PAUL SCHERRER INSTITUT

PSI

Daniela Kiselev, Michael Wohlmuther: PSI
Jean-Christophe Davide: CEA-Saclay
Alfredo Ferrari: CERN
Tatsumi Koi: SLAC

Po-production in lead: A benchmark between Geant4, FLUKA and MCNPX

SATIF13, Dresden, Germany, 10.10.-12.10.2016

Motivation

- Disposal of the radioactive Pb-waste (SINQ-target,n-ToF):
  - Authorities need complete (calculated) nuclide inventory of long-lived isotopes (T1/2 > 60 d)
  - Predictions have to be (partly) validated/justified.
  - Particularly interesting are risky isotopes like α-emitters and volatile elements → **Po**
- Benchmarking of codes
  - estimate of reliability and uncertainties
  - comparison with exp. data (taken at SINQ spallation source at PSI)
    - → requires a detailed/complicated geometry
    - → difficult to acquire statistics
    - → usually only 1 code is used for predictions
  - several codes need a lot of effort (geometry, statistics)
    - → use simple model for benchmark → **SINQ Toy model**

Talk on SATIF12:

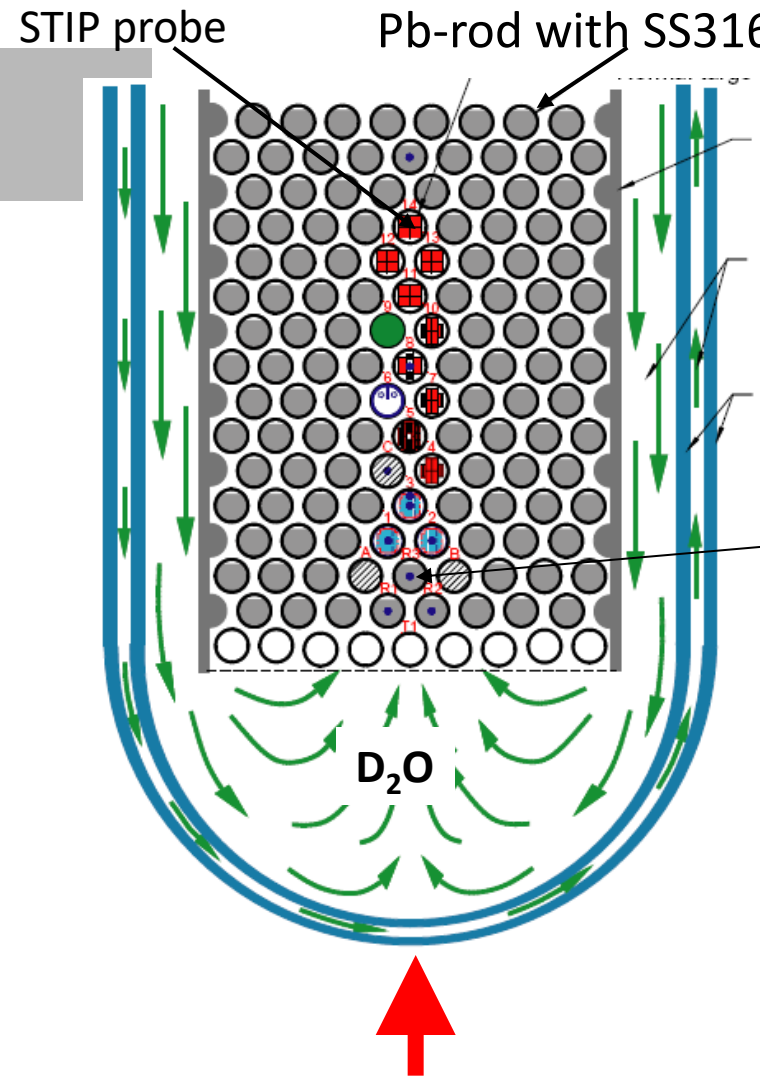
Po-production in lead:

Calculation and measurement on SINQ-samples

just comparing with MCNPX and different c.s. models

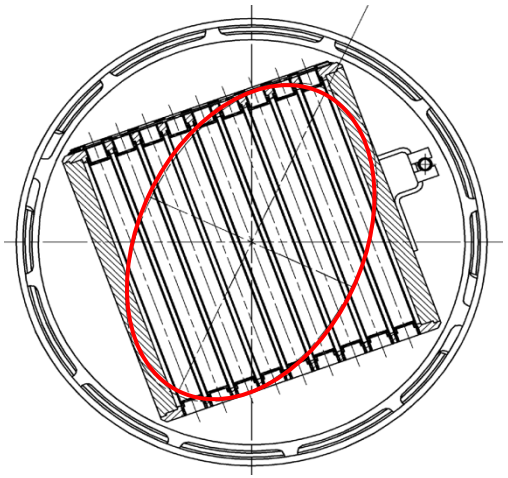
SINQ facility: neutron spallation source

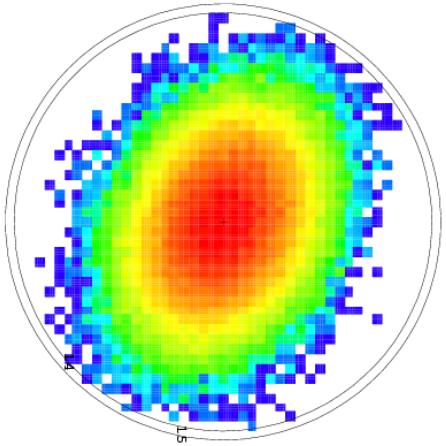
Target 4: March 2000-Dec. 2001 → 10.03 Ah



Rod3: Pb: Activity of Po isotopes was measured (D. Schumann, T. Lorenz (PSI))

Footprint on target:





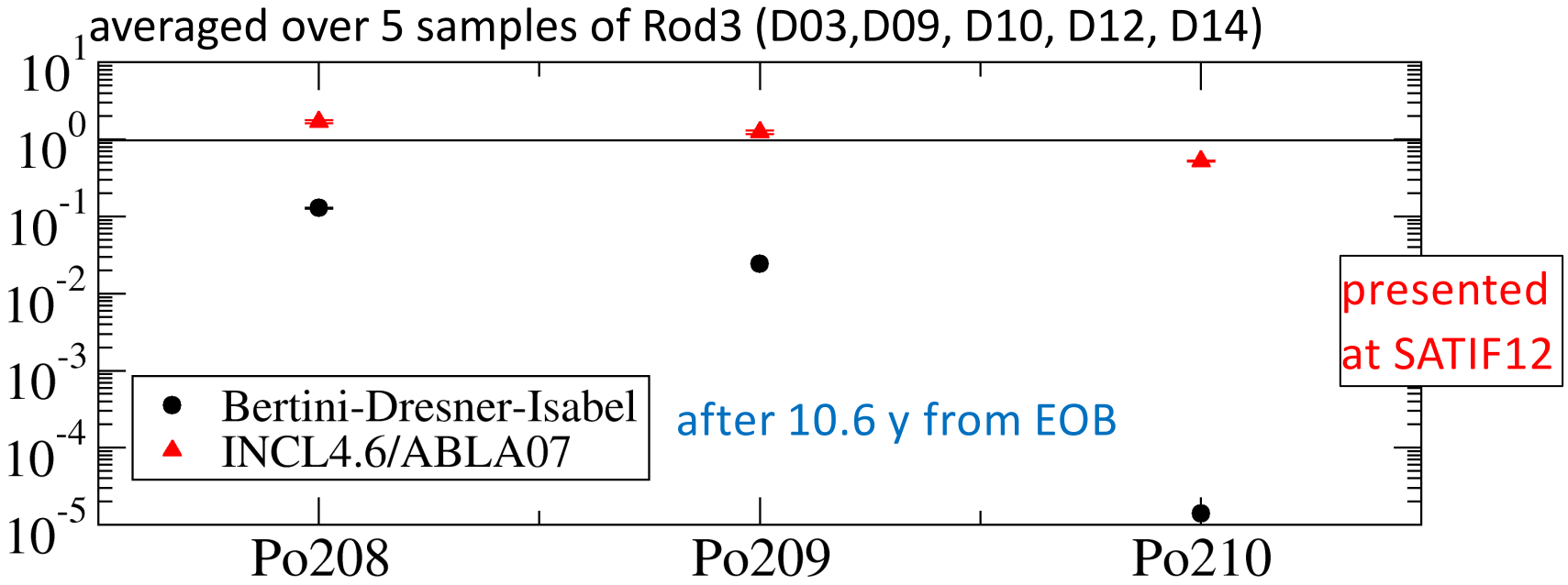
~ Gaussian:

