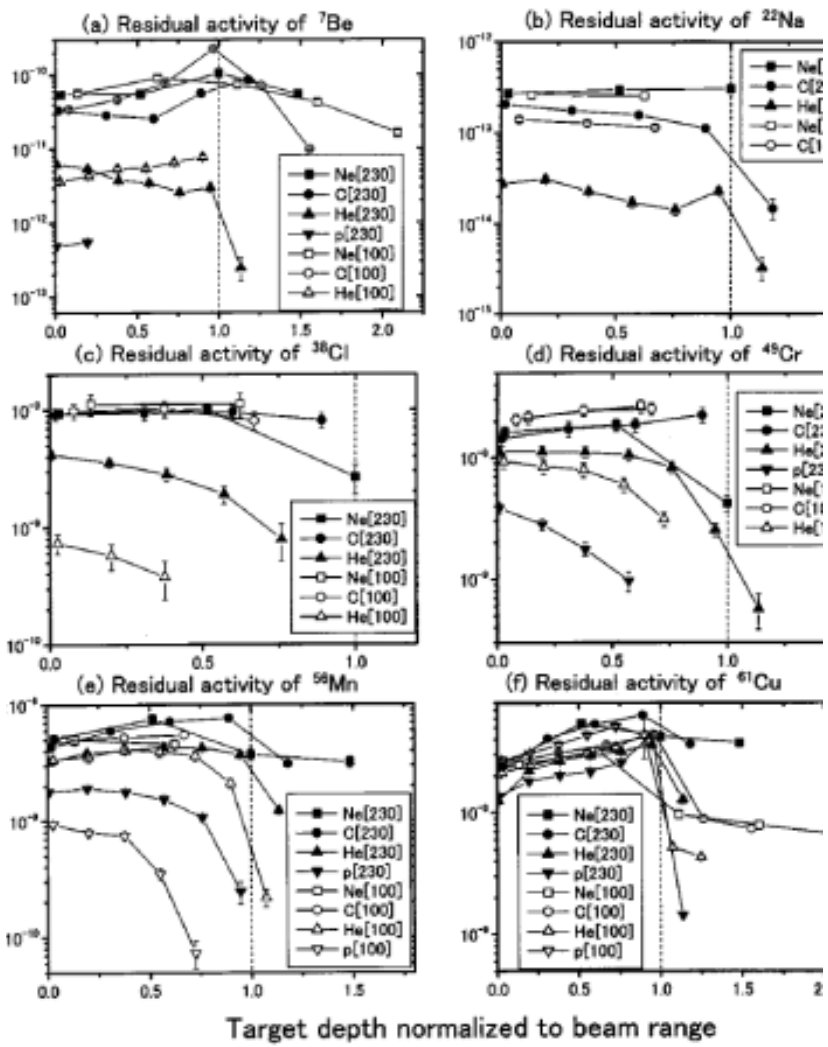
Data used for this benchmark

Measuring radioactive spallation products in a thick Cu target were obtained for 230 and 100 MeV/nucleon Ne, C, He, and p ions.

"Projectile dependence of radioactive spallation products induced in copper by high-energy heavy ions" Yashima H. el al, PHYSICAL REVIEW C 66, 044607



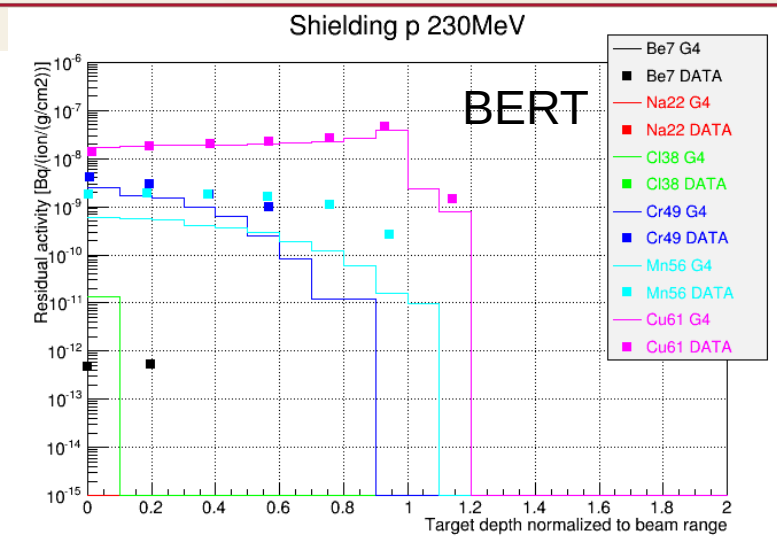
Residual activities of various nuclides

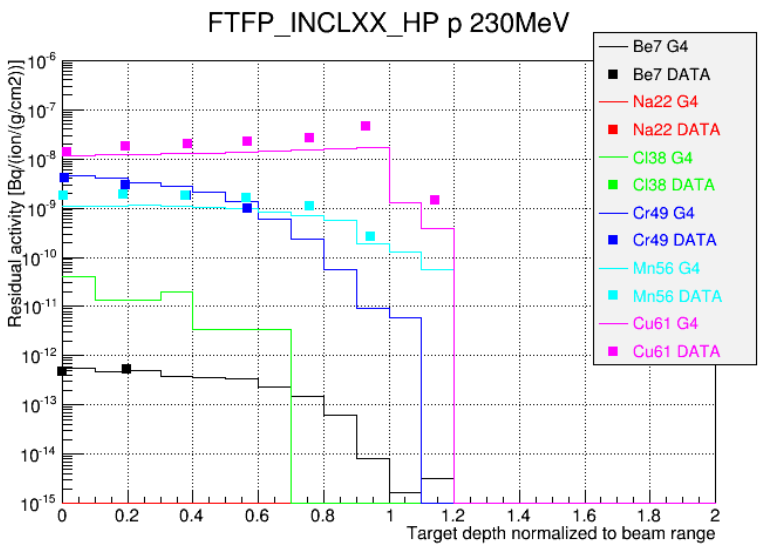


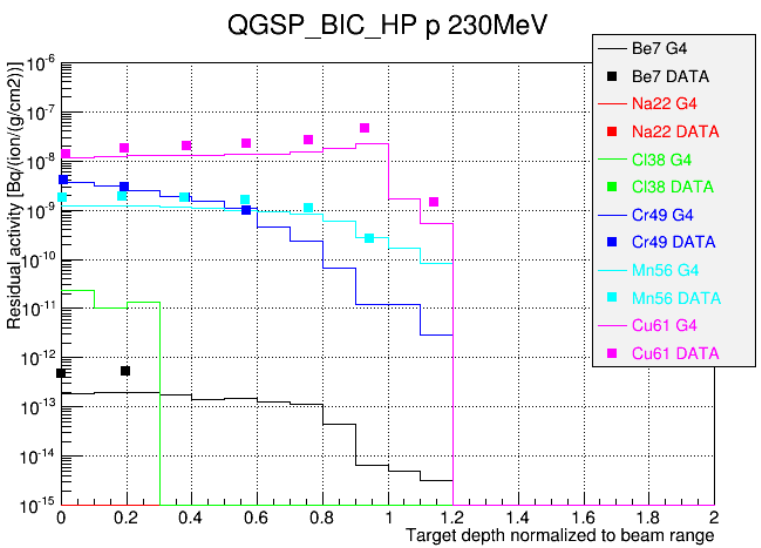
Residual nuclides	Type of Yield	Gamma-ray energy [keV]	Branching ratio [%]	Half-life
7Be	*I*	477.61	10.5	53.29*D*
22Na	*C*1	1274.53	99.9	2.6019*Y*
38Cl	*C*2	1642.71	31.9	37.24*M*
49Cr	*C*1	90.64	53.2	42.3*M*
56Mn	C2	1810.72	27.2	2.5785*H*
61Cu	*C*1	282.96	12.2	3.333*H*

