Validation of particle_hp

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Introduction

What is particle_hp?

neutron_hp package uses evaluated nuclear data bases for neutron interactions:

- ✓ Total cross sections
- ✓ Inelastic channel cross sections
- ✓ Double differential spectra of outgoing particles
- ✓ Gamma emission because of nuclear level transitions

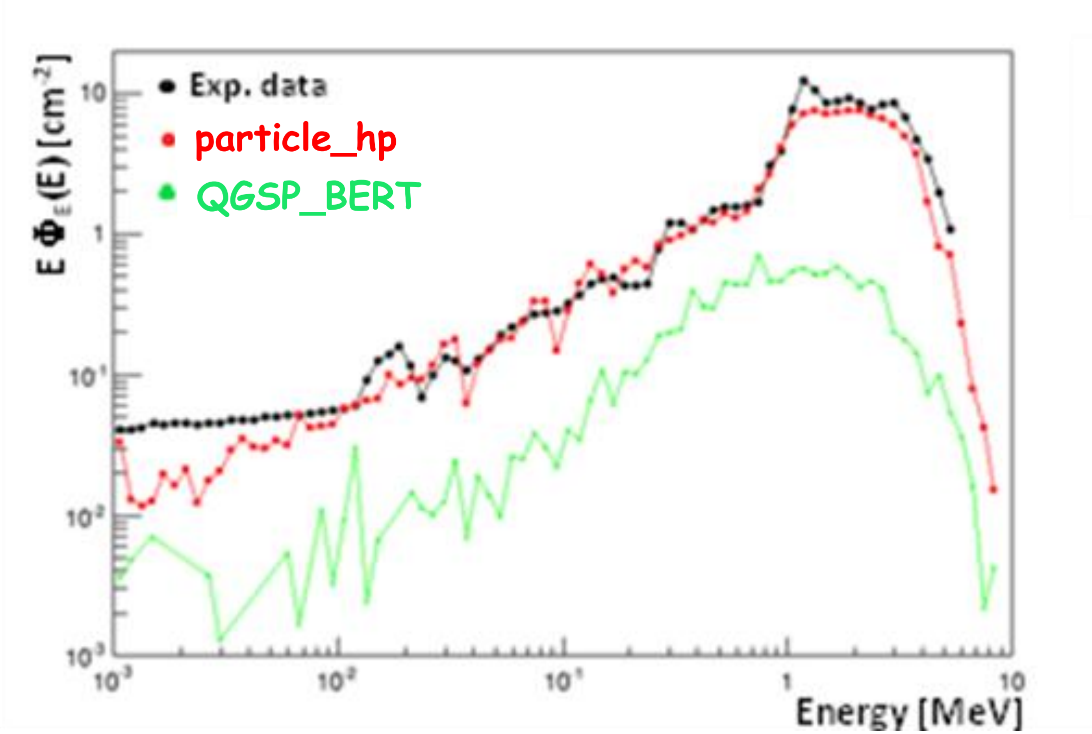
particle_hp: do the same for (**inelastic**) interactions of other particles (p, d, t, He3, α)

Inelastic interactions of p/d/t/He3/α particles E < 200 MeV from evaluated nuclear databases

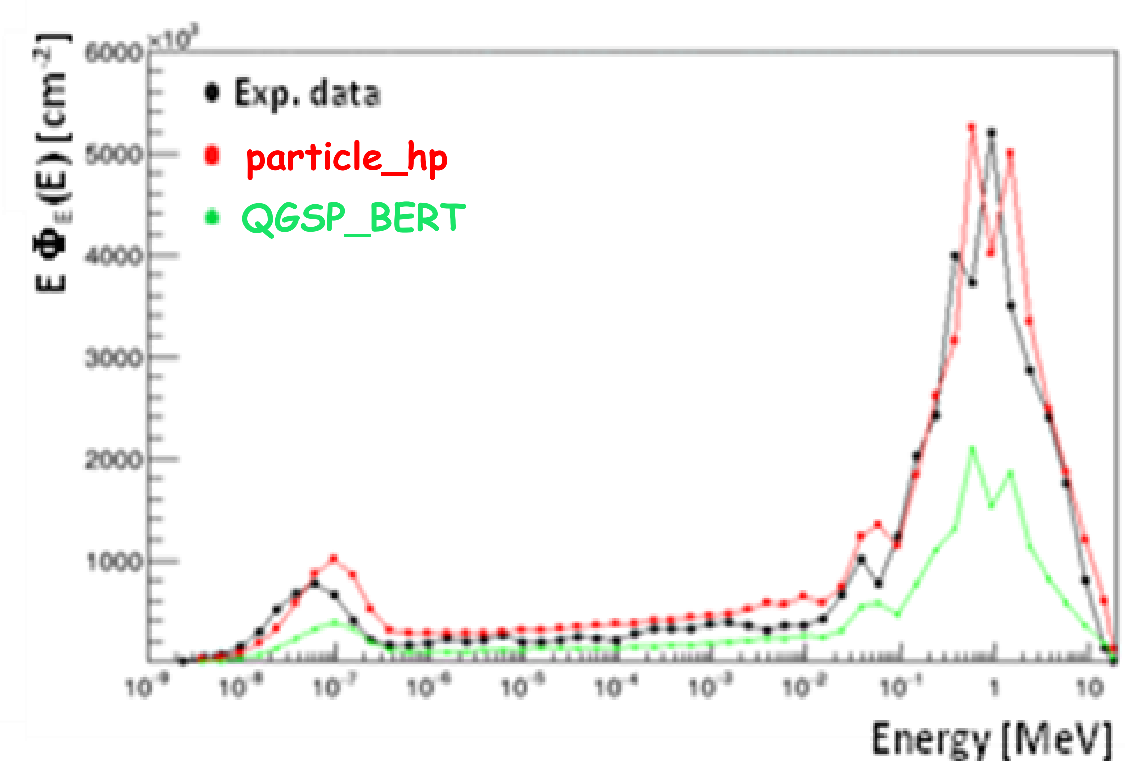
Why particle_hp?