σ_x= 2.1 cm,
σ_y= 3.0 cm

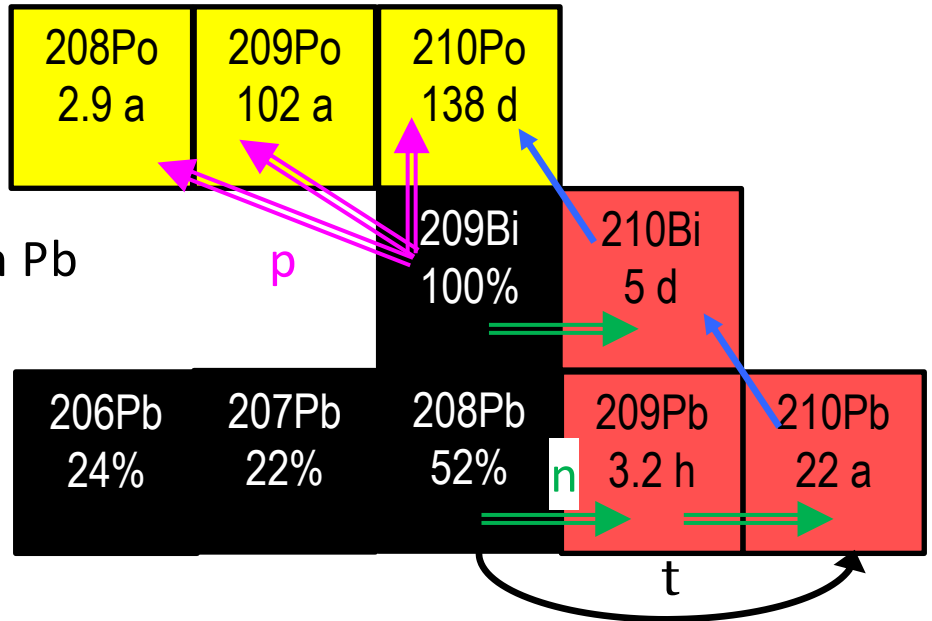
Beam distribution in MCNPX model

Comparison presented at SATIF-12

Ratio MCNPX2.7.0(SINQ-model) to exp. data



Great improvement using INCL4.6/ABLA07:



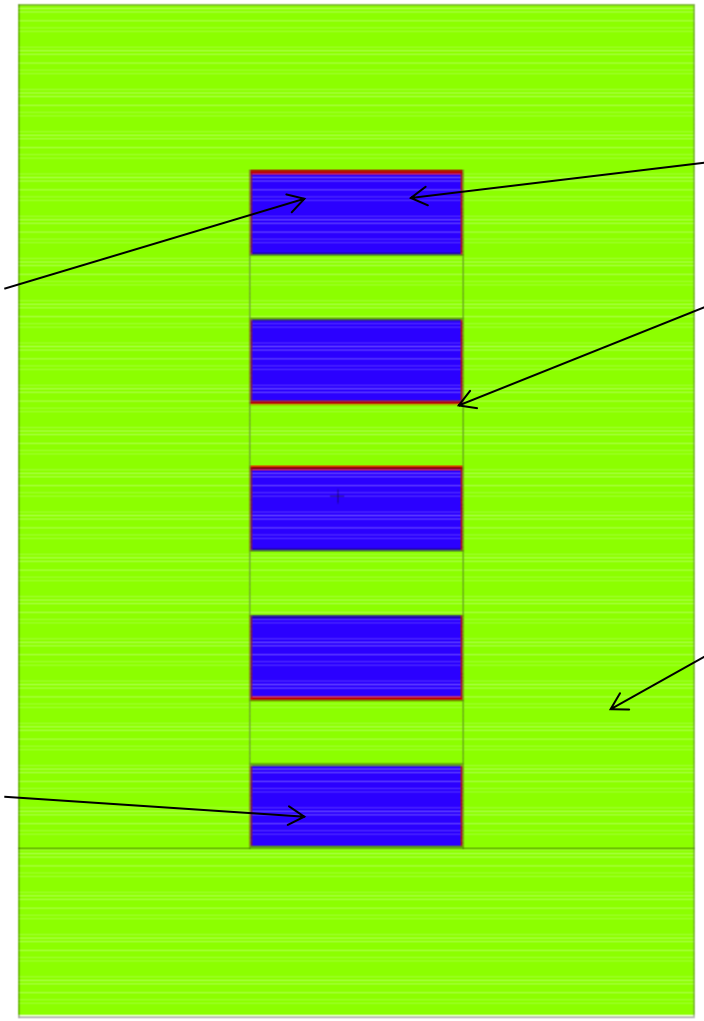
Reason:

- Production of Po208, Po209 by alphas on Pb
- Production of Po210 by tritium capture

→ Check:

- Alpha and triton spectra
- Production cross sections

Simplified SINQ model → Toy model



Block 5

Block 1

Pure Pb cladded with
1 mm Steel

Steel cladding:
avoids direct contact with D, H3

D_2O

Inner Part ~ SINQ Target
~ 57% Pb + Steel
~ 43% D_2O

p-beam (pencil)
575 MeV

MCNPX2.7.0 + buildup&decay

Monte Carlo particle transport program **MCNPX2.7.0** n,p,γ,α,π,d,^{3}H....

Input: *dedicated geometry, material compositions,*
cross sections: for n<20MeV ENDF-B, otherwise ***Bertini-Dresner***

Output: n-fluxes (E<20 MeV), residual nuclei production rates
with **rnucs-card** (former active htape) in *.o file
- avoids huge histp file (can be several GB)
- developed by F. Gallmeier & M. Wohlmuther
- patch in the Cinder2008 release on RSICC

activation script

M. Wohlmuther et al., Proc. AccApp *2007*, Pocatello, p. 226.
F.X. Gallmeier, dito, p. 207

Cinder + c.s. library or **SP-Fispact** + EAF2010 or **Orihet3**

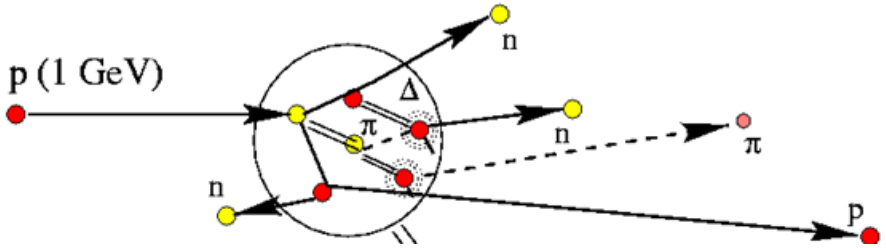
+ *irradiation history*

→ nuclide inventory

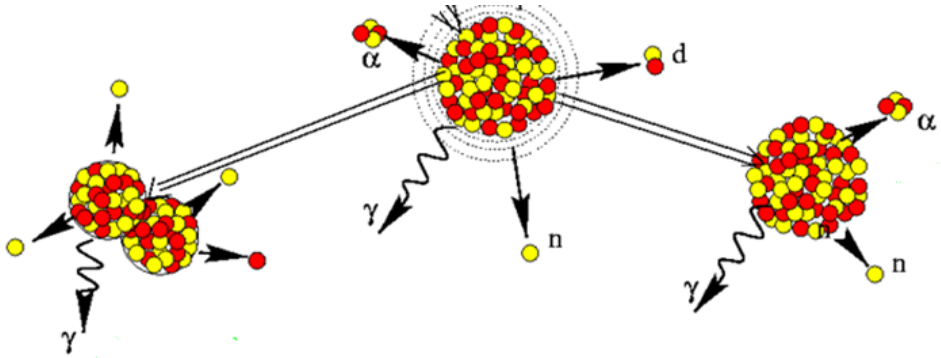
Using FISPACT10/EAF2010: negligible difference to Cinder & Fispact07/EAF2007