I :independent
*C*1:cumulative positron
*C*2:cumulative electron

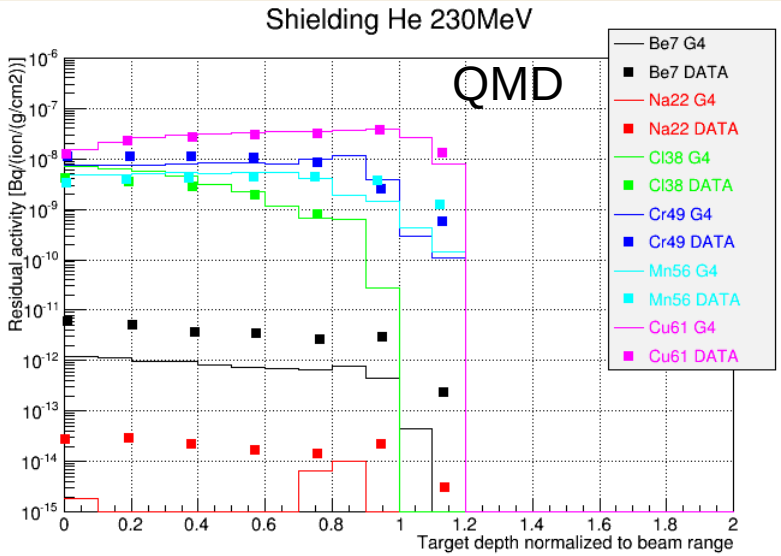
Depth distribution of residual activities in Cu target Proton 230MeV

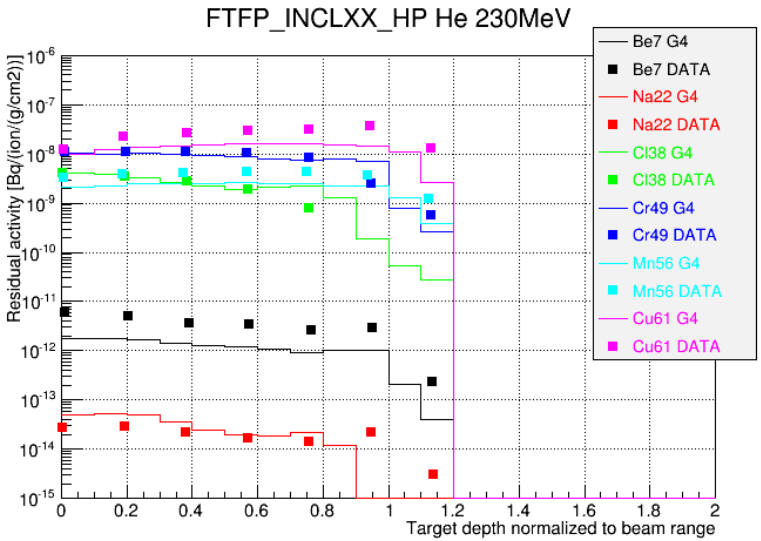


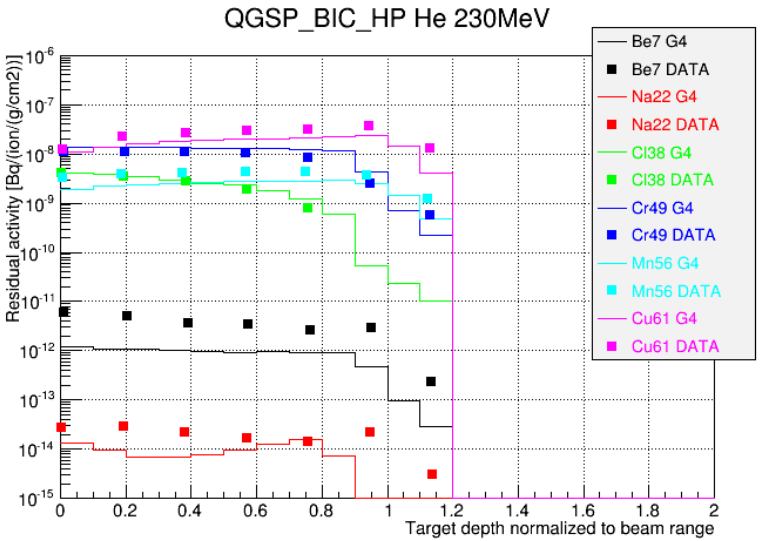




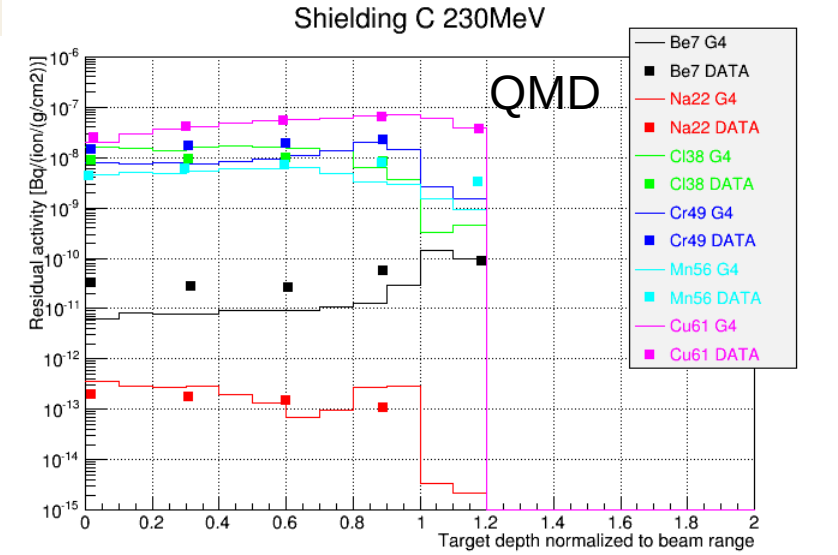
Depth distribution of residual activities in Cu target Helium 230MeV/n

