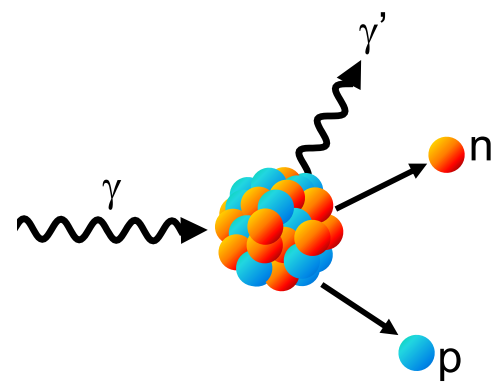


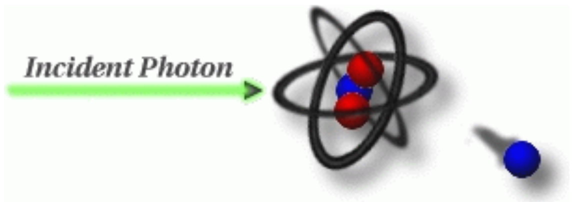
COMPARISON OF THE VALIDATION OF PHOTO-NUCLEAR PREDICTIONS WITH GEANT4, FLUKA AND MCNP FOR SELECTED TEST CASES IN HIGH ENERGY RANGE

L. Quintieri (ENEA-Casaccia), M. G. Pia (INFN-Genova) , M. Augelli (CNES-Toulouse), P. Saracco (INFN-Genova), M. Capogni (ENEA-Casaccia), G. Guarneri (ENEA-Portici)

SATIF13-Helmholtz-Zentrum Dresden-Rossendorf

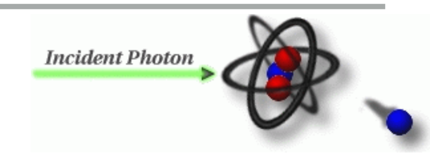
October 10-12, 2016

SUMMARY

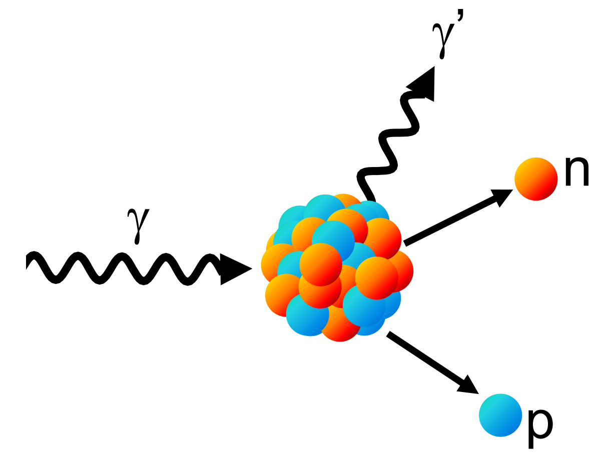


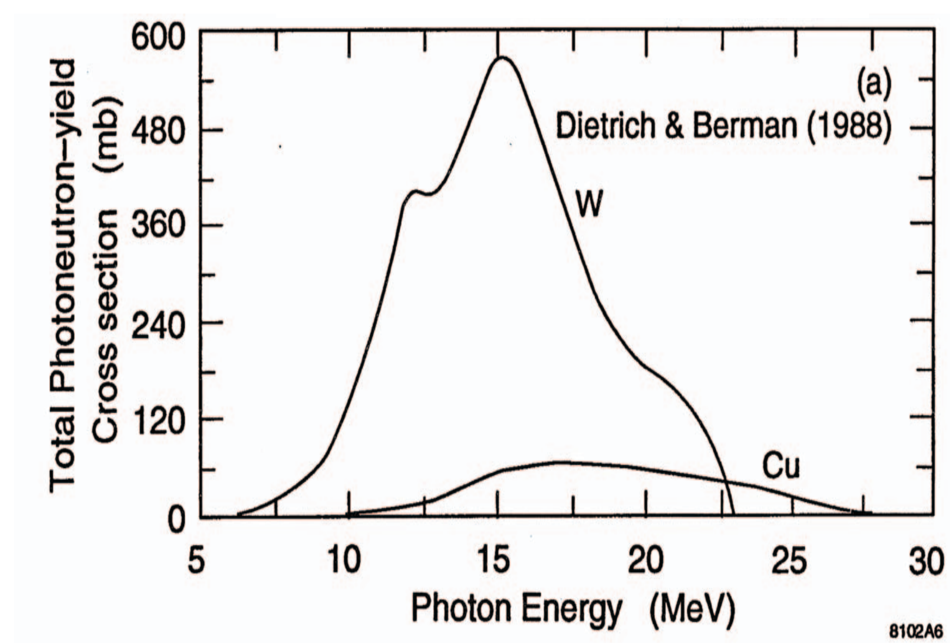
- **Photo-nuclear physics** and its relevance in high energy applications
- **Implementation** of photo-nuclear physics in MC codes
- The **experimental context** of this work
- Photo-nuclear physics in **Fluka, Geant4 and MCNP:** a brief **introduction**
- **Statistical approach** to compare code prediction capabilities in rigorous and quantitative way
- **Photo-nuclear cross sections** implemented in the selected codes **compared** to experimental ones (when available) or evaluated data: **some preliminary analysis results and considerations**

PHYSICS OVERVIEW



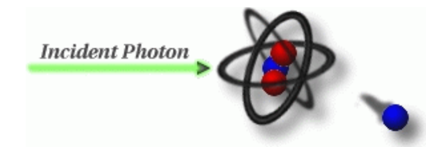
- Photons interact with nuclei causing the emission of nucleons (neutron, protons, pion, etc)
- Photon energy levels above the nuclei binding energy (5-15 MeV) are necessary. Photo-nuclear interactions are threshold reactions: threshold is lower for heavy nuclei
- In heavy nuclei photo-nuclear reactions are almost equivalent to photo-neutron ones. Protons can be emitted, but the presence of a large Coulomb barrier strongly repress this channel.
- Below Z=20, proton yield is in general larger than the neutron yield. The contrary happens for heavy nuclei.