Selected physics models in MCNPX

1) Intra-Nuclear Cascade:



2. Evaporation/Fission



1) MCNPX default option:

- for n & p: < 3.5 GeV

  BERTINI (INC) + Dresner (evaporation) + RAL (fission):

  - **BERTINI**: based on Serber's model, spacelike realization
  - **DRESNER**: EVAP-A, based on Weisskopf's statistical model
  - **RAL** (Atchison): fission in between of the evaporation stages
- for light ions (d, t, α): < 1 GeV

  ISABEL (INC) + Dresner + RAL:

  - ISABEL: based on Serber's model, timelike realization

2) ISABEL (INC) + Dresner + RAL:

- for all incident particle types
- developed by Yariv & Fraenkel

Selected physics models in MCNPX

INCL4.6 + ABLA07: «private» version of MCNPX2.7.0

Large improvements compared to INCL4.2+ABLA
implemented in standard version of MCNPX2.7.0

INCL4.2	n, p, π	no ^{3}H (t)
ABLA	n, p, α	
INCL4.6	n, p, π, d, t, ^{3}He, α and A ≤ 8	
ABLA07	n, p, d, t, ^{3}He, α and clusters (IMF)	

INCL4.6: allows for incident clusters
coalescence in phase space → emitting clusters

Newest MCNPX2.7.0 INCL4.6/ABLA07 version:
handles also metastable isotopes according to data from file (PHTLIB)

INCL4.6: A. Boudard et al., Phys. Rev. C. 87, 014606 (2013)
ABLA07: M. V. Ricciardi, A. Kelić, K-H. Schmidt, Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions„ held in Trieste, Italy, 4-8 January 2008, p. 181

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Geant 4

- Version: Geant4 v10.02.p02 compiled by gcc-4.8.5 and running on RHEL6-64
- **Physics List: QGSP_INCLXX_HP**
  - Quark Gluon String Model (QGSP) is used for high energy (>>1GeV)
    - High energy model does not change result
  - Geant4 version of INCL model (INCLXX) is used for intermediate energy
    - Selection of cascade model changes result → important!
    - Results from other cascade models (Bertini-like and Binary cascade)
      → **talk of Tatsumi Koi on Tuesday**
    - High Precision (HP) package for low energy (<20MeV) neutron transport
  - RadioactiveDecay module is added to the physics list by physics constructor

Details of Geant4 simulation for Toy SINQ Model

Two step calculation:

- First step
  - Protons hits toy SINQ Model
  - Energy spectra of triton and alpha in lead blocks are accumulated

- Second step
  - Production rates in the lead blocks are derived from convolution of the particle spectra with the production cross sections
  - The production rates are fed into Cinder07 taking into account the intensity profile (Buildup & decay)

FLUKA Hadron-nucleus interactions: PEANUT*

**PreEquilibrium Approach to NUclear Thermalization*

PEANUT handles hadron-nucleus interactions from threshold (or 20 MeV neutrons) up to several tens of TeV

Sophisticated Generalized IntraNuclear Cascade → GINC

↓

Smooth transition (all non-nucleons emitted/decayed + all secondaries below 30-50 MeV)

↓

Prequilibrium stage

↓

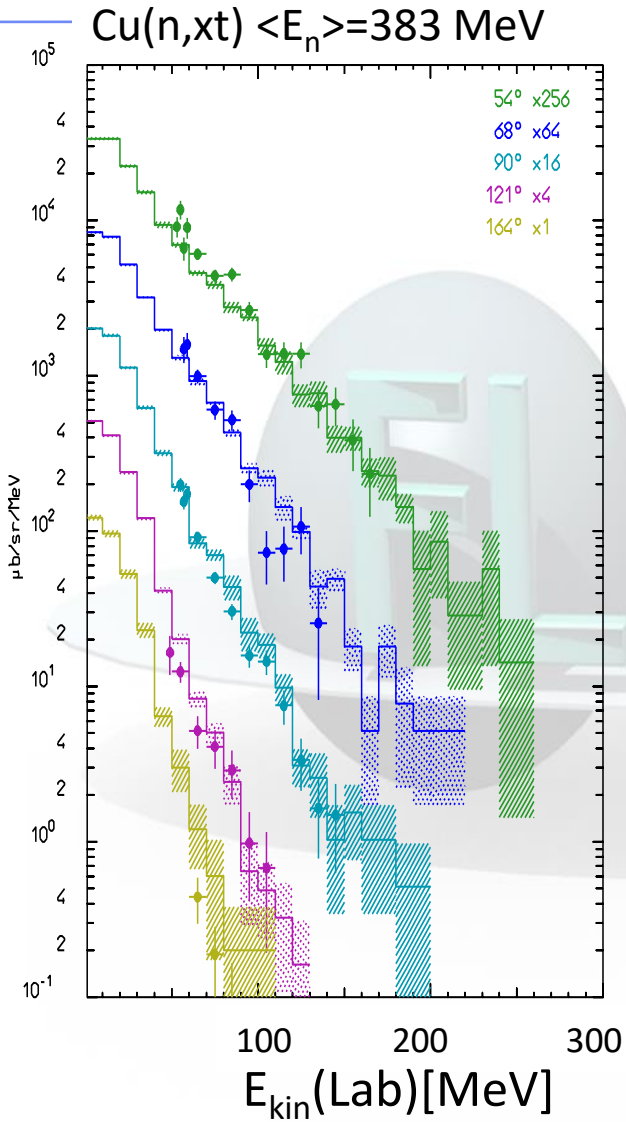
Standard Assumption on exciton number or excitation energy

↓

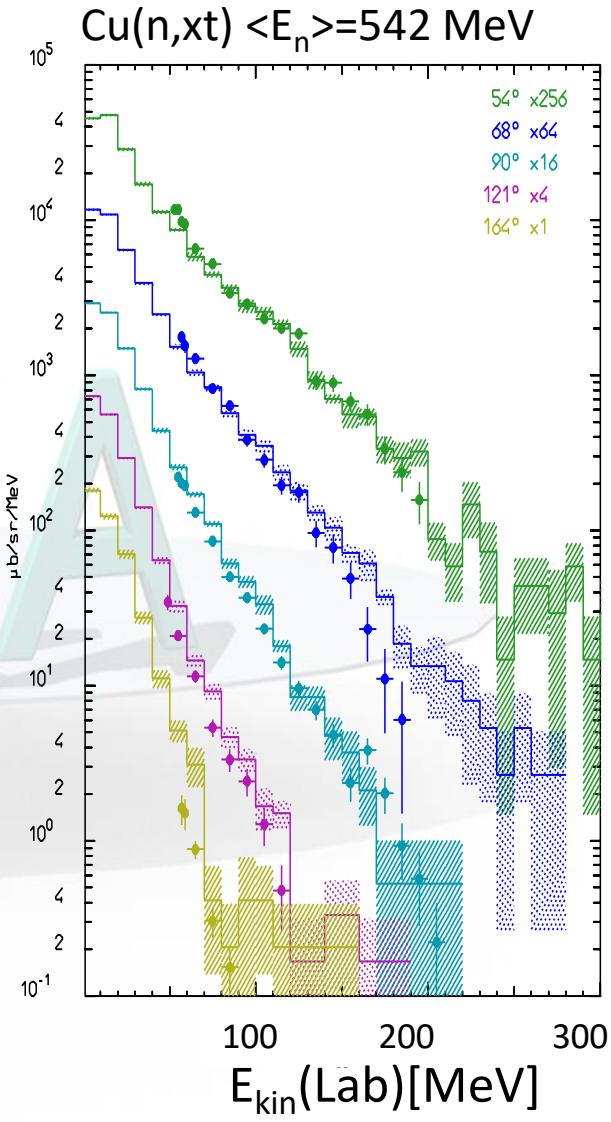
Common FLUKA Evaporation/Fragmentation/Fission models

(600 possible emitted particles/states (A<25) with an extended evaporation/fragmentation formalism, spin-dependent Fermi break-up for A<18)

Secondary light fragments: coalescence in PEANUT



Coalescence is an essential ingredient in producing energetic composite particles, d, t, ^{3}He, α, which are very much relevant for this intercomparison