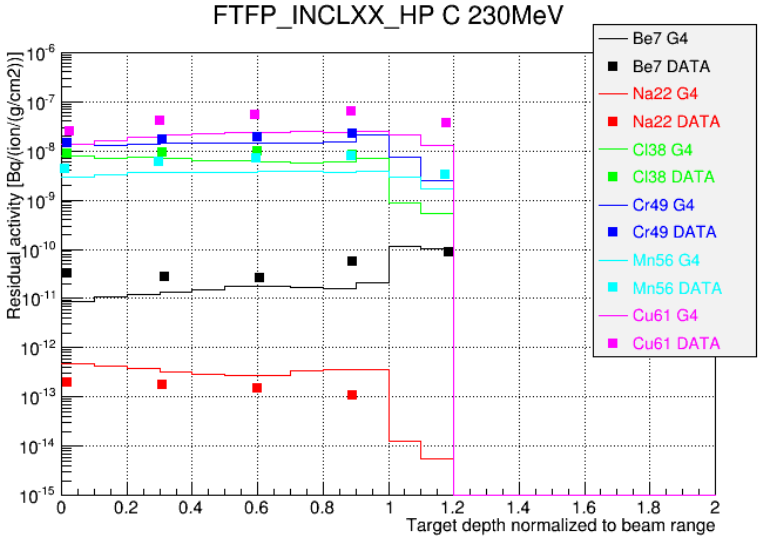


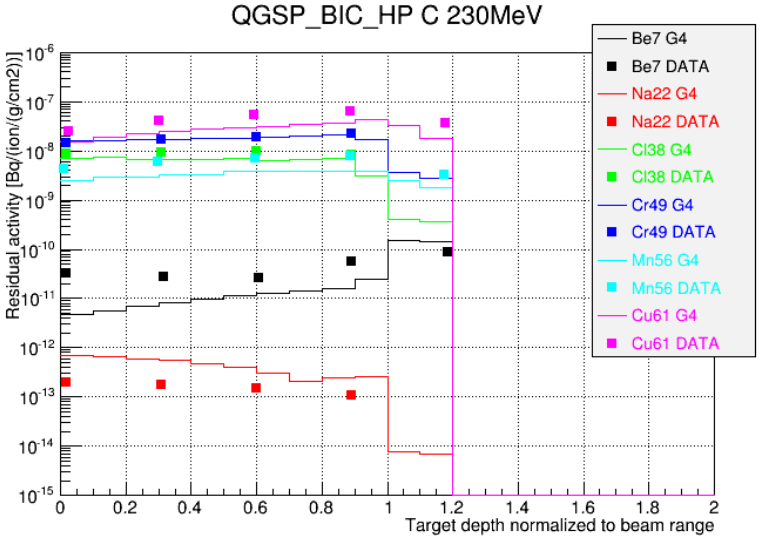




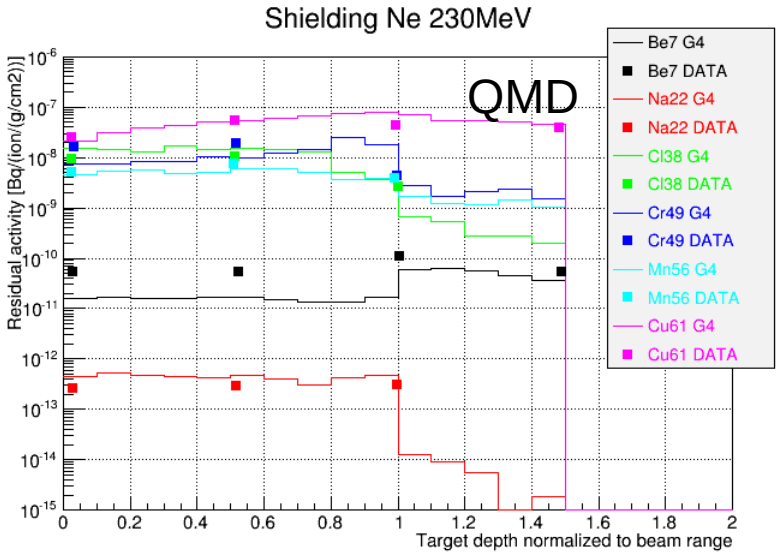
Depth distribution of residual activities in Cu target Carbon 230MeV/n