Theory models or semi-empirical models sometimes cannot reproduce experimental data at low (10-100 MeV), specially for low Z elements (J.M. Quesada agrees):

n spectra from p (10MeV) + AL6082



n spectra p(18 MeV) + ^{18}O



Differences w.r.t. neutron_hp

❖ **No new classes**: only modify neutron_hp package

1. Interpolation of 2ary spectra double differential tables

NEUTRON ENERGY	neutron_hp	particle_hp
5.9 MeV	Table for 6 MeV	Interpolates 5 MeV & 6 MeV tables
6 MeV	Table for 7 MeV	Table for 6 MeV

2. G4PHP_DO_NOT_ADJUST_FINAL_STATE affects adjusting of ALL photons

3. Particle yield in an interaction is not sampled in neutron_hp (except for gammas):
   - Integer value is taken 2.43 → 2

➢Environmental variable DO_NOT_SET_PHP_AS_HP to run as neutron_hp (default particle_hp = neutron_hp)

Validation :

neutron_hp = particle_hp?

Verification strategy

Goal: Check particle_hp is **exactly** the same as neutron_hp for incident neutrons

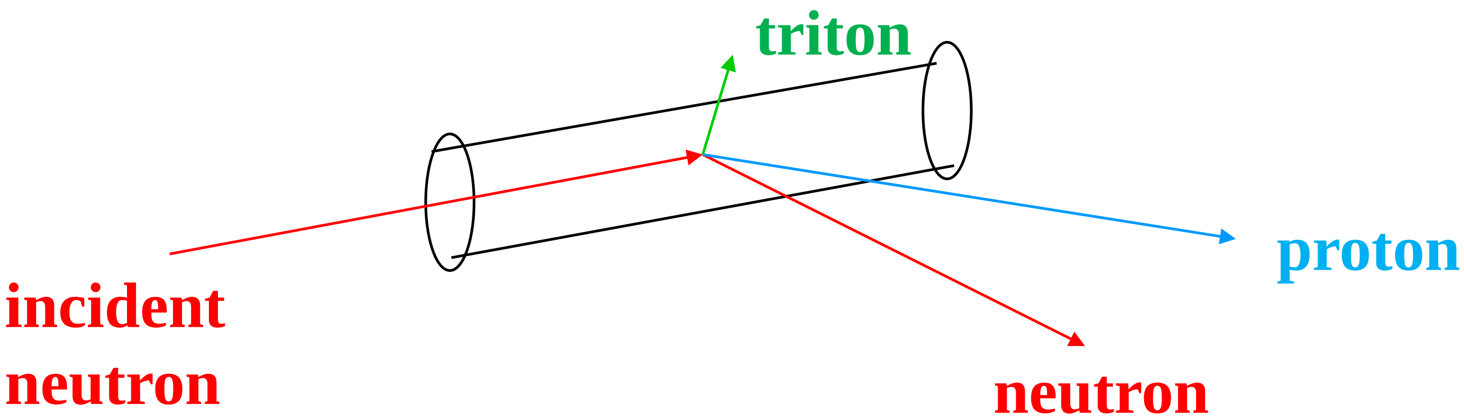
Procedure: the same used in previous verification processes (neutron_hp).

- ❖ neutrons along cylinder with negligible radius

⇒ Every secondary particle goes out of the cylinder after the first interaction

- ❖ Energy 10^{-10}-20 MeV, isolethargicaly
- ❖ A different simulation is performed for each isotope

➢ Plot energy and angle of secondary particles (n, γ, p,d,t,^{3}He,α)



Verification strategy

Simulations have been performed with the following versions of the GEANT4 code:

- ❑ geant4.10.01.p02, using G4NeutronHP gcc version 4.1.1
- ❑ geant4.10.01.ref08, using G4NeutronHP gcc version 4.9.1
- ❑ geant4.10.01.ref08, using G4ParticleHP, "PHP_AS_HP" (default)
  - ▪ Two random seeds to check statistical differences
- ❑ geant4.10.01.ref08, using G4ParticleHP, not "PHP_AS_HP"

INSTALLATION/RUNNING OPTIONS:

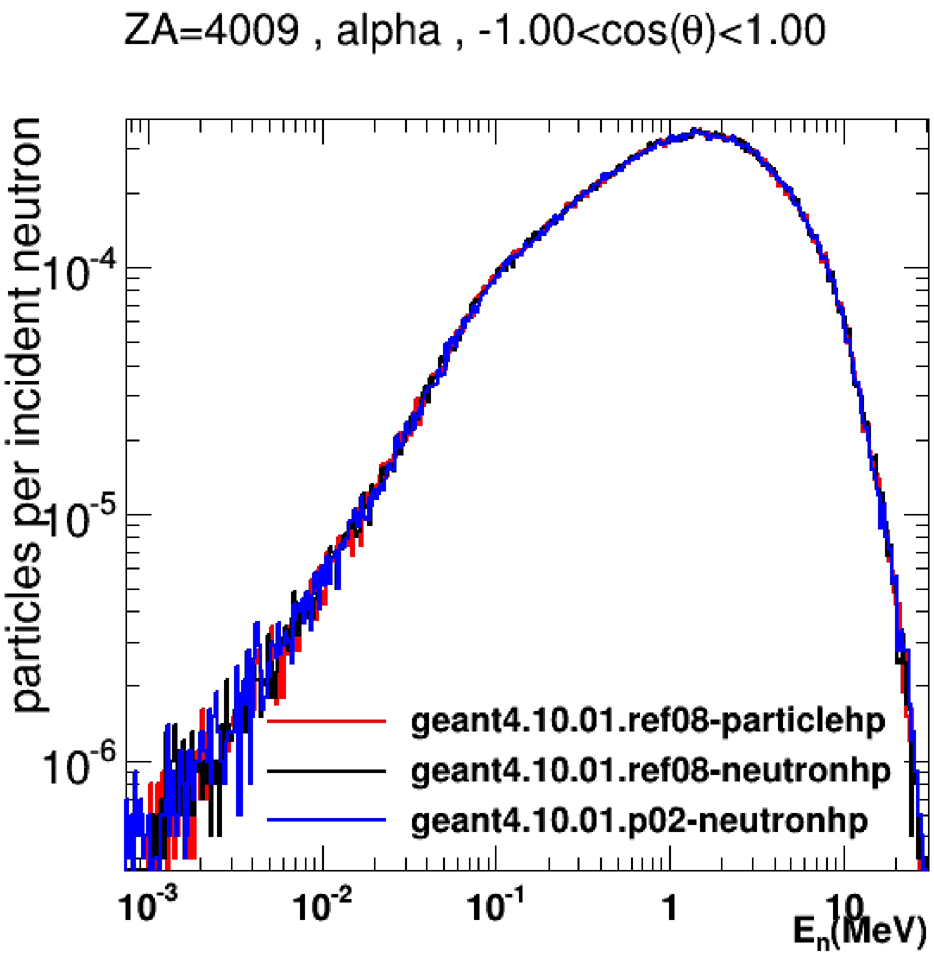
- ➢ -DBUILD_SHARED_LIBS=OFF -DBUILD_STATIC_LIBS=ON
- ➢ -DGEANT4_USE_OPENGL_X11=ON
- ➢ OFF:

G4NEUTRONHP_USE_ONLY_PHOTONEVAPORATION
G4NEUTRONHP_SKIP_MISSING_ISOTOPES G4NEUTRONHP_NEGLECT_DOPPLER
G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE
G4NEUTRONHP_PRODUCE_FISSION_FRAGMENTS

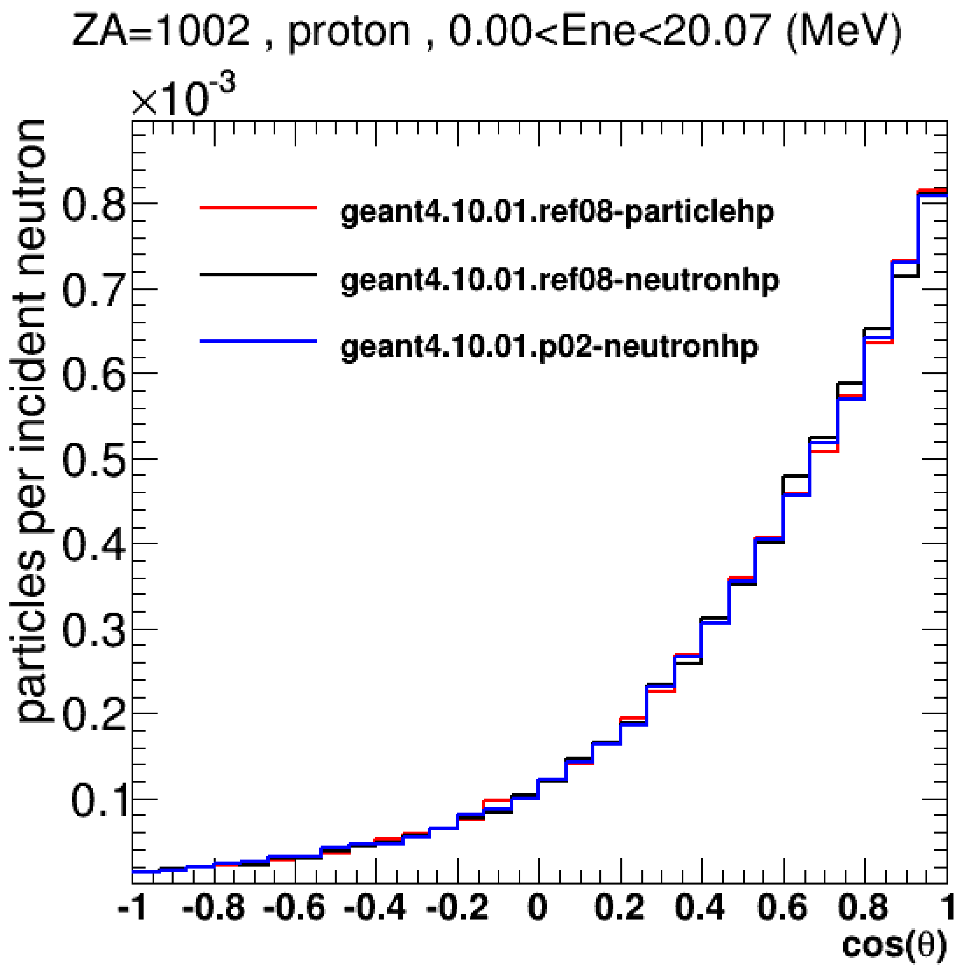
- ➢ G4NDL 4.5

Verification strategy

- All 355 isotopes in G4NDL4.5 (excluded 3 isomers)
- 10^7 source neutrons.



Energy distributions of the alpha particles in the n+^{9}Be reaction.



Angular distributions of the protons in the n+^{2}H reaction.

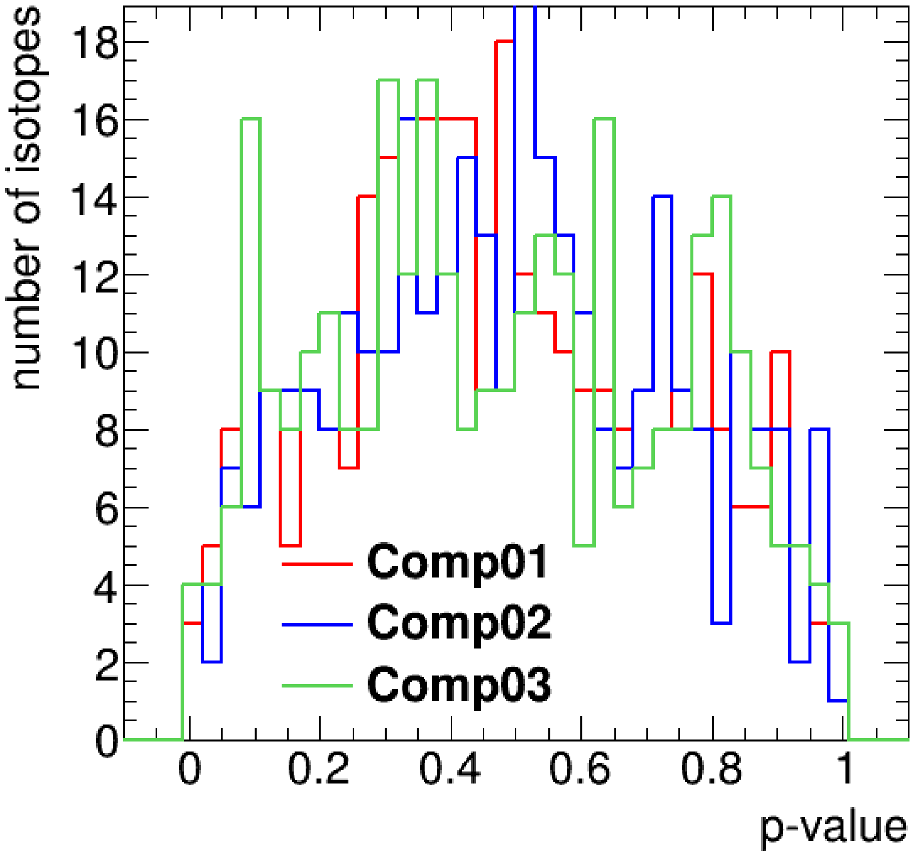
Results: χ^2 checks

- Comp01: geant4.10.01.ref08-G4ParticleHP with itself but using a different seed.