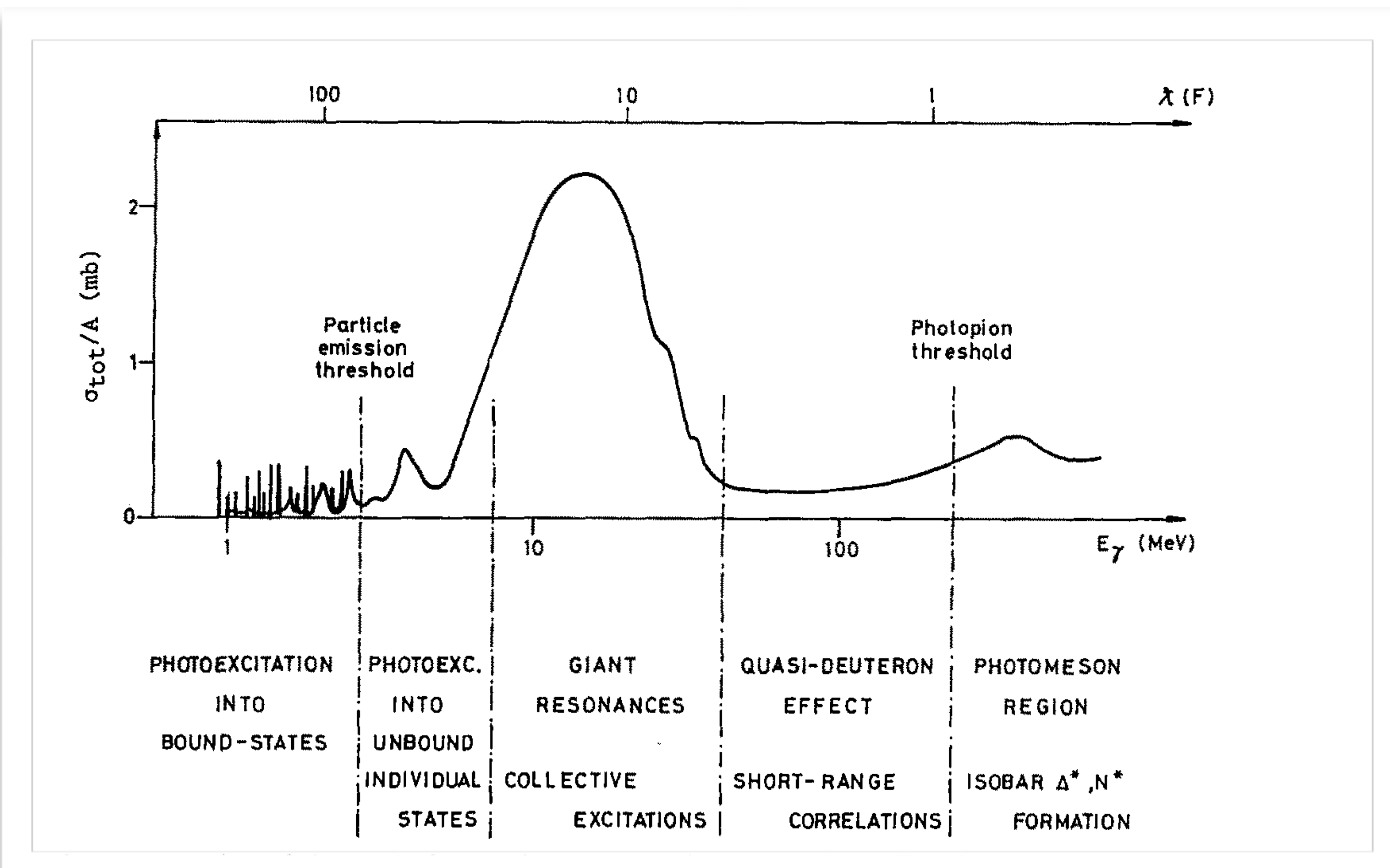


Typical photo nuclear photoneutron cross section behaviour for medium (Cu) and high (W) Z materials

NUCLEI ENERGY DEPENDENT DE-EXCITATION PROCESSES



A photonuclear interaction begins with the absorption of a photon by a nucleus, leaving the nucleus in an excited state. The excited nucleus then undergoes the de-excitation process, emitting secondary particles and possibly undergoing fission.



Nuclear Resonance Fluorescence (NRF)
E<2 MeV

Giant Dipole Resonance
relevant for photon energies in the range 12-16 MeV

Quasi-Deuteron Absorption
relevant for photon energies < 140 MeV

Delta Resonance
E>140 MeV (pion mass)

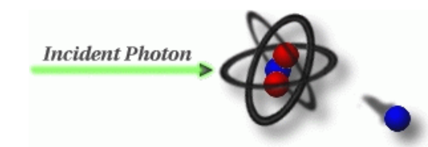
$$\sigma(\gamma+p\to p+\pi^0)\equiv\sigma(\gamma+n\to n+\pi^0)$$
$$\sigma(\gamma+p\to n+\pi^+)\equiv\sigma(\gamma+n\to p+\pi^-).$$

PION PRODUCTION BECOMES POSSIBLE

Photo-Meson
Region E>350 MeV

WHY THE INCREASING INTEREST IN PHOTO NUCLEAR PHYSICS?

Photo-induced reaction cross section data are of importance for a variety of current and emerging applications:



Radiation Shielding Design

In medical and industrial linear electron accelerators, high energy accelerator complex, reactors (of particular concern are photo-neutrons produced by photons in high atomic number material with energies above the neutron separation energy-typically above 8 MeV)

Neutron Sources

Need of new cost effective intese neutron sources.
Accelerator driven neutron sources for radiopharmaceutical production.