Double differential triton production from <E>=383 MeV (left) and 542 MeV (right) neutrons on Copper (Nucl. Phys. A510, 774 (1990)). Symbols are exp. data, histograms FLUKA

FLUKA: the BME Model for nucleus–nucleus interactions below 150 MeV/n

The BME (Boltzmann Master Equation) model

It works for $A_{proj}, A_{targ} \geq 3$, $E \leq 150$ MeV/A

1. COMPLETE FUSION

Fragment(s) : **pre-equilibrium** de-excitation according to the BME theory (where available) or to the PEANUT exciton model

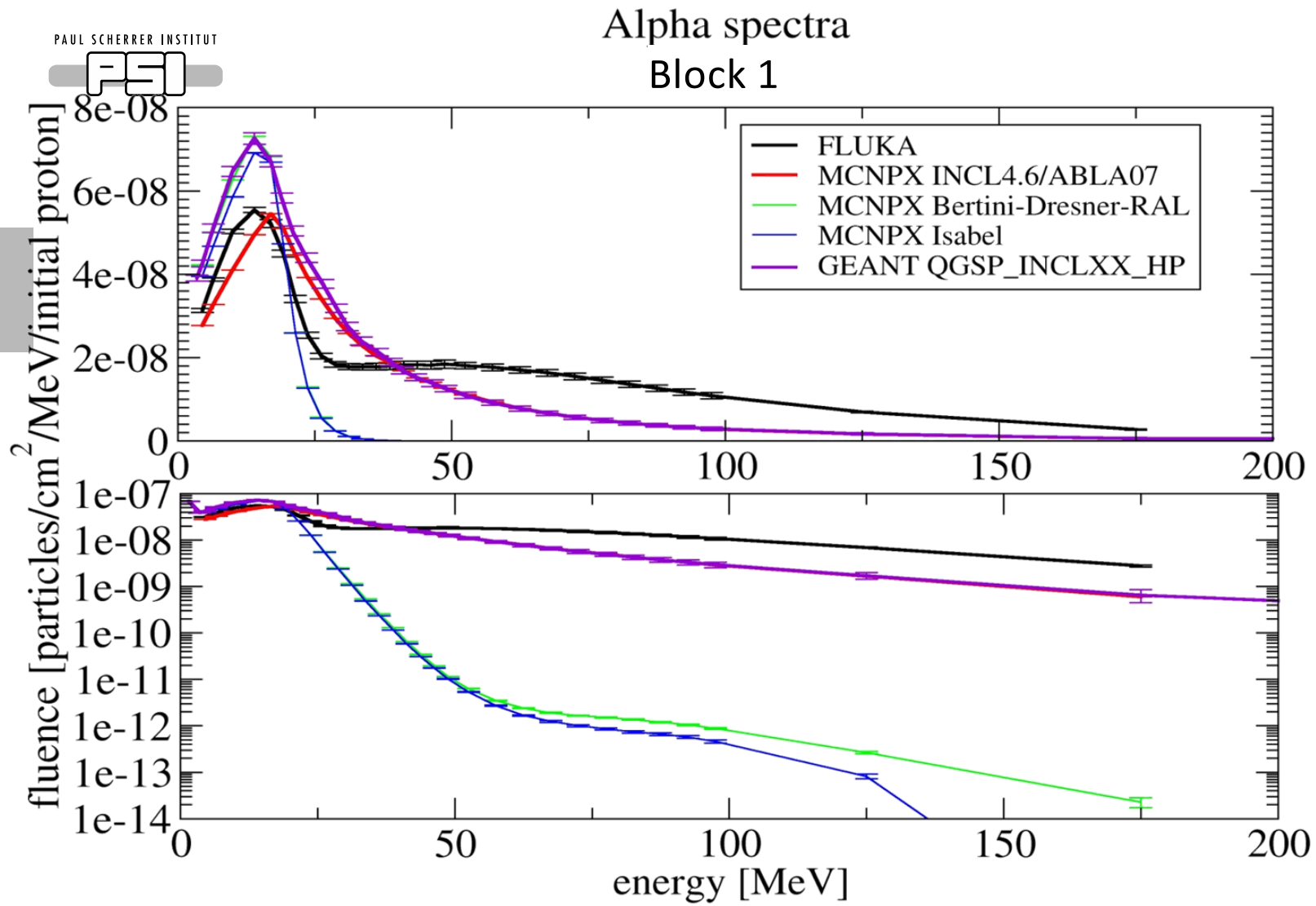
evaporation/fission/fragmentation/ gamma de-excitation, same as for hadron-nucleus interactions

2. PERIPHERAL COLLISION

- *three body mechanism*
- *incomplete fusion*
- *one nucleon break-up and possibly transfer* (at high *b*)
- *pickup/stripping* (for asymmetric systems at low *b*)

The kinematics is suggested by break-up studies.

Fluka2016.5 with the latest versions of PEANUT and BME has been used for this intercomparison

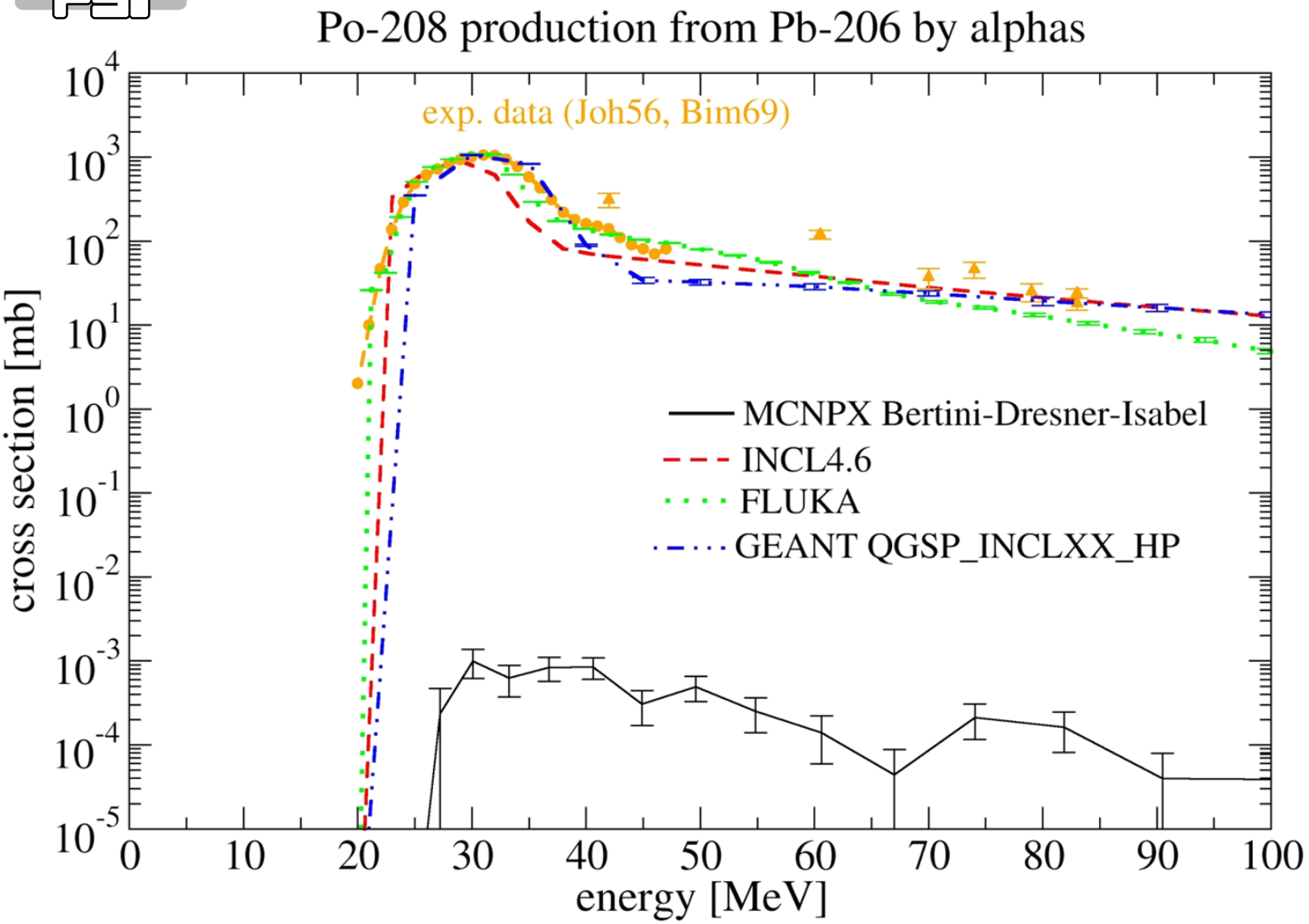


Bertini + Isabel: missing the tail = high energetic particle due to forward emission