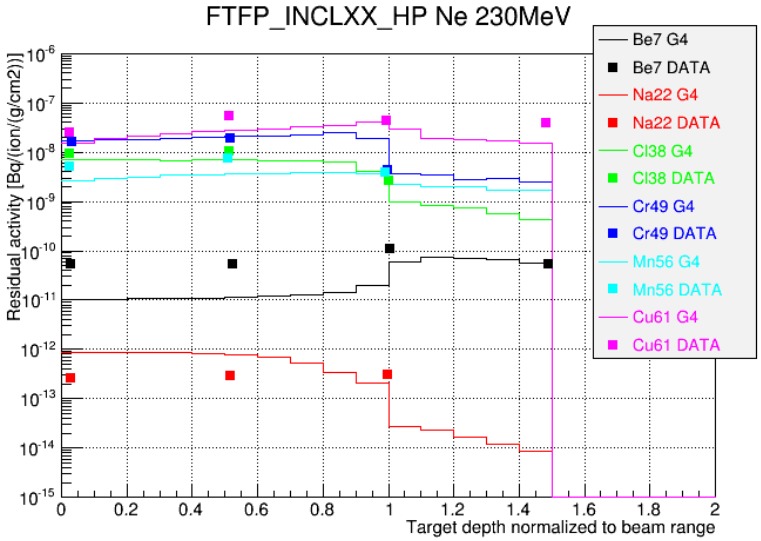


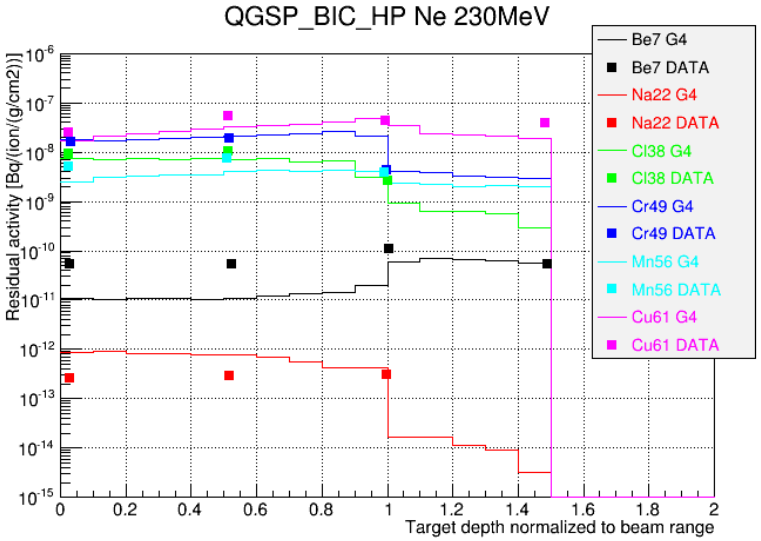




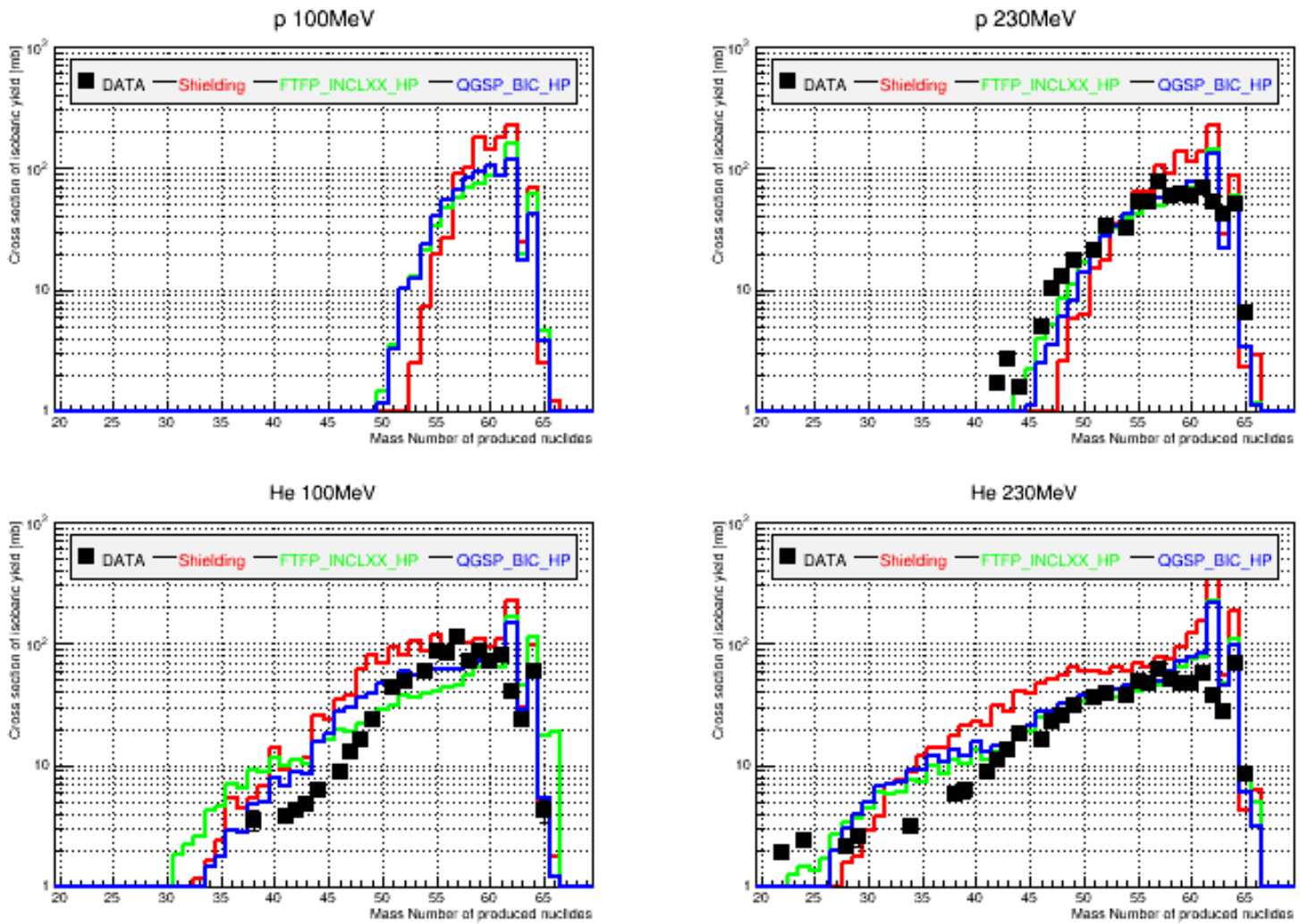
Depth distribution of residual activities in Cu target Neon 230MeV



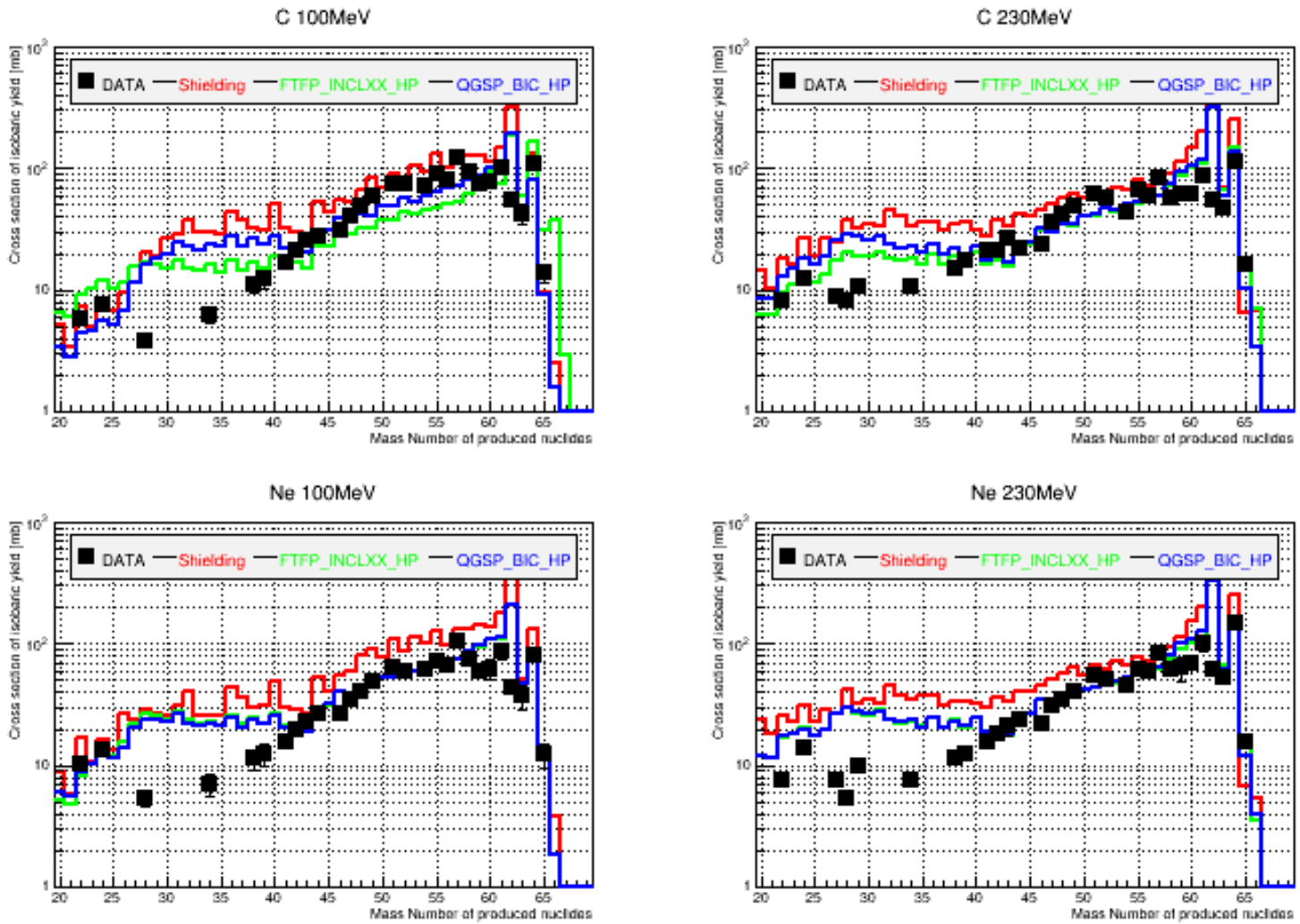




Comparison of mass yield curve to measurement
Proton and Helium projectiles



Comparison of mass yield curve to measurement Carbon and Neon projectiles



Geant4 MT

Geant4 supports (optional) event-level parallelism for multi-threaded application since version 10.00 (released in 2013 Dec).

- In a multi-threaded application, at the end of first kernel initialization, worker threads are started and initialized.
- These worker threads are responsible for simulating events.

The objects that consume the largest fraction of memory (geometry and static physics tables) are shared among threads, while all other objects (in particular user-action and sensitive detectors) are thread-private.