Absorbed dose

Calculation of absorbed dose in the human body during radiotherapy

Nuclear waste

Transmutation of nuclear waste either directly by photons or by neutrons created from photo-nuclear reactions (ADS applications)

Fission reactors

New generation physics and technology of fission reactors (i.e new lead cooled fast reactors): influence of photo reaction on neutron balance

Electron beam-dumps

Design of electron beam-dumps in high energy physics context (es. ELI high brilliance laser facility should foresee dump for 800 MeV electrons)

Activation analysis

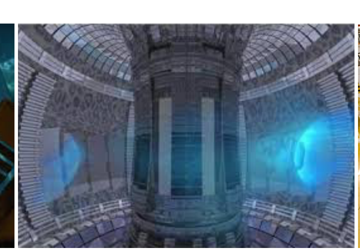
Activation analyses, safeguards and inspection technologies (identification of materials through radiation induced by photo-nuclear reactions using portable bremsstrahlung devises

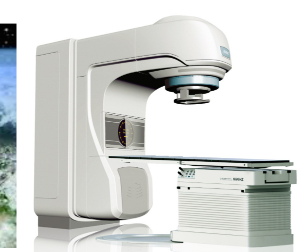
Nuclear astrophysics

Photo-nuclear reactions play an important role in stellar nucleosynthesis

Plasma diagnostics

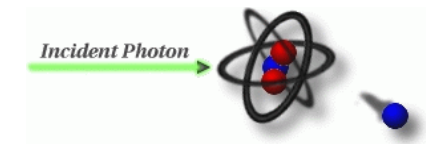
In fusion energy technologies

CODE IMPLEMENTATION OF PHOTO NUCLEAR PHYSICS

Computational issues of photo-nuclear physics in particle transport and interaction codes have been mainly related to:



1. **For a long time photo-nuclear processes were neglected mainly due to the lack of complete evaluated data for applications.**
    - Experimental photo-nuclear data from different laboratories (Lawrence Livermore National Laboratory, Commissariat à l'Energie Atomique, Saclay, Argonne National Laboratory, Illinois etc.) often show(ed) discrepancies that must be resolved in the evaluation process
    - Only a few measurements of the energy- and angle-dependent spectra of secondary particles emitted in photo-nuclear reactions. Most of the existing spectral measurements are for bremsstrahlung, while measurements from mono-energetic sources give emission spectra directly useful for cross-section evaluations
2. **Photo-nuclear data are isotopic in nature, the cross sections showing irregular dependence on atomic number (Z) and atomic mass (A).** Thus while photo-atomic data are readily tabulated by element, instead photo-nuclear data must be tabulated for each isotope of an element
3. **A relatively complete photo-nuclear data file in ENDF format for 164 isotopes became available only "recently", in 2000** (ENDF-6 formatted files containing complete interaction descriptions, i.e., double differential cross sections, suitable for use in transport calculations)

FLUKA Geant 4 mcnp PHITS Particle and Heavy Ion Transport code System TRIPOLI CODE

IAEA REPORT TEDOC-1178 (2000)

"Handbook on photo nuclear data for applications, cross-sections and spectra"..

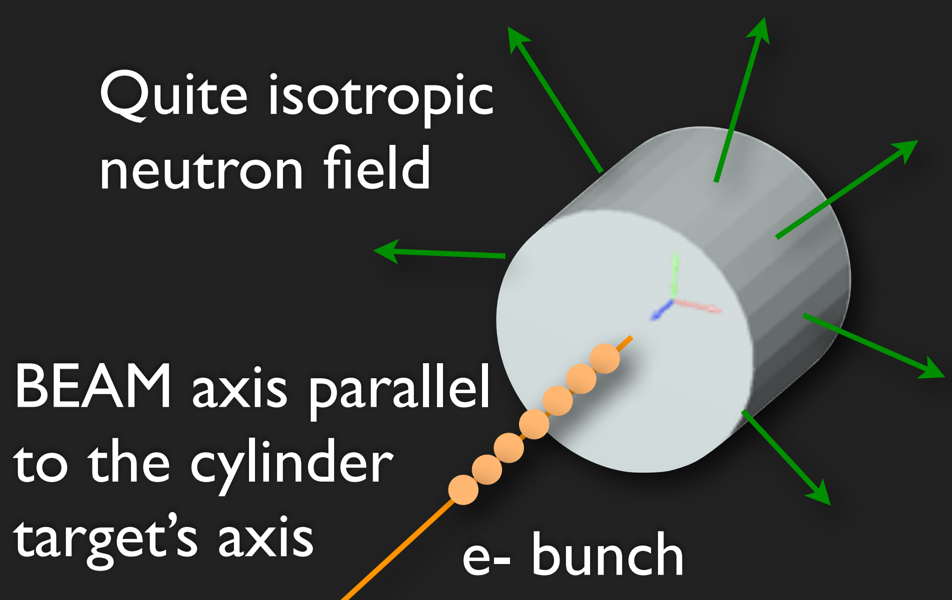
The IAEA Photonuclear Data Library is consisted of files originated from five laboratories.