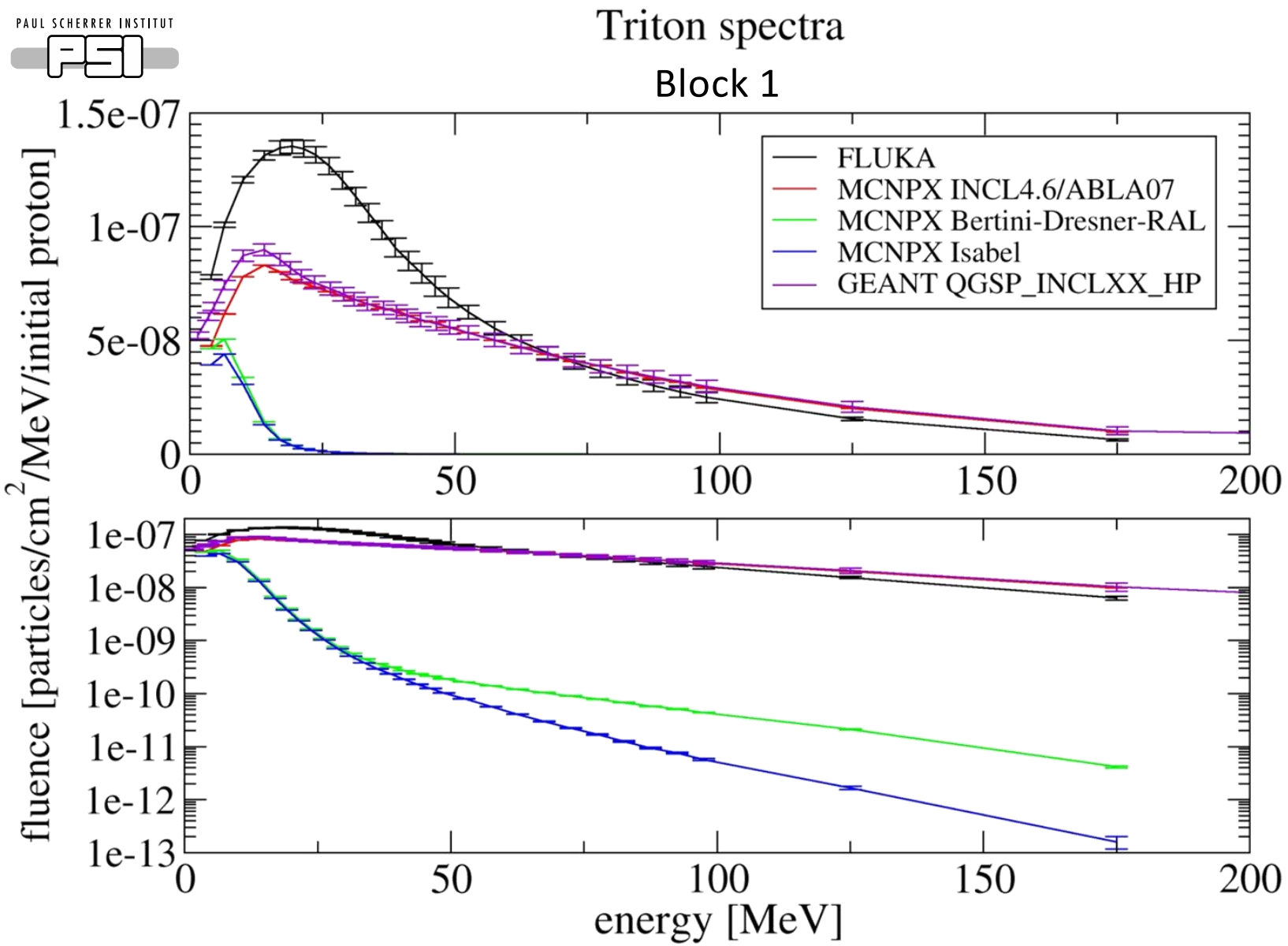
MCNPX INCL4.6 & GEANT INCLXX: same tail, different peak

MCNPX INCL4.6 & FLUKA: same peak, different tail

FLUKA: extra bump in tail



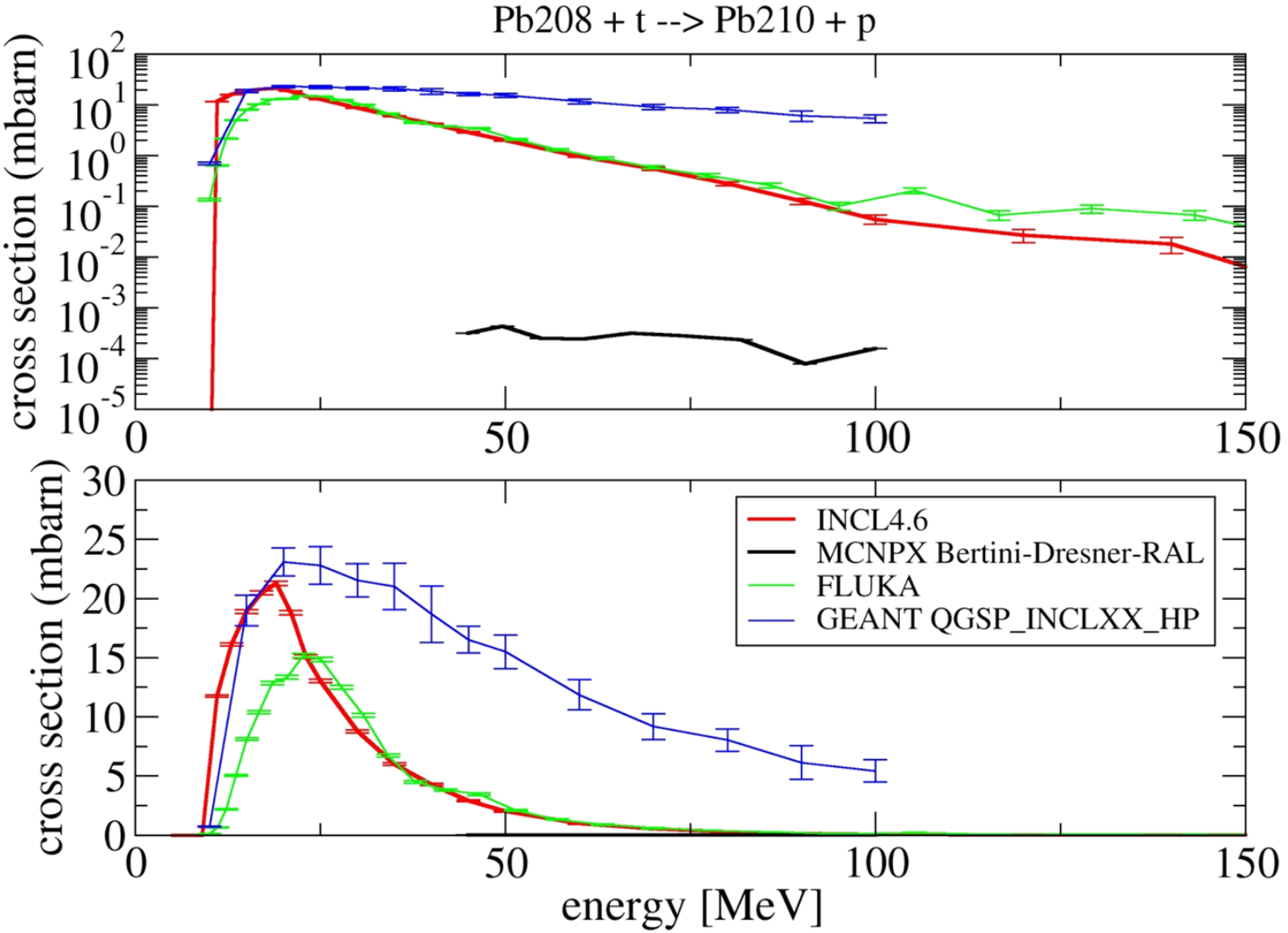
Except for Bertini-Dresner the other cross section models lead to very similar results and are in agreement with the exp. data.