- Exploits full performance of multi-core CPU(s) with less memory consumption

Testing MT performance on application for production of radioactive nuclides

CPUs

- Intel(R) Xeon(R) CPU E5-2620 v2 @ 2.10GHz x 2
  - total 12 physical core

Memory size

- 32GB

OS

- CentOS release 6.5 64bit

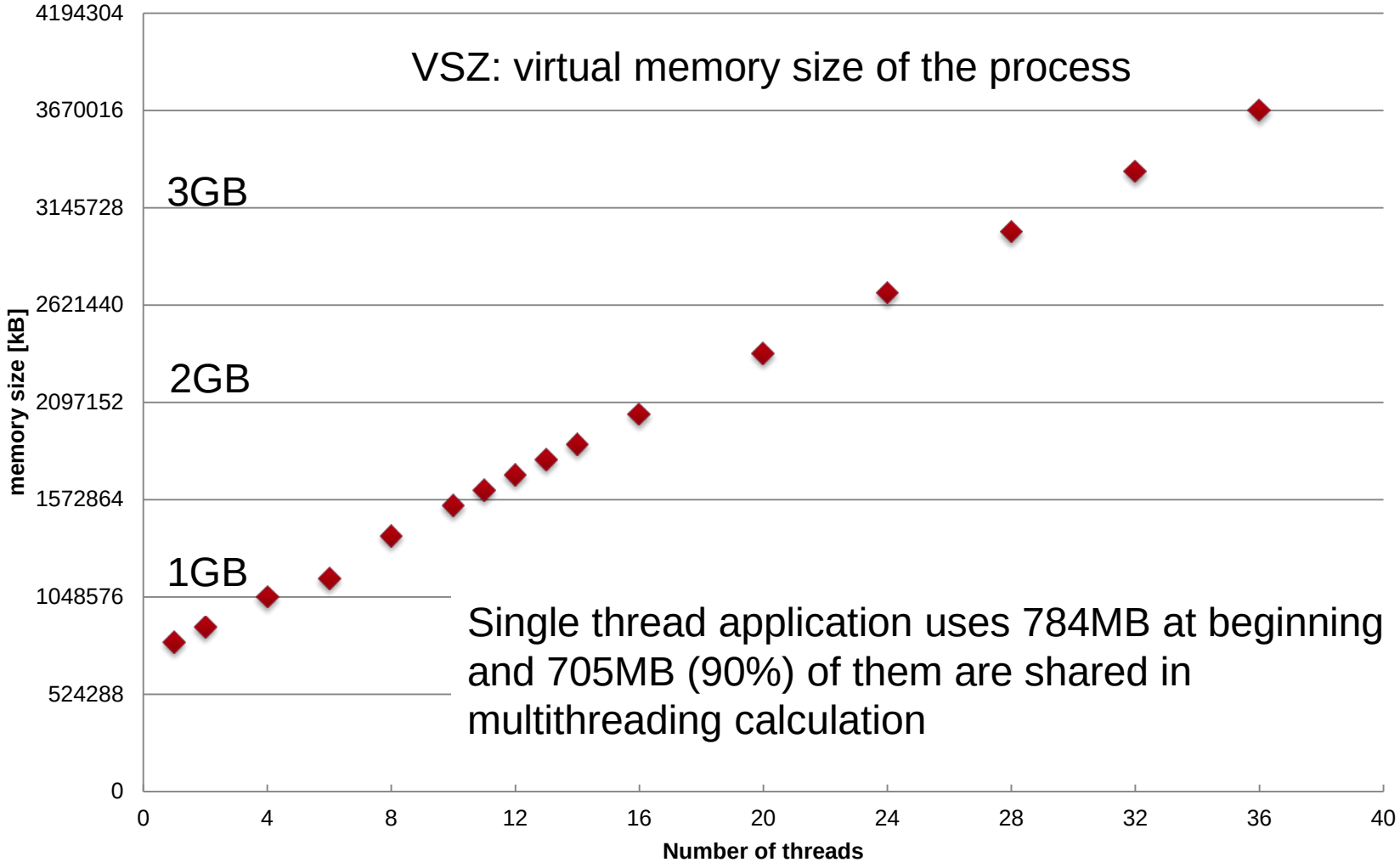
Compiler

- gcc 4.4.7

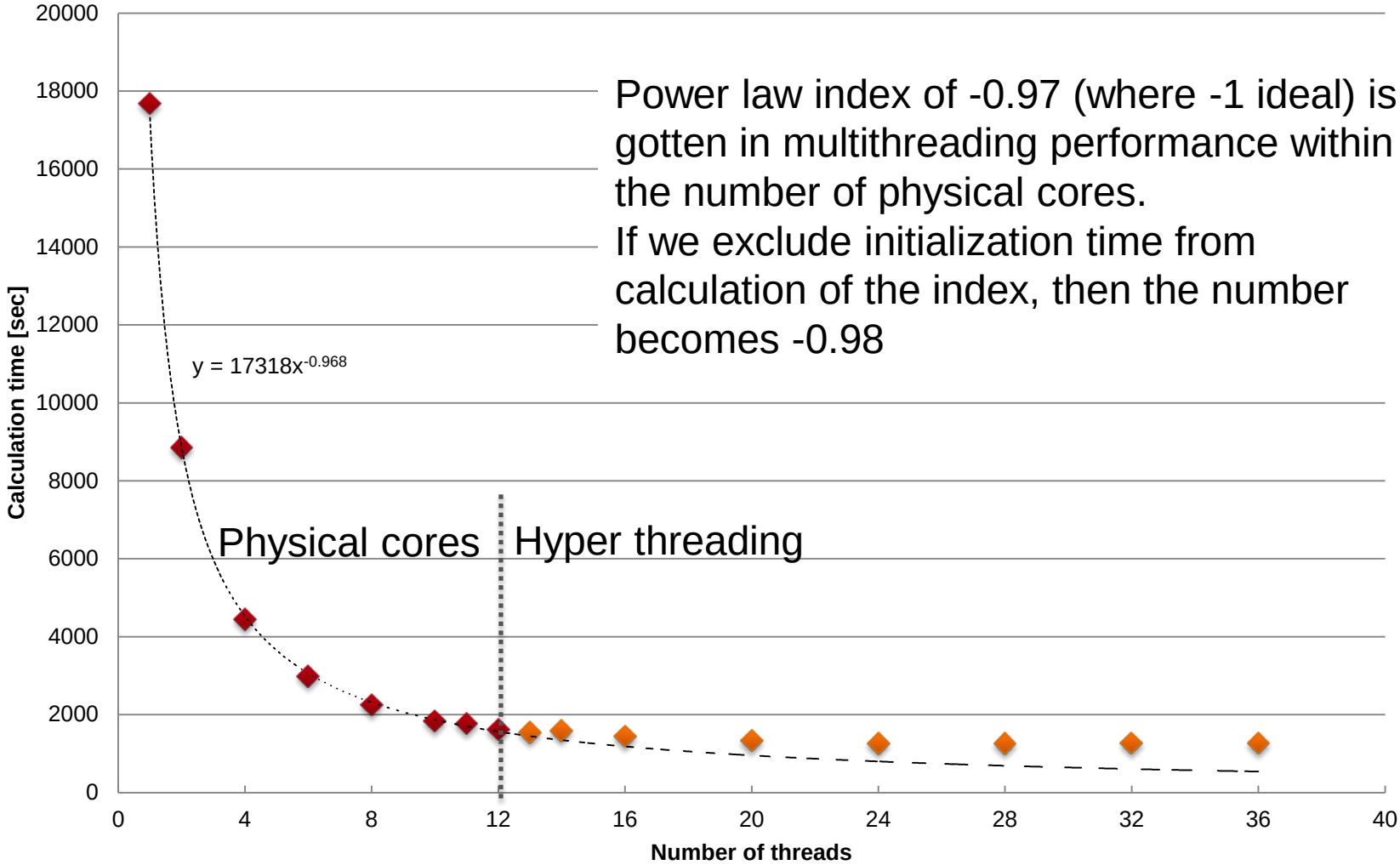
Testing application

- Multi-threaded application for production of radioactive nuclides on Geant4 v10.01.p01
  - 256k events of 230MeV/n Carbon bombarding Cu target