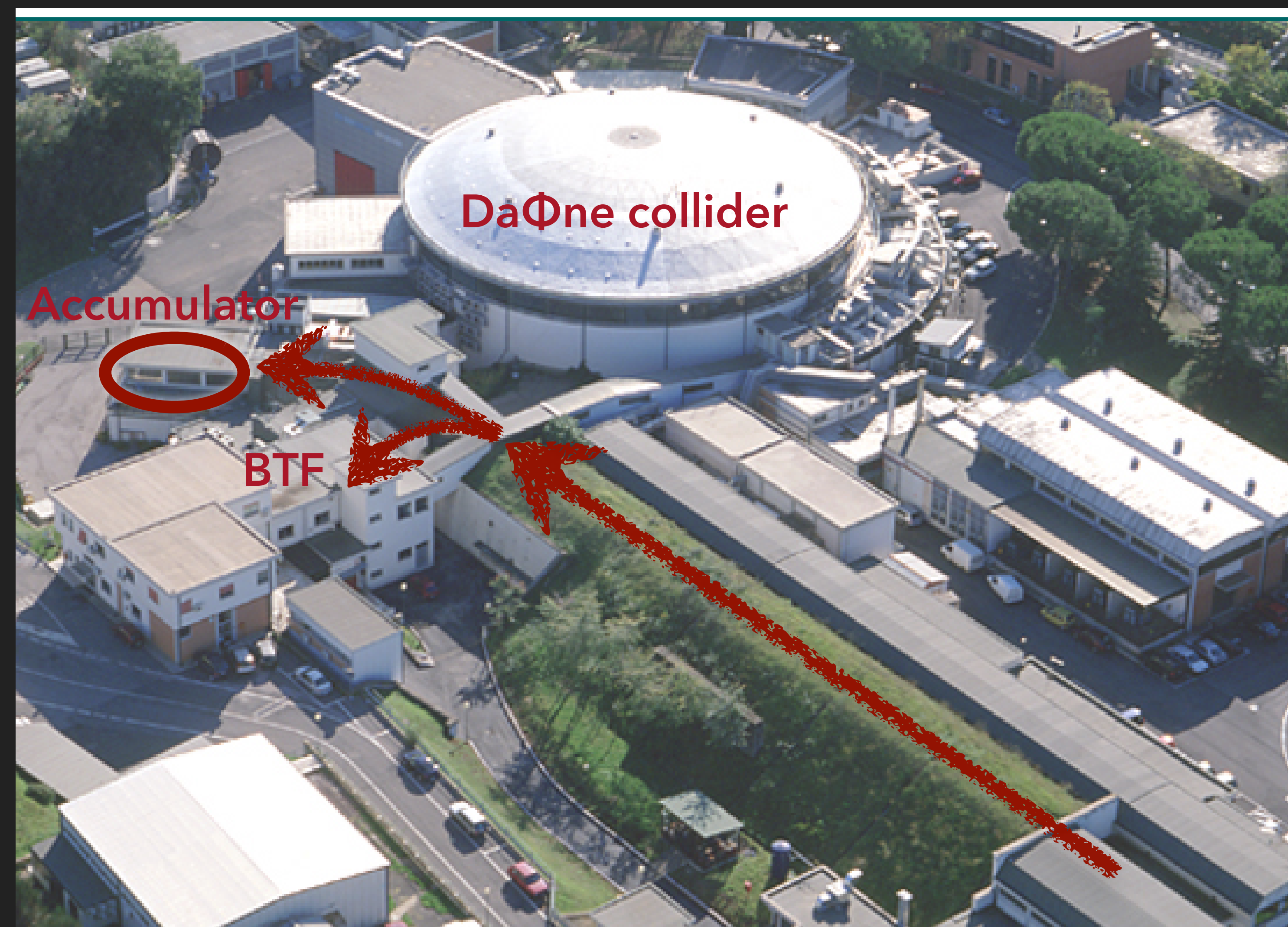
A selection of the worldwide experimental measurement has been accurately performed to provide to scientific community a "Reccomended" photo nuclear data

https://www-nds.iaea.org/photonuclear/

THE EXPERIMENTAL CONTEXT THAT MOTIVATED THIS WORK:

USE OF MC CODE TO DESIGN A LOW INTENSITY PHOTO-NEUTRON SOURCE AT LNF-INFNF FRASCATI NATIONAL LABORATORIES





High current Linac:

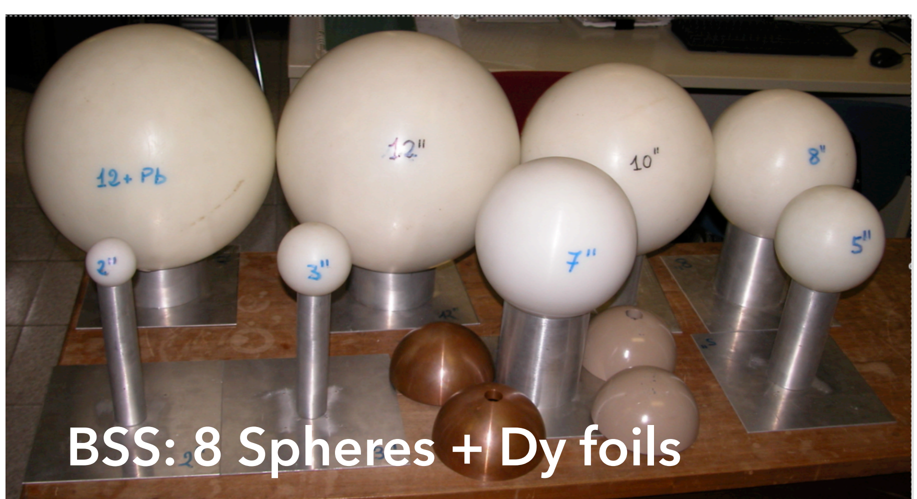
- 500mA for e^-
- 200mA for e^+
- 1 - 10 ns pulses (10^9 particles pe pulse)

PHOTO-NUCLEAR PRODUCTION AT HIGH ENERGY

EXPERIMENTAL MEASUREMENT AT LNF DAΦNE: N@BTF

BTF main e- beam parameters

Parameter	Value
Energy Range	25-750 MeV (e-) 25-510 MeV (e+)
Transverse emittance @ 510MeV (both planes)	1mm mrad (e-) 10 mm mrad (e+)
Energy Spread @ 510 MeV	1% (e-) 2 % (e+)
Repetition Rate	1-50 Hz
Number of particles per pulse	1-10^10
Macro Bunch duration	1 or10 ns
Spot size (mm)	2mm (single particle) 2 cm (high multiplicity)