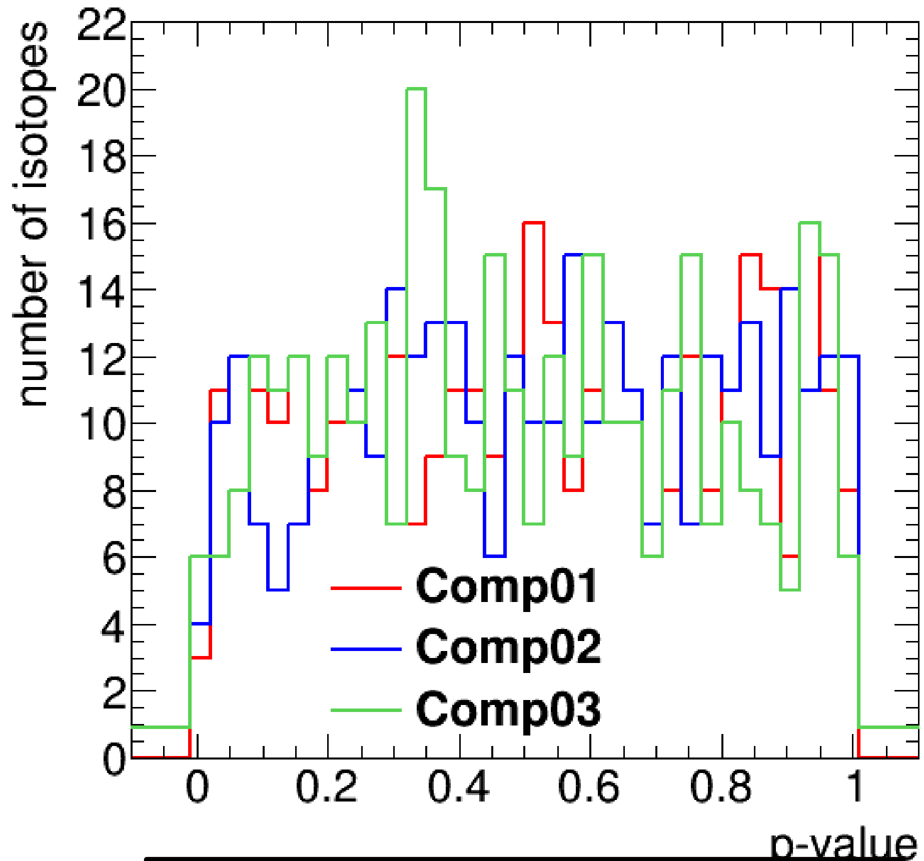
- Comp02: geant4.10.01.ref08-G4ParticleHP (PHP_AS_HP) VS geant4.10.01.ref08-G4NeutronHP.

- Comp03: geant4.10.01.ref08-G4ParticleHP (no PHP_AS_HP) VS geant4.10.01.p02-G4NeutronHP (no PHP_AS_HP).

➢ No any extremely low p-value, with the exception outgoing gamma particles



p-value for energy distributions of the outgoing alpha particles.

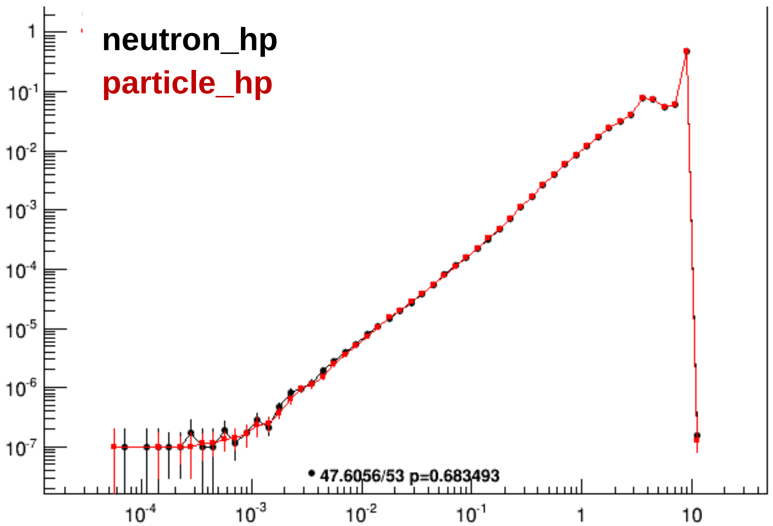


p-values for angular distributions of the outgoing neutrons.

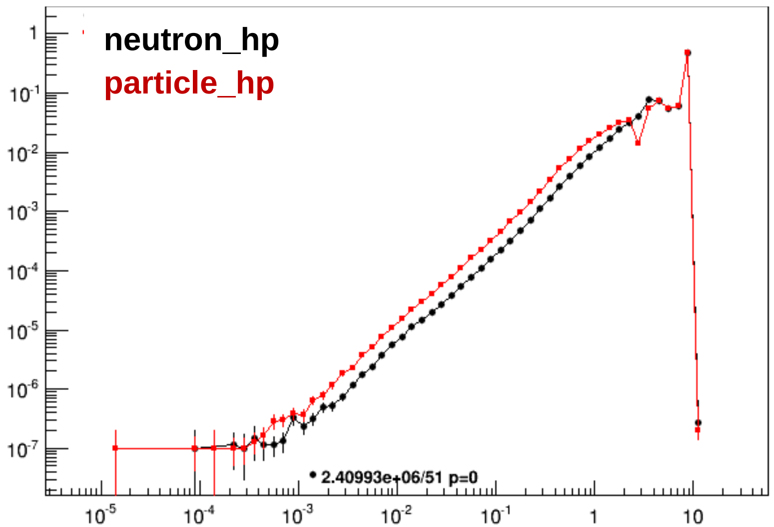
Results: no PHP_AS_HP

- Differences mainly at high incident energy
- Differences depend on isotope target