Memory consumption

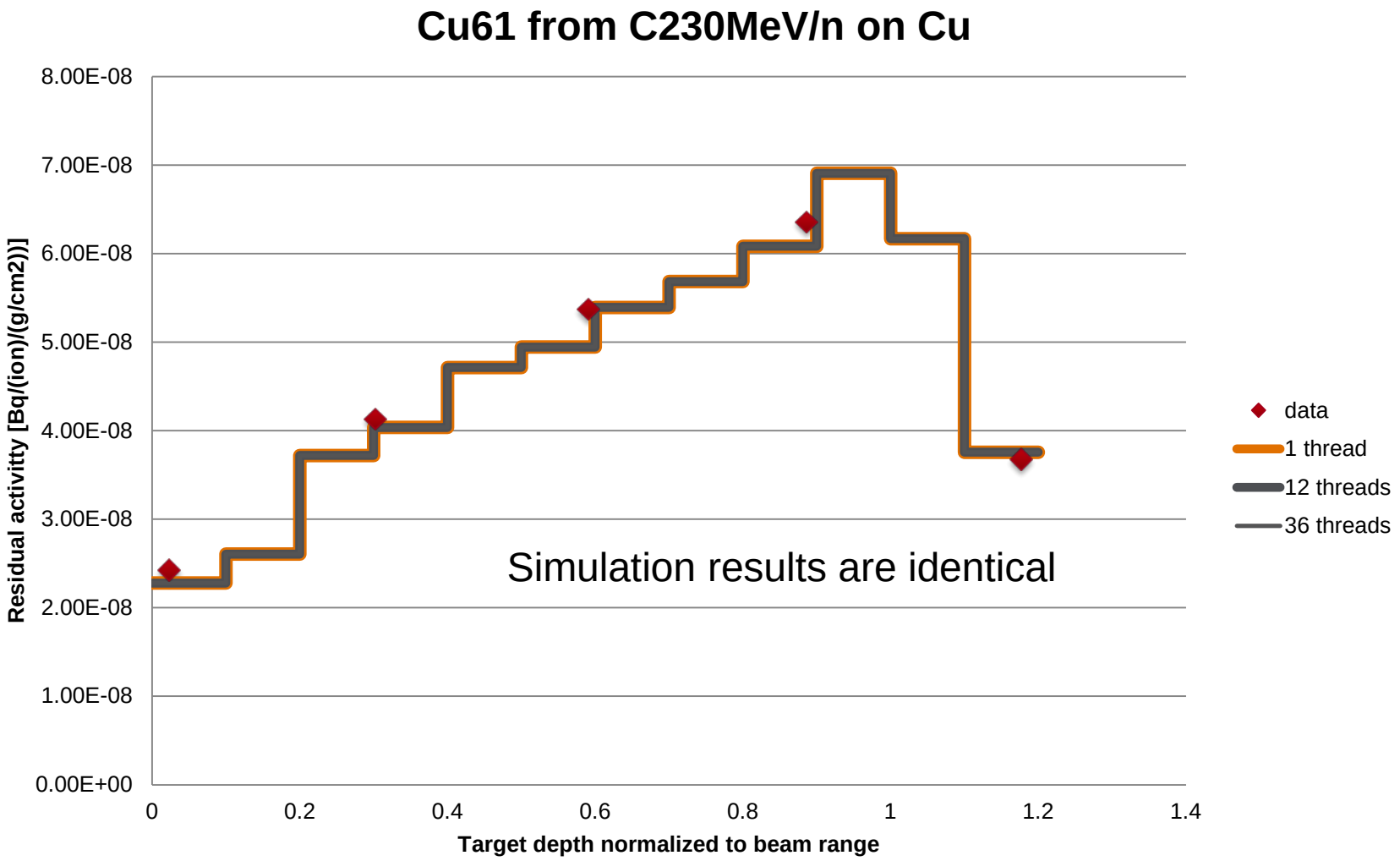


Computing Performance



Power law index of -0.97 (where -1 ideal) is gotten in multithreading performance within the number of physical cores.
If we exclude initialization time from calculation of the index, then the number becomes -0.98

Physics Performance



Summary

Geant4 is a toolkit for the simulation of the passage of particles through matter.

- Provide multiple choice for users in many aspects

A validation against measurement of radioactive products induced in copper by high-energy heavy ions is shown

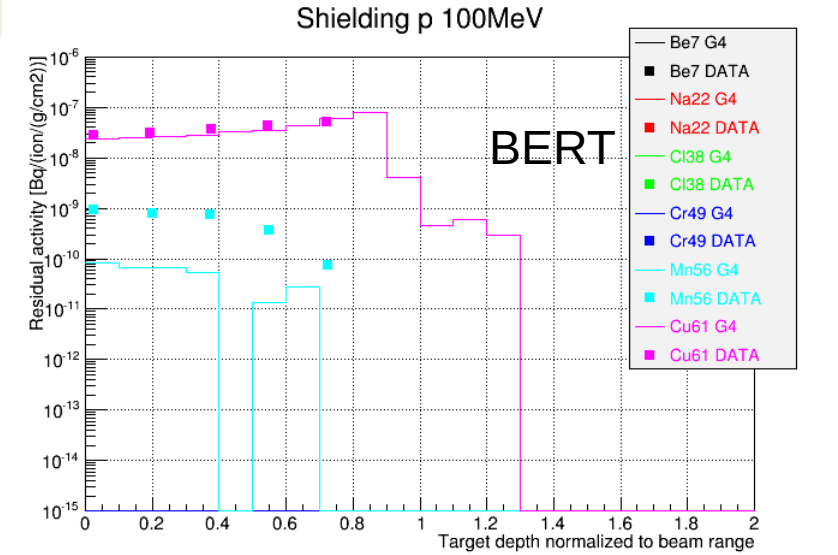
- Getting reasonable agreements to measurement in all models
- ***We are happy to provide other validations***

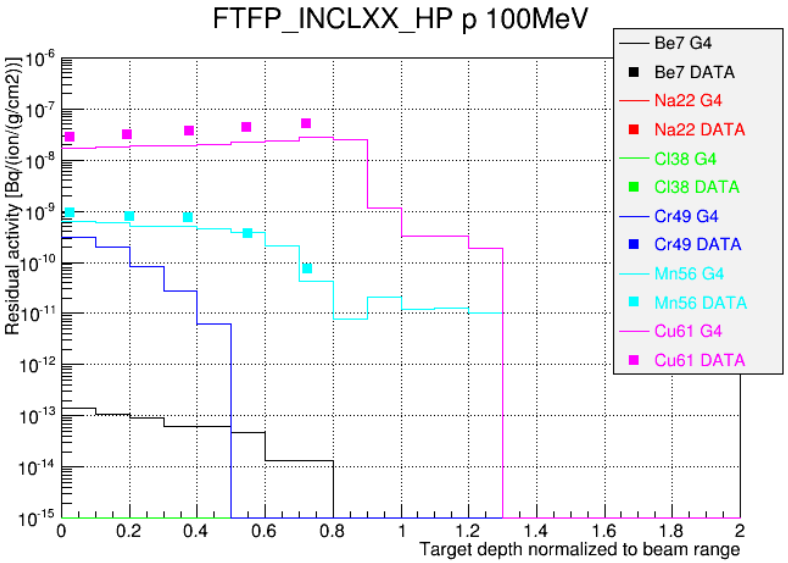
Tested performance of multi-threaded application for production of radioactive nuclides