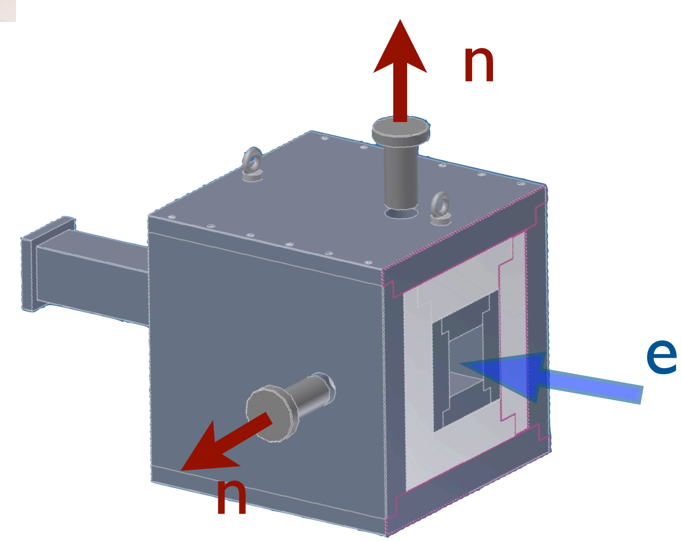


BSS: 8 Spheres + Dy foils

W-nat target:

R =3.5 cm, L=6 cm

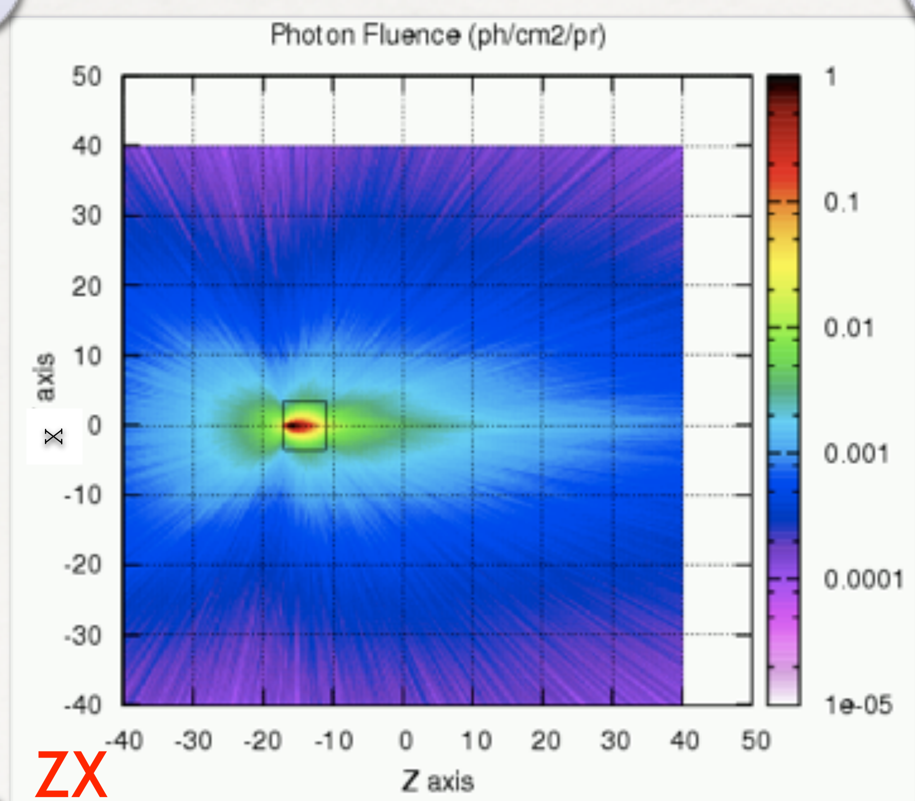
First Measurements May 2010

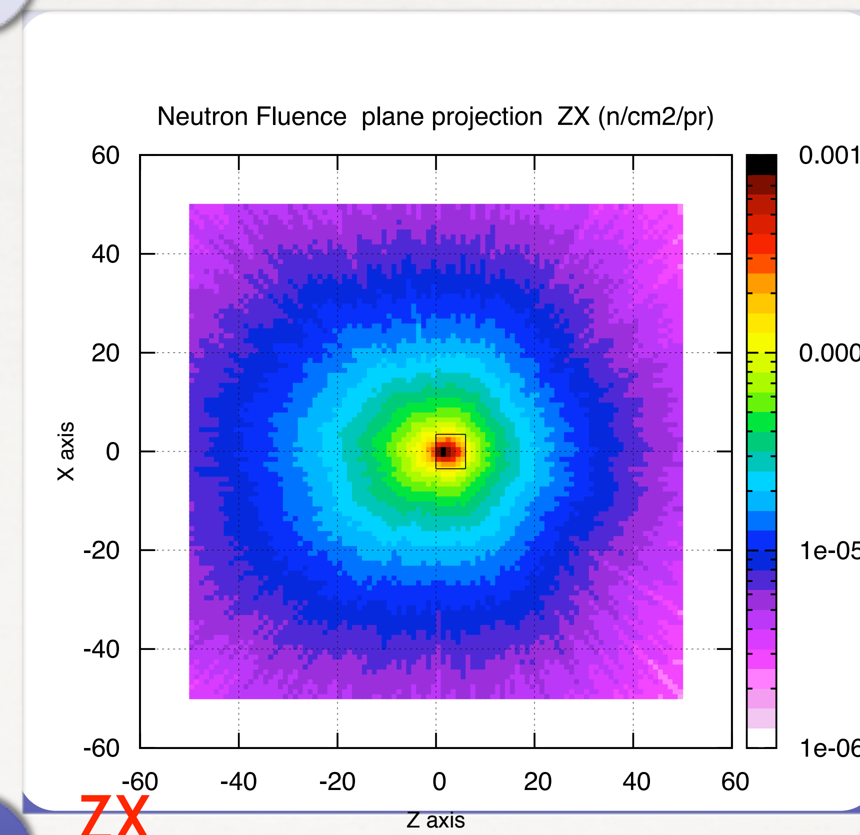


2 Extraction Lines @ 90° wrt the beam direction (Φ_{hole}=70 mm)

Expected Neutrons and Photons:
(target in vacuum)