Bertini + Isabel: missing the tail = high energetic particle due to forward emission in direct reactions

MCNPX INCL4.6 & GEANT INCLXX very similar

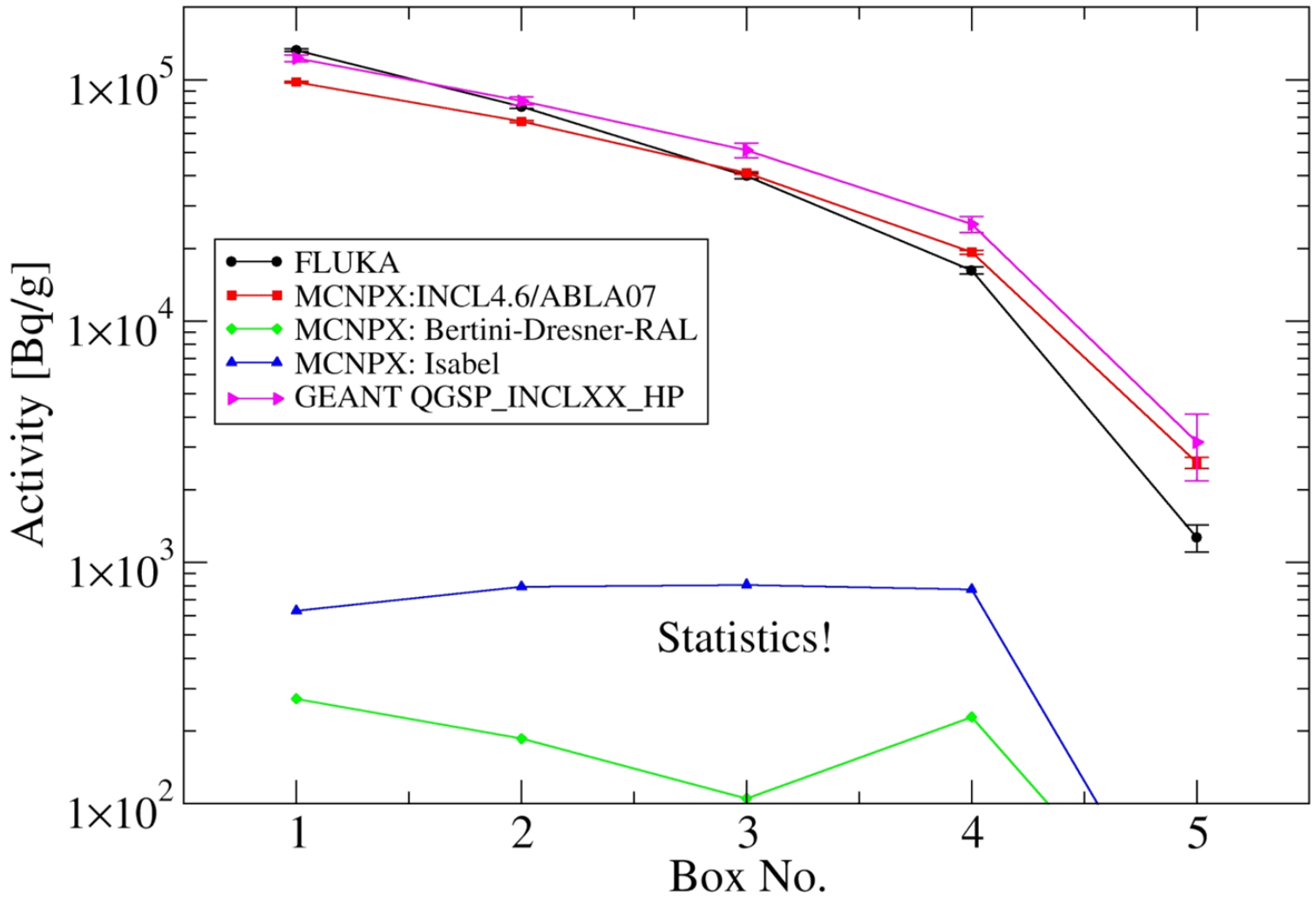
Production cross section of Pb210 via tritons



- MCNPX Bertini c.s. 4 orders of magnitude smaller
- GEANT INCLXX has a larger tail