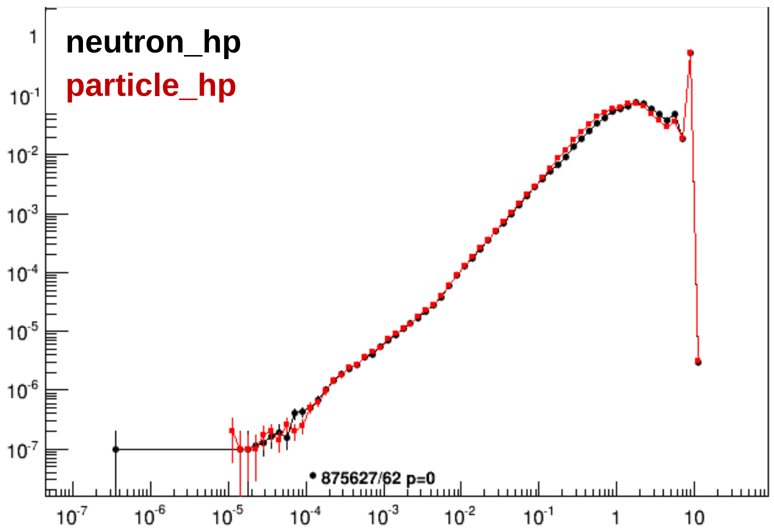
PHP_AS_HP: n from p 10 MeV on Al27



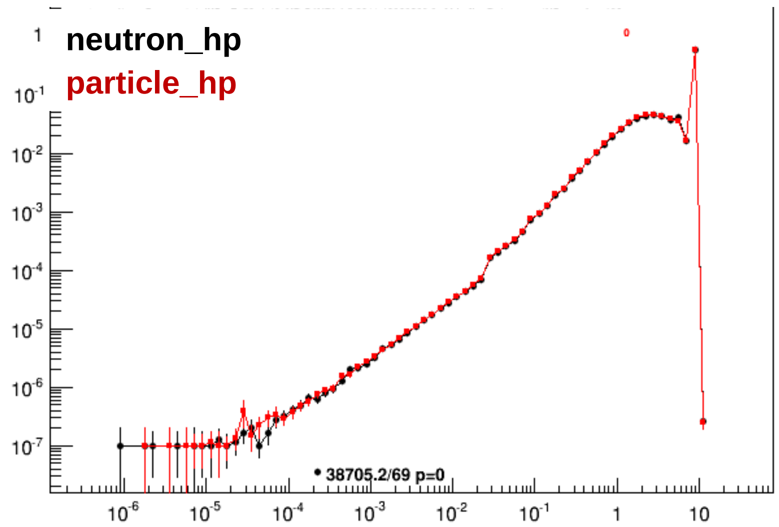
No PHP_AS_HP: n from p 10 MeV on Al27



No PHP_AS_HP: n from p 10 MeV on Pb208



No PHP_AS_HP: n from p 10 MeV on Fe56



We willl to provide full set of plots: all isotopes, all energies (X10), all secondary particles

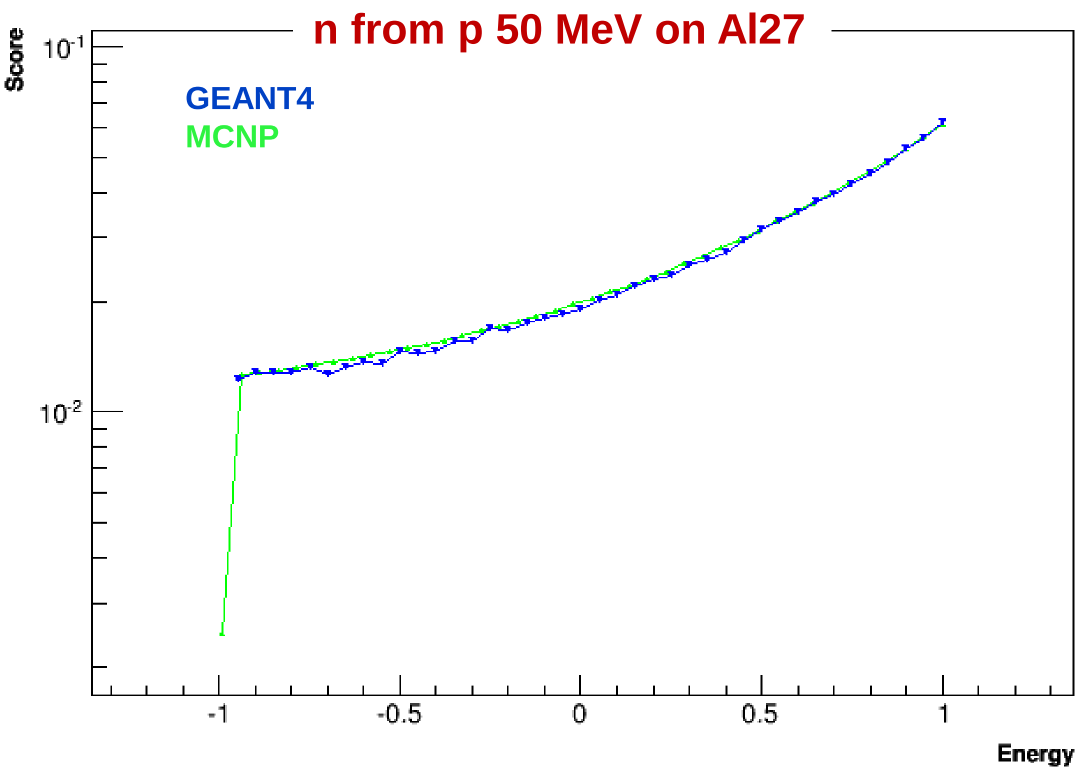
protons:

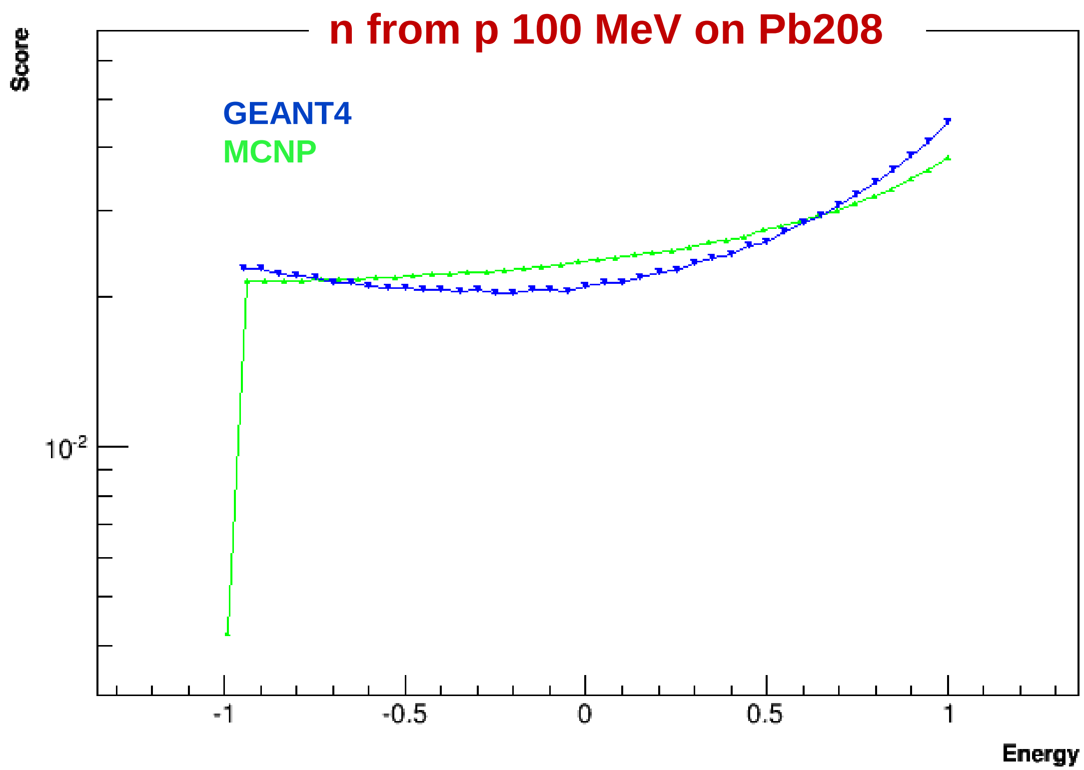
Check with MCNP6

Tests: compare with MCNP

Secondary angle spectra (neutrons)

- Send protons of fixed energy and let them interact until they lose all energy
  - All start along X axis
- Score neutrons/gammas as they reach a sphere: do not let them interact