Spatial distribution





Higher intensity and hardest Gammas
in forward direction. More than 2 order of magnitudes
of difference in photon fluxes @ 90° and 0 °
wrt beam direction

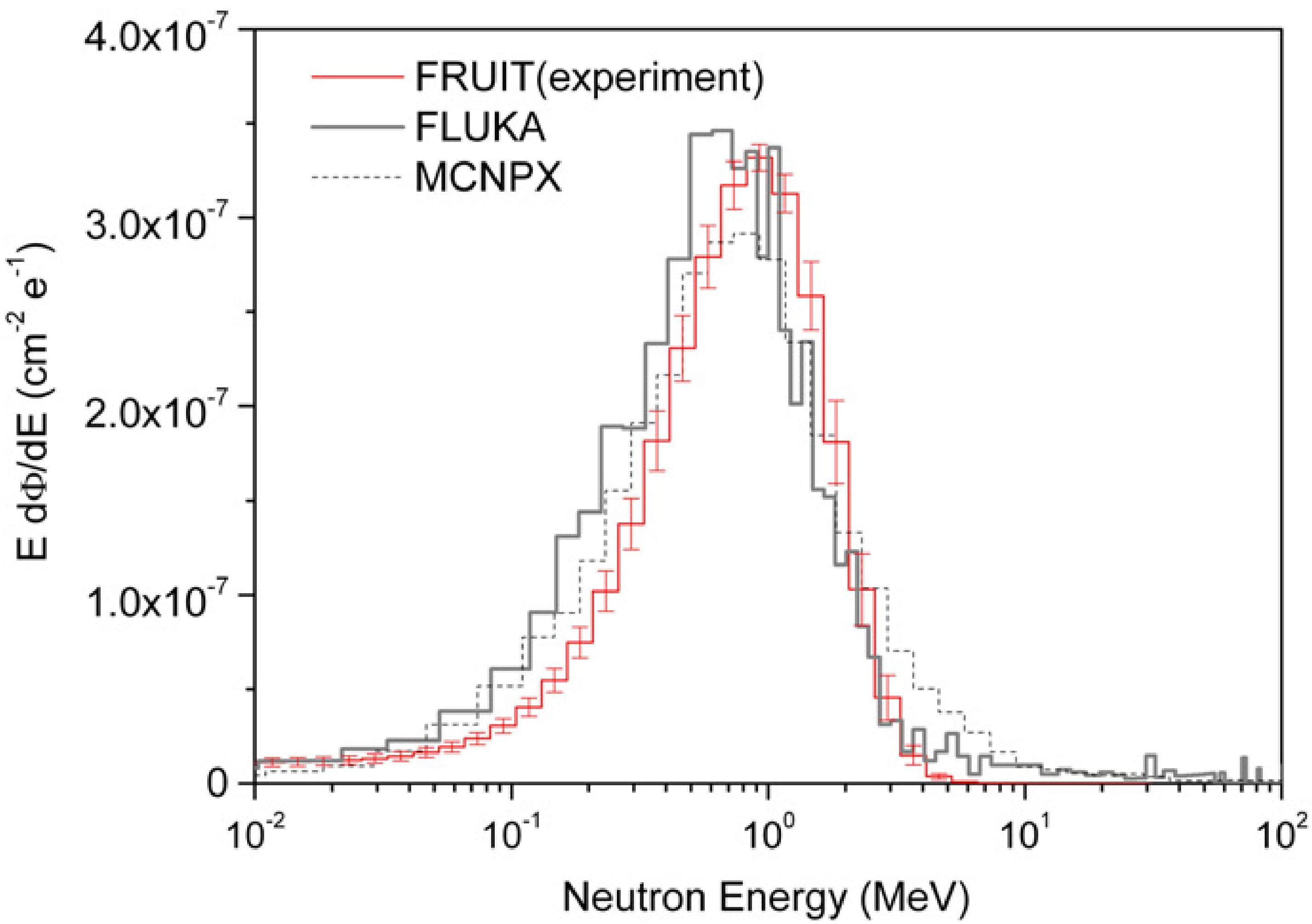
Quite well isotropic

EXPERIMENTAL AND COMPUTATIONAL RESULTS

Ref: Nuclear Instruments and Methods in Physics Research A 659 (2011) 373-377

The measurement point twas at ~150 cm from the target and at 90° wr to the impinging electron beam line

Lethargic (dΦ/dE)*E spectrum normalized to the total flux



Total Neutron Flux per primary particle		
Ex. Measurement	FLUKA	MCNPX
8.04E-7 ±3%	8.10E-7 ±4%	8.02E-07 ±0.2%

The flux above 10 keV is 6.53E-7 /cm2/pr

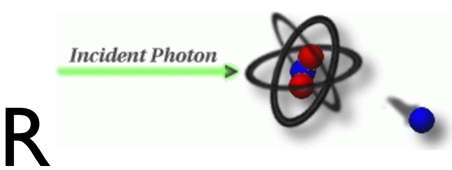
As expected, more than 80% is found around the Giant resonance (from 10 KeV up to 20 MeV)