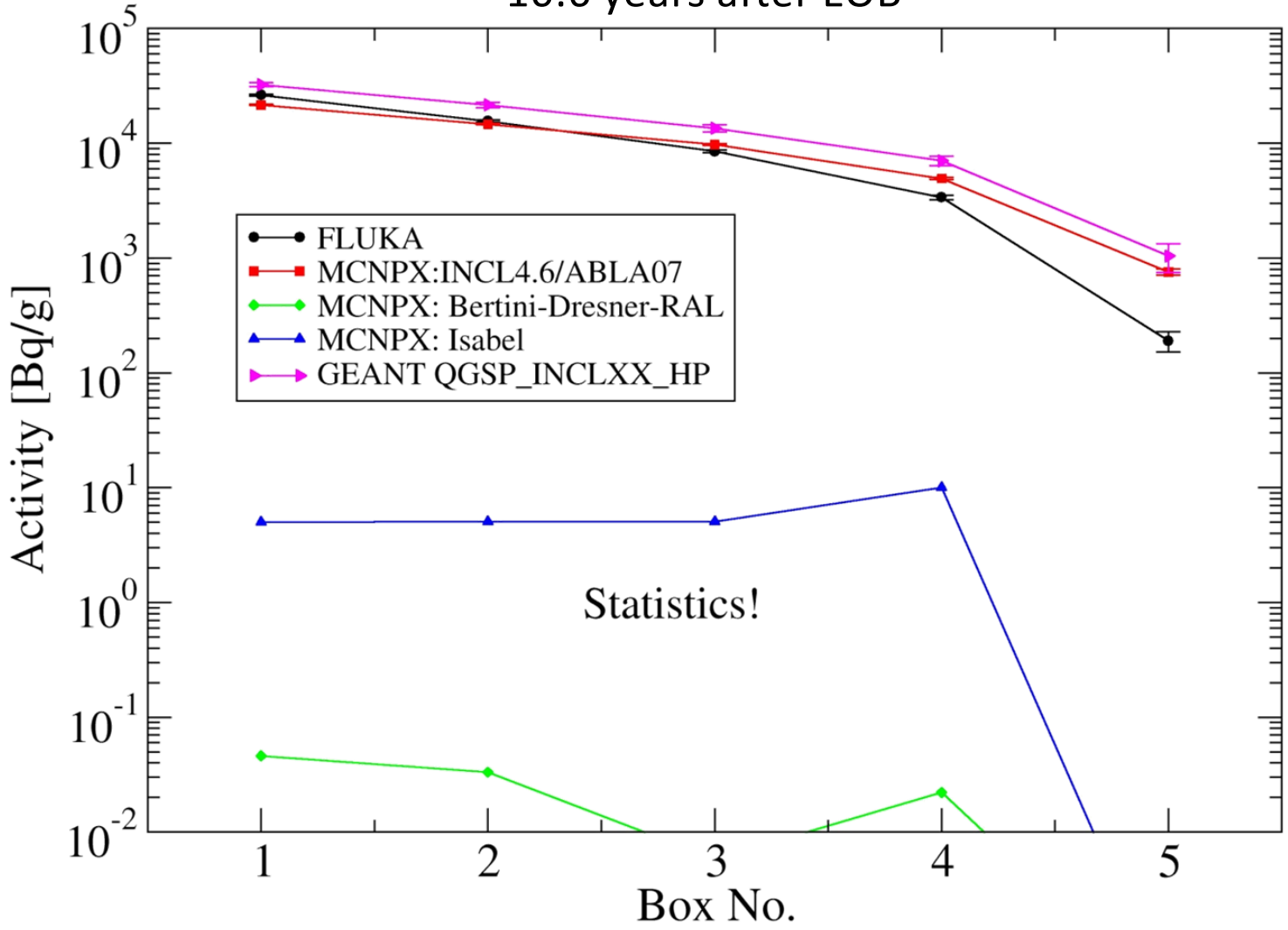
Po208 production in Lead

10.6 years after EOB



FLUKA & MCNPX INCL4.6 & GEANT INCLXX lead to quite similar for Po208

Po209 production in Lead
10.6 years after EOB



FLUKA & MCNPX INCL4.6 & GEANT INCLXX lead to quite similar for Po209

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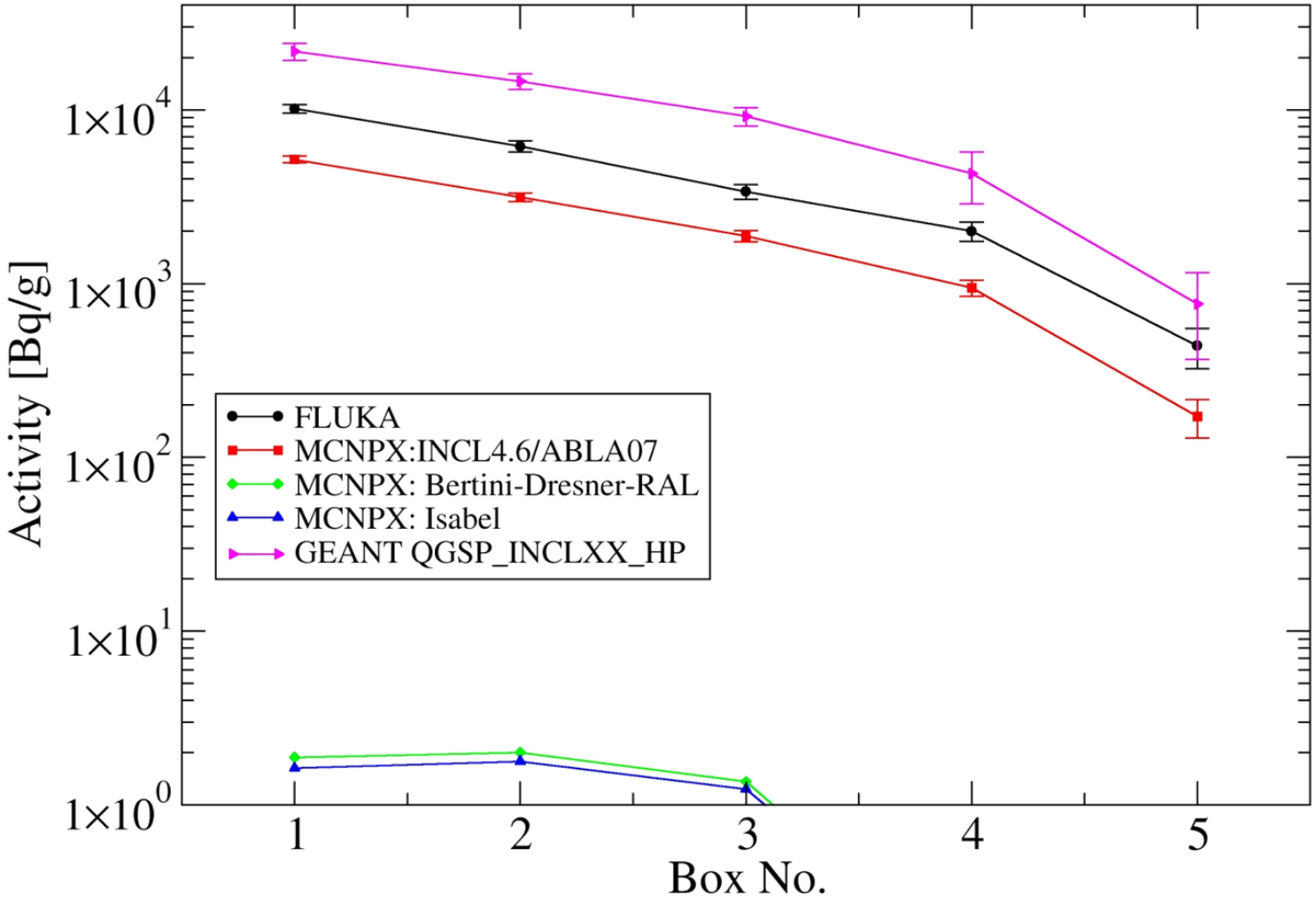
Po210 production in Lead

10.6 years after EOB → direct Po210 production is decayed

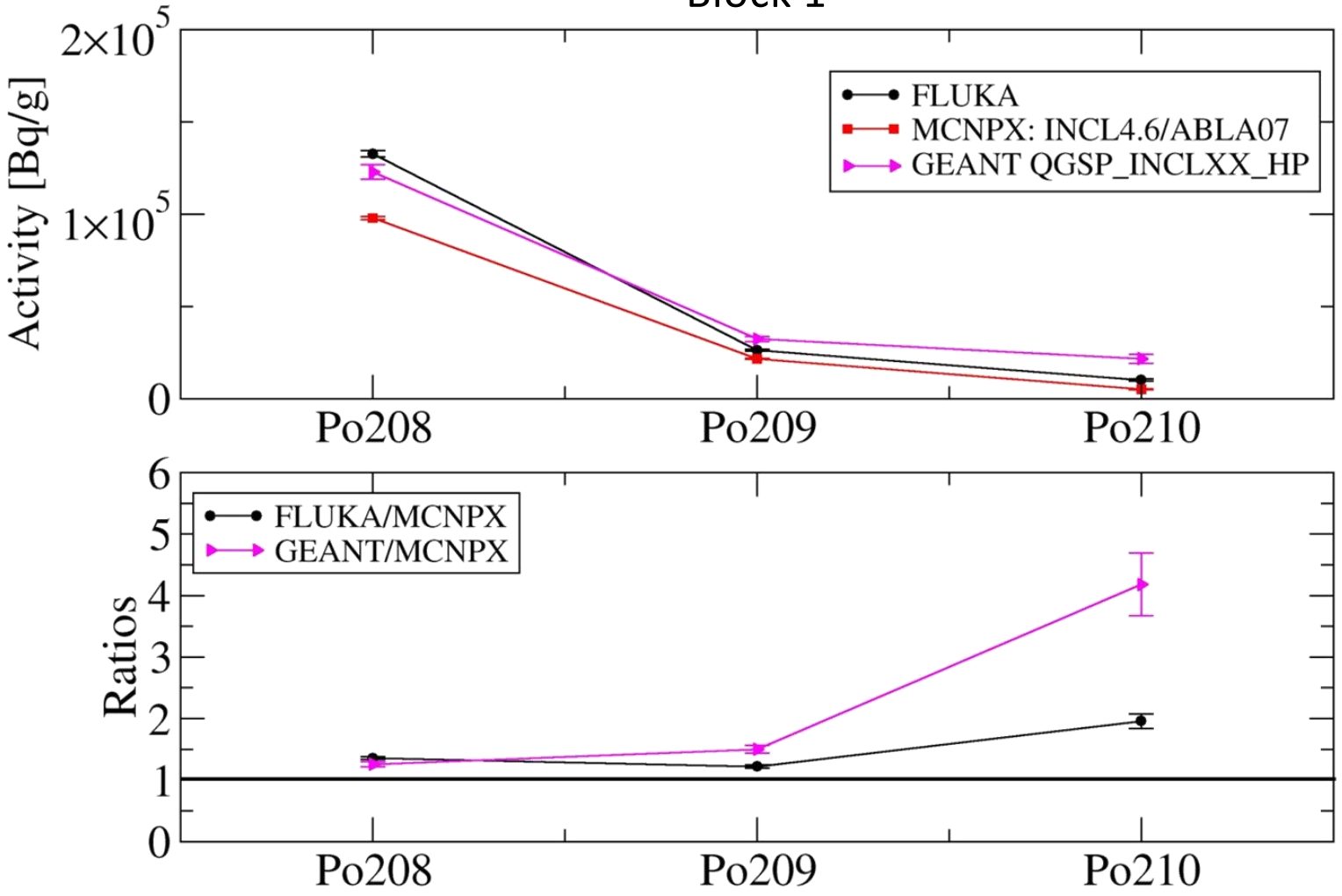


Compared to Po208, Po209 (production due to alphas)

the codes show the larges differences for Po210 (production by tritium via Pb210)