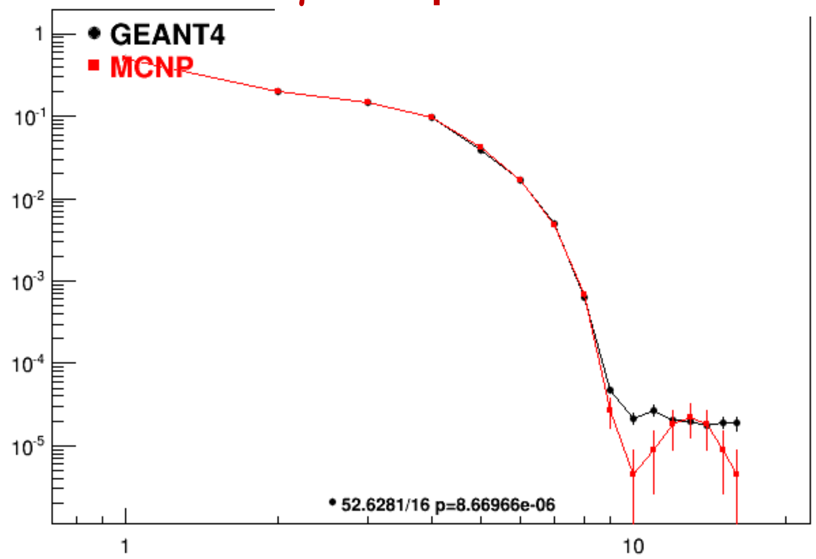


Tests: compare with MCNP

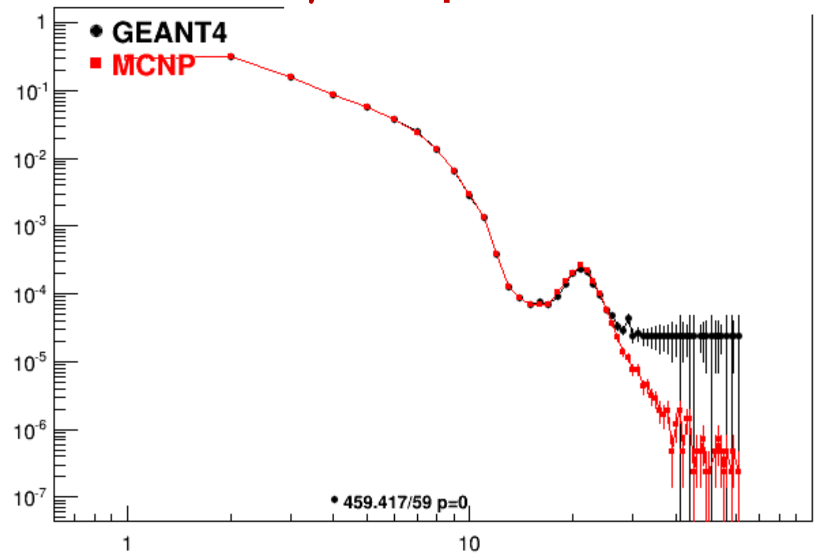
Secondary energy spectra

- Send protons of fixed energy and only activate “protonInelastic” process

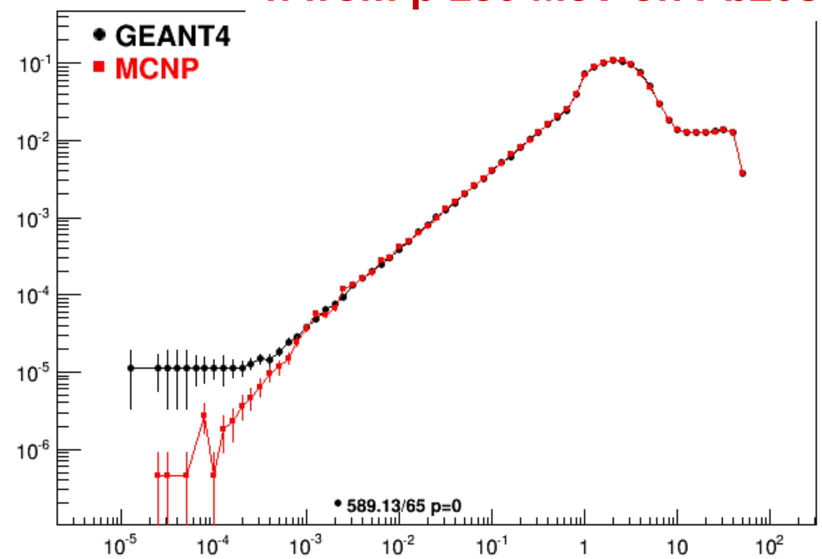
γ from p 10 MeV on Fe56



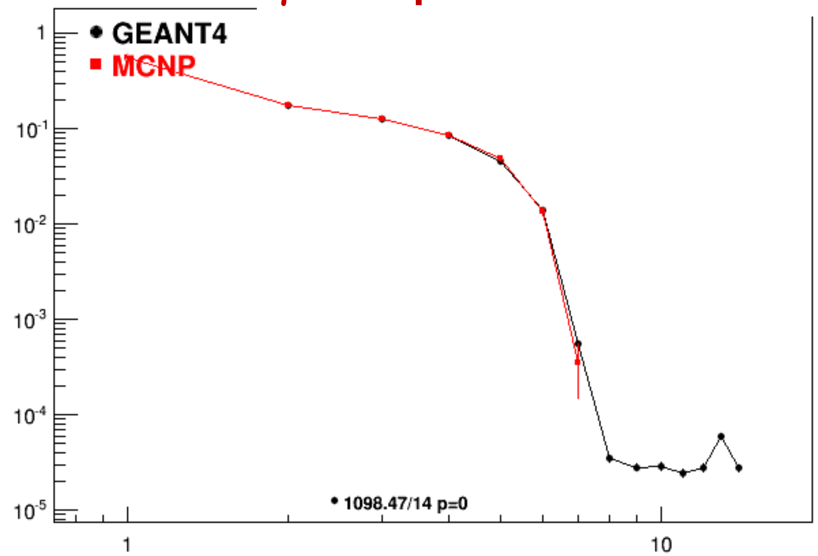
γ from p 50 MeV on Al27



n from p 150 MeV on Pb208



γ from p 10 MeV on Pb208

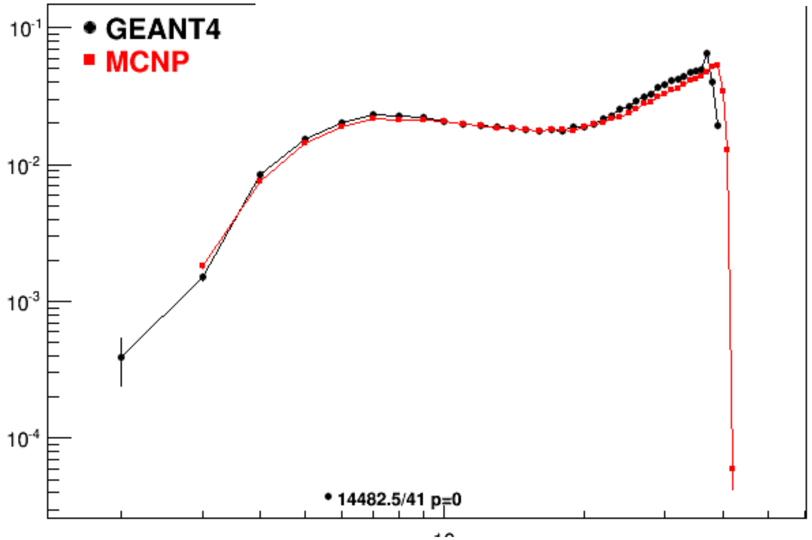


Tests: compare with MCNP

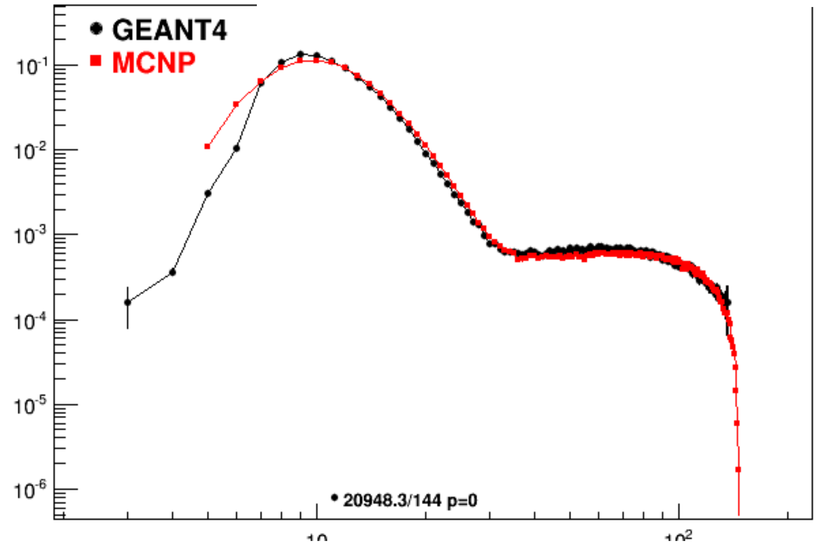
Secondary energy spectra

➢ Send protons of fixed energy and only activate “protonInelastic” process

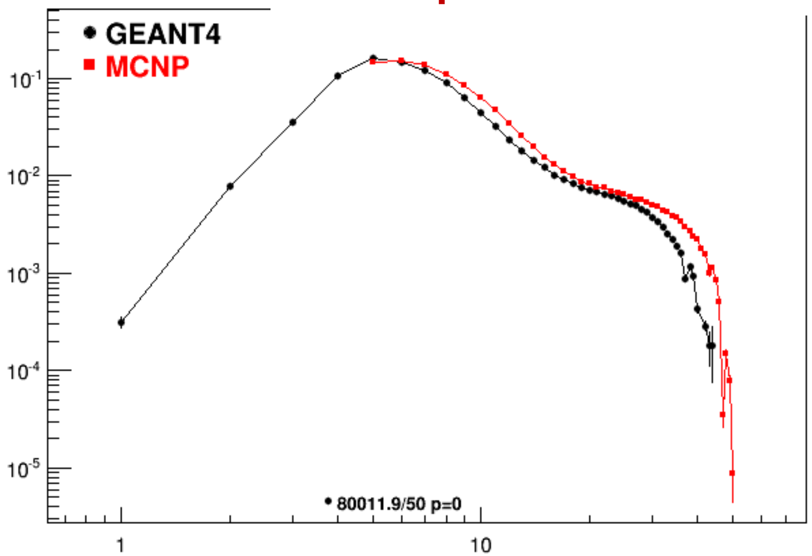
d from p 50 MeV on Fe56



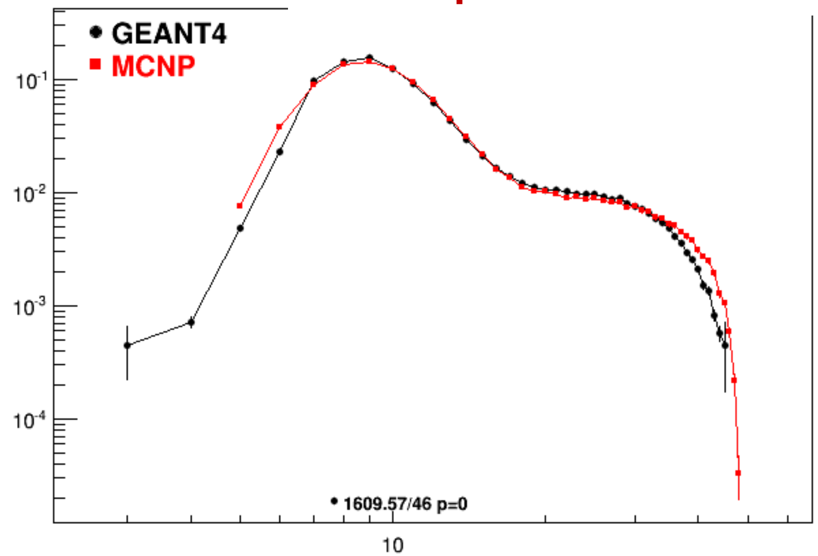
α from p 150 MeV on Fe56



α from p 50 MeV on Al27



α from p 50 MeV on Fe56

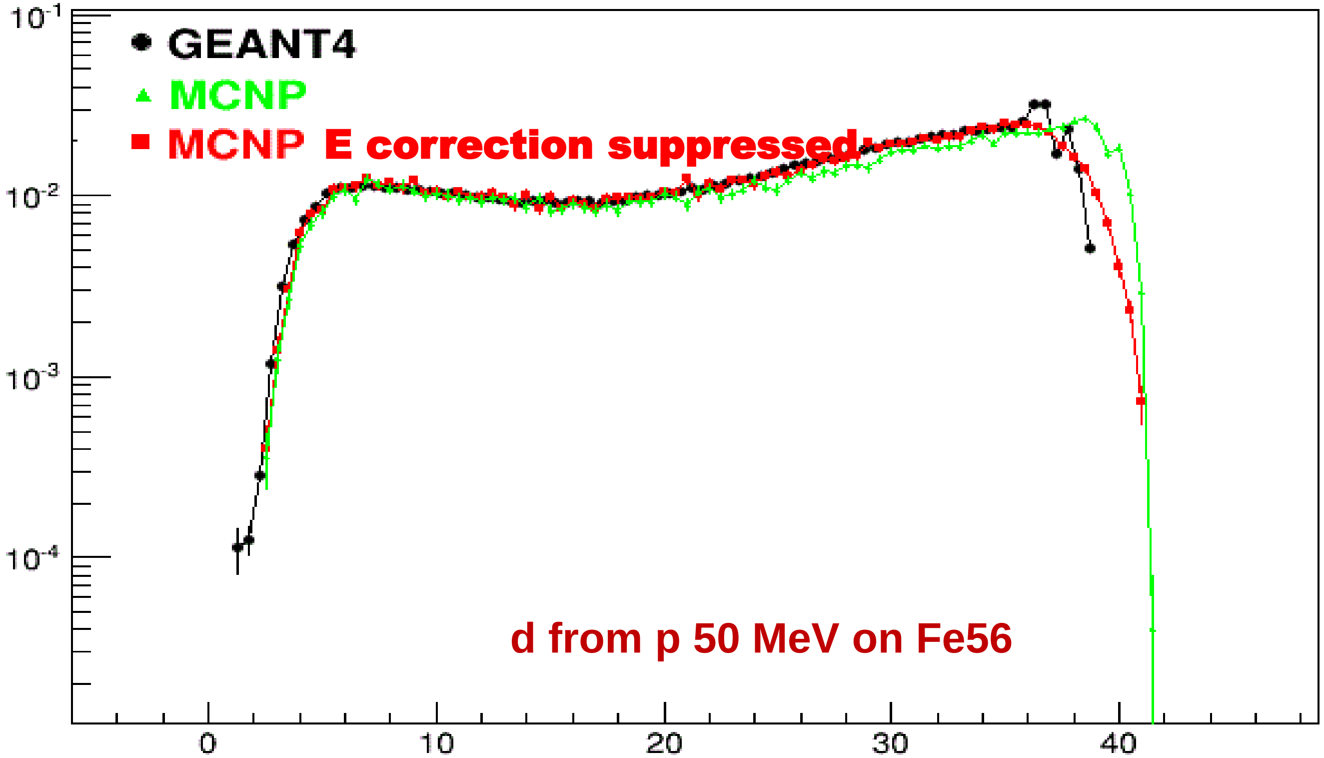


Tests: compare with MCNP

Differences in secondary energy spectra

- For each isotope, for each secondary particle type, for each incident energy data for secondaries:
  - GEANT4 uses **3** parameters
    - Energy
    - Probability
    - Angle parameter
  - MCNP uses **5** parameters
    - Energy
    - Probability
    - Cumulative probability $\sum_{k=0}^{n}(P_{k-1} - P_k)/2$
    - Angle parameter
    - Energy correction?!

Good idea, GEANT4 calculates the cumulative probability on the fly, for each interaction!



Conclusions

- Geant4 (and other MC) theoretical models do not work well for charged particle (p, d, t, He3, α, γ) inelastic interactions at low energy O(10-100 MeV)

- Alternative implemented: use evaluated data bases: particle_hp
  - Also serves for neutrons

☺ Some improvements w.r.t. neutron_hp

☺ It gives the same results as neutron_hp (when improvements not applied)

☹ Differences w.r.t. MCNP have to be understood

particle_hp will is meant to replace neutron_hp from release geant4.10.2

- **Data sources for charged particles under discussion (TENDL/ENDF)**
  - **For neutrons G4NDL will be kept**