Statistical uncertainty in the calculations less than 4%

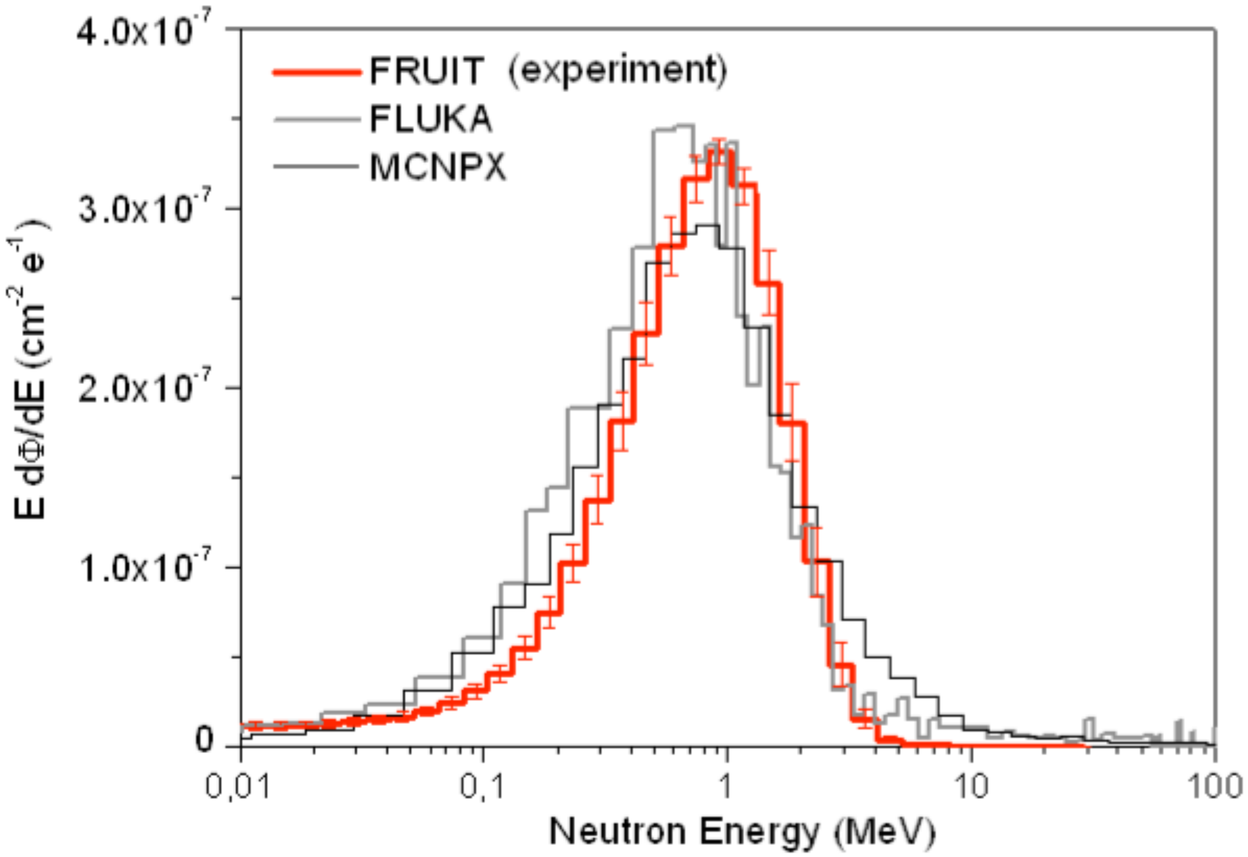
Max neutron Flux currently available in BTF

Neutron Flux at 1.5m from shield = 4E+5 n/cm2/s corresponds to Equivalent Dose=45 mSv/h

MC ACCURACY WR TO EXPERIMENTAL DATA



GoF tests to asses quantitatively the accuracy around the GDR



	Neutron fluence per incident electron $\Phi(10^{-7}\,\mathrm{cm}^{-2})$
FRUIT (experiment)	8.04 ± 0.25
FLUKA	8.12 ± 0.04
MCNPX	(Tally F4) 8.06 ± 0.04
	(Tally F5) 8.020 ± 0.002

Both FLUKA and MCNPX provide an accurate reconstruction of the experimental resonance, both in energy position and amplitude

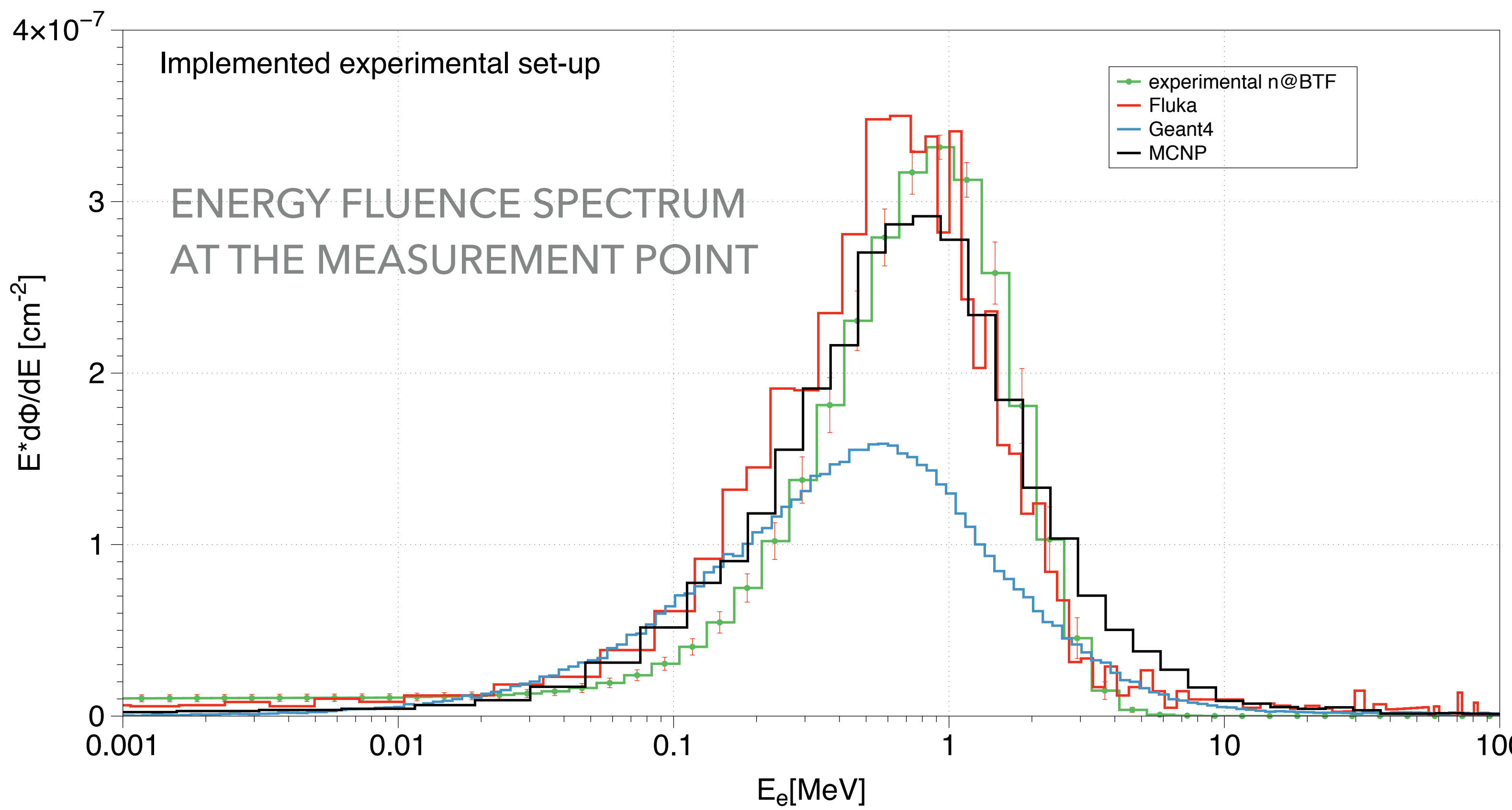
$$\chi^2=(MC^2-Exp^2)/(\sigma^2_{MC} + \sigma^2_{Exp})$$