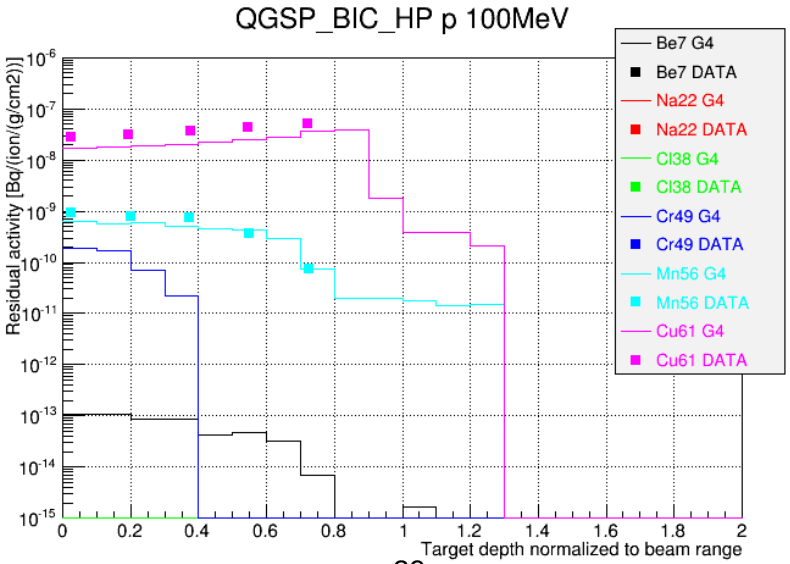
- Getting very good computing performance both in CPU and memory consumption with unchanged physics performances
- An easy way to use full power of your machines

Appendix

Spatial distribution of residual activities in Cu target Proton 100MeV







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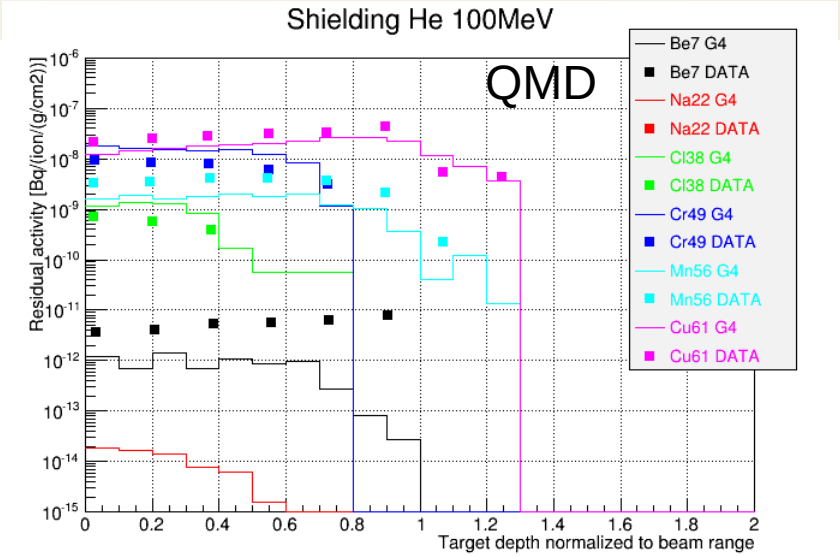
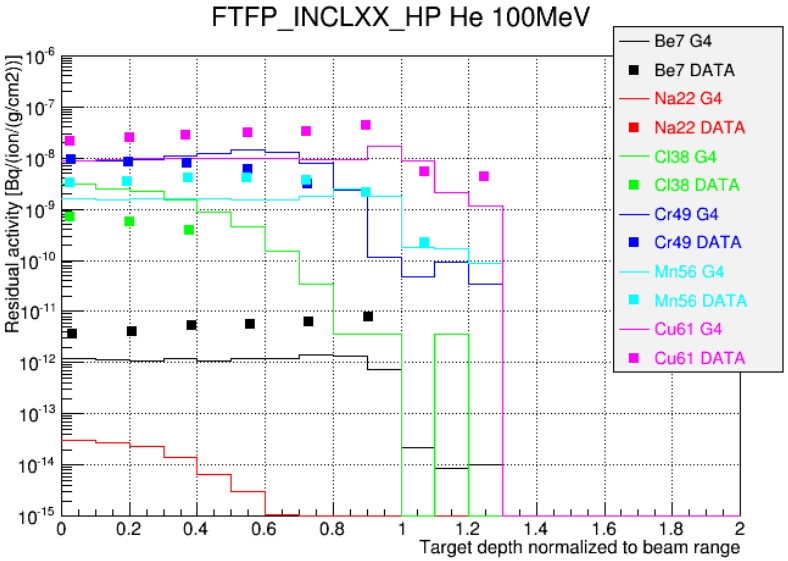
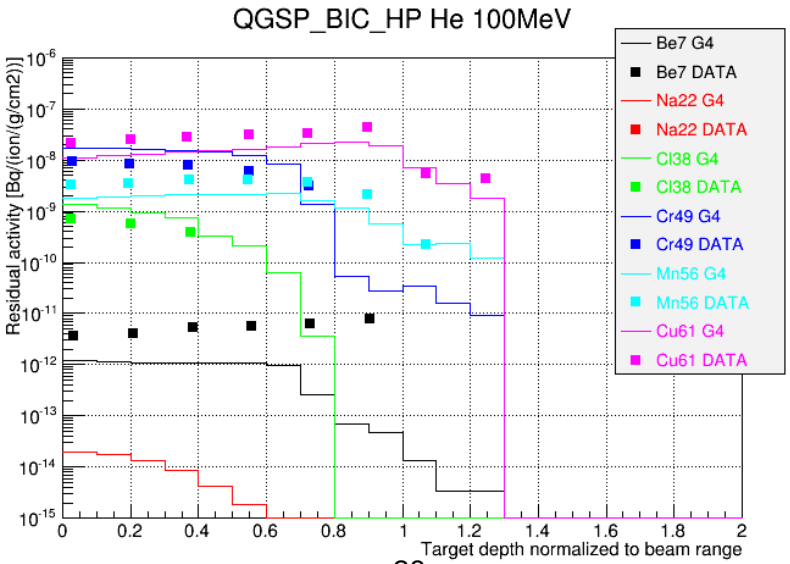
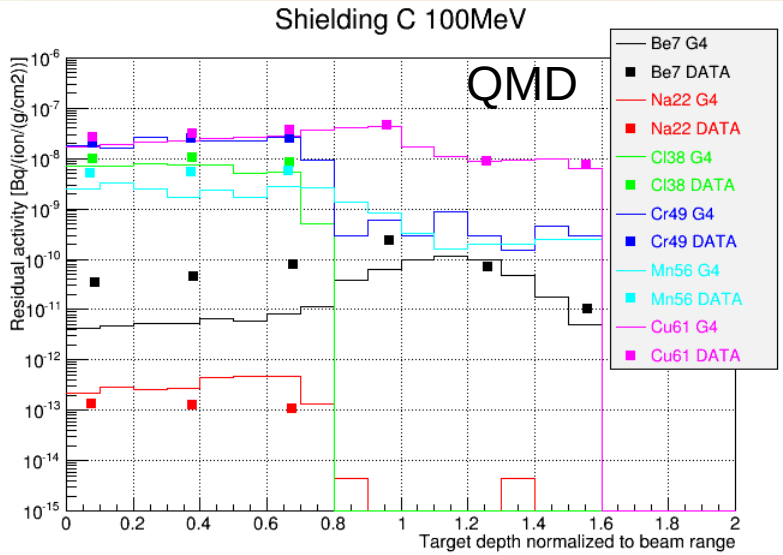
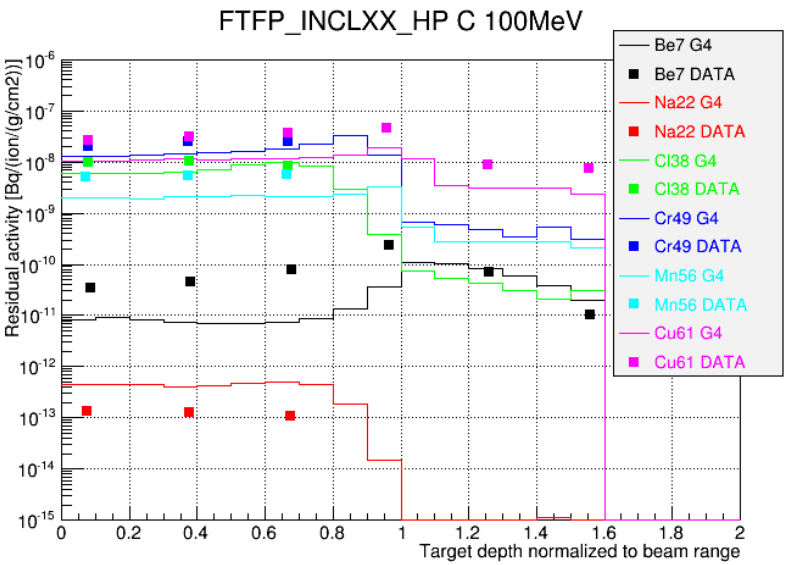