Comparison of FLUKA, GEANT, MCNPX

Block 1



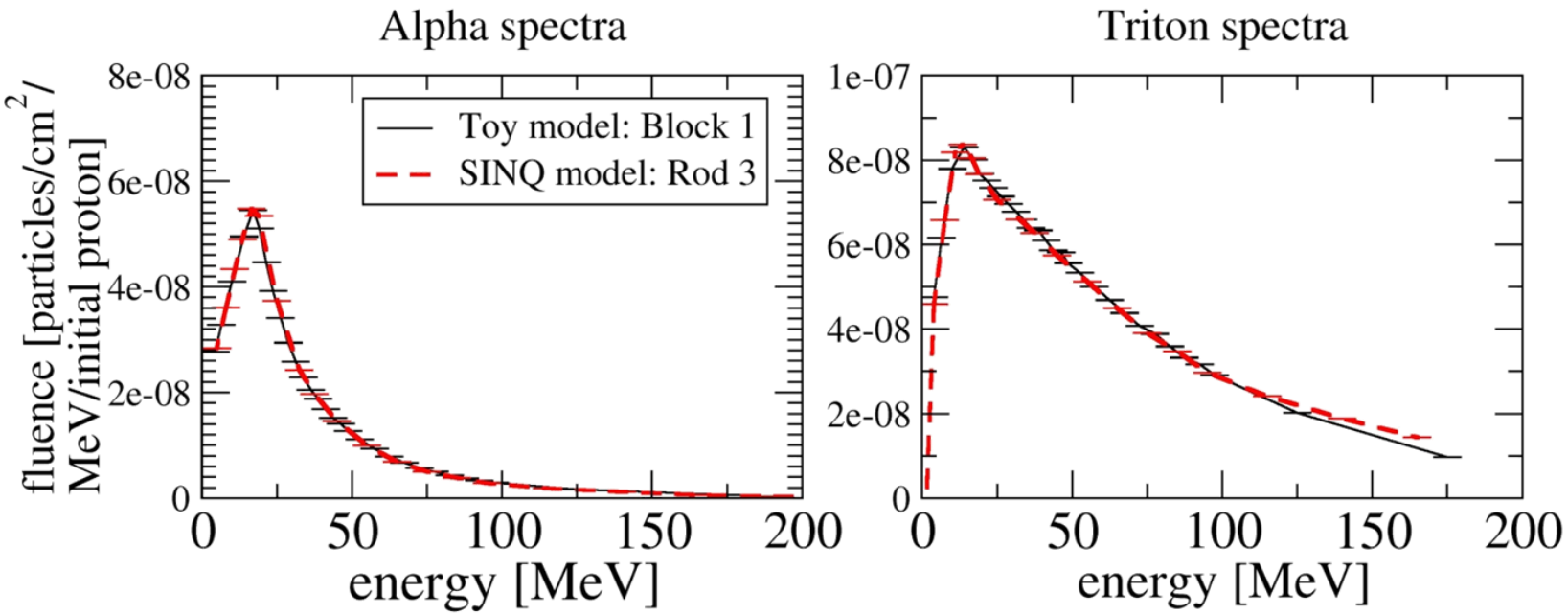
FLUKA/MCNPX: 1.2 to 2

GEANT/MCNPX: 1.2 to 4

Predictions are very close to each other

- despite of these more difficult reactions

Comparison Toy model and SINQ model using MCNPX INCL4.6/ABLA07



Spectra for Alphas and for Tritons obtained in

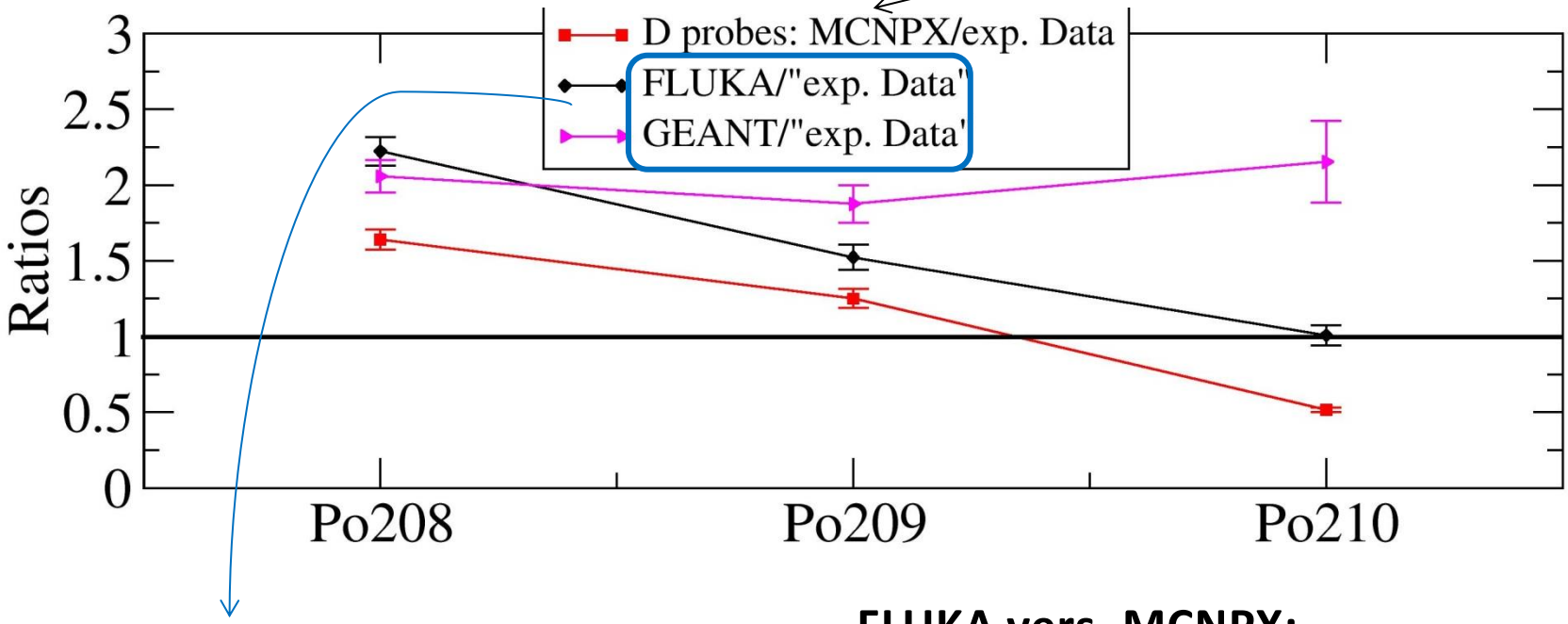
- Block 1 of simplified Toy model
- Rod 3 with detailed SINQ model (Normalization scaled)

almost identically.

→ Comparison of activities
in Block 1 of Toy model with exp. data in Rod 3 justified.

Comparison with exp. Data taken at SINQ

Simulation using the detailed SINQ model



$$\frac{\text{FLUKA}}{\text{MCNPX(Toy m.)}} \qquad \frac{\text{MCNPX(SINQ m.)}}{\text{exp. Data}}$$

FLUKA vers. MCNPX:

- more conservative
- better prediction for Po210
- max. deviation from data: 2 for both models

Geant vers. MCNPX:

- more conservative
- max. deviation from data: 2 (almost constant)

Summary

Benchmark of MCNPX, FLUKA, GEANT using different models for c.s.

- Main primary reaction: 575 MeV p on bulk Pb
- Main goal:

  Comparison of the Po208, Po209 and Po210 activities.

Production via alpha and triton capture on Pb isotopes

Good agreement of all 3 codes using modern cross section models !

Comparison with exp. data taken on Rod 3 in SINQ:

Alpha and triton spectra are very similar in the toy and SINQ model

→ Scaling of the exp. data and comparison with toy model results

→ Maximum deviation of the Po activities predicted by all 3 codes from the exp. data is 2!

Acknowledgement

- Dorothea Schumann
- Tobias Lorenz

for providing the exp. data

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Po-210 production in the central part of Rod3