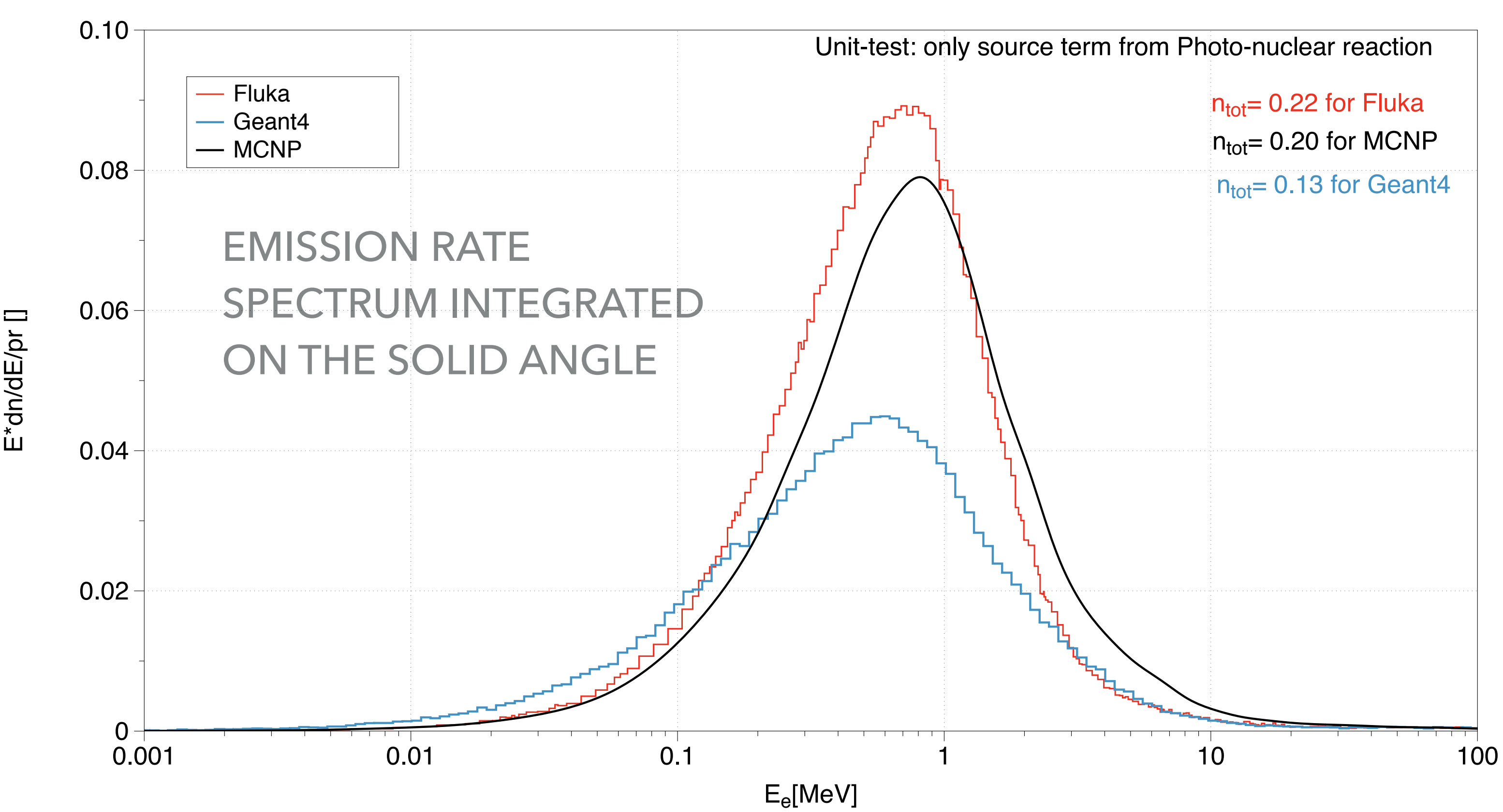
TEST FLUKA-EXP
χ2 TEST: P VALUE 0.967

TEST MCNPX-EXP
χ2 TEST: P VALUE 0.996

WHAT ABOUT GEANT4 PREDICTIONS?

SIMULATION OF THE OVERALL EXPERIMENTAL APPARATUS