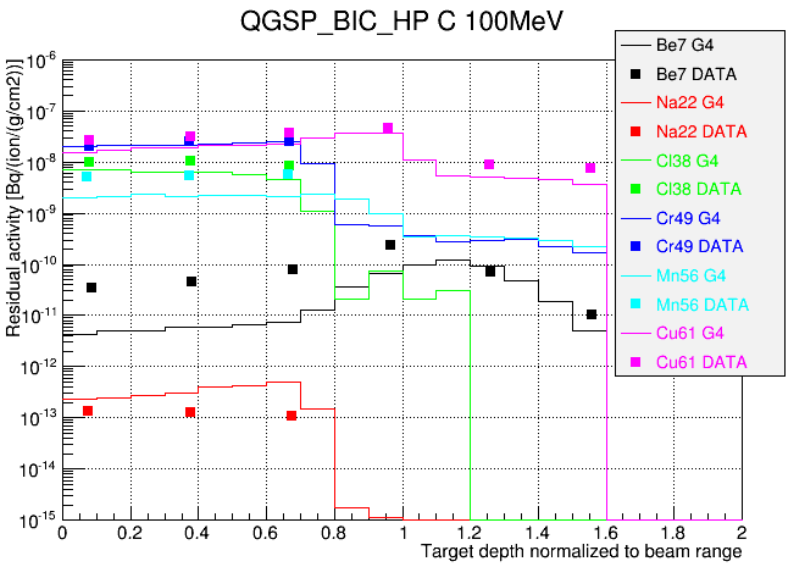
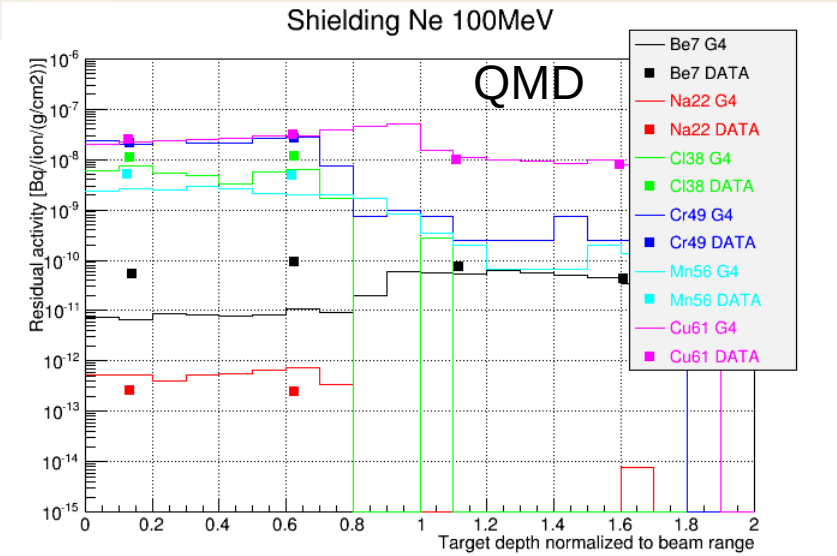
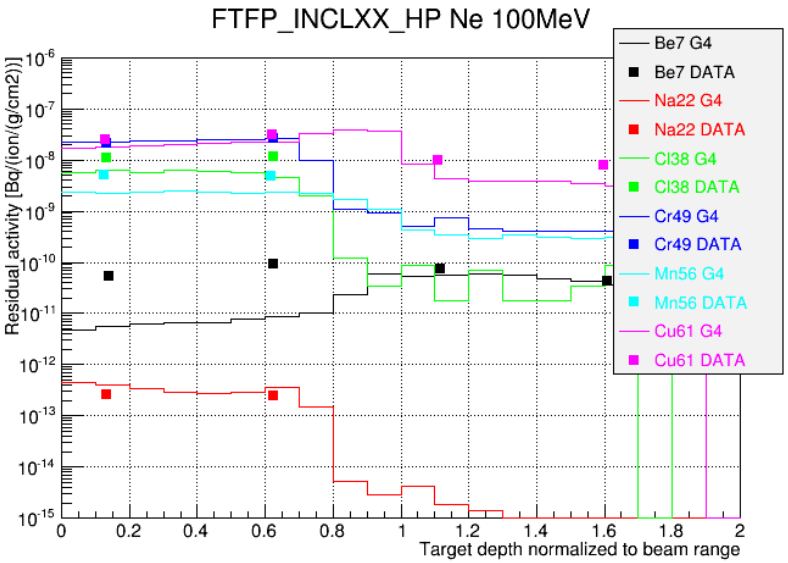
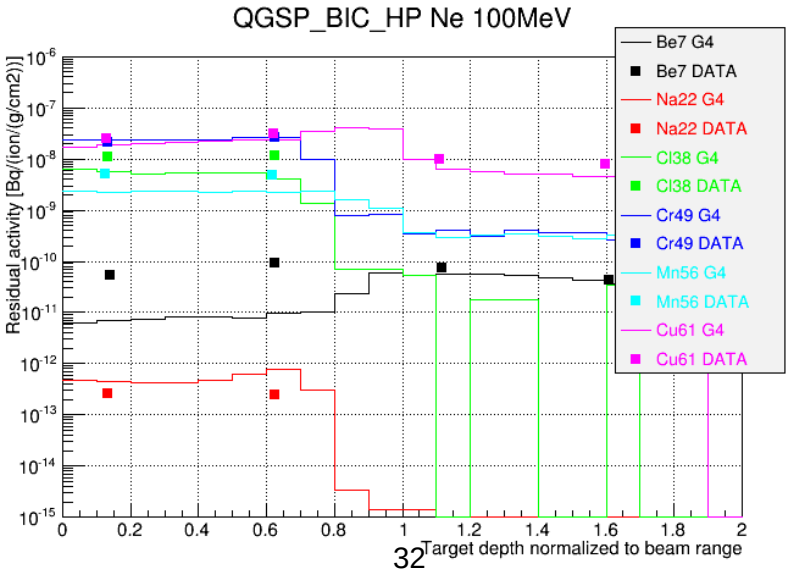




Spatial distribution of residual activities in Cu target Carbon 100MeV/n







Spatial distribution of residual activities in Cu target Neon 230MeV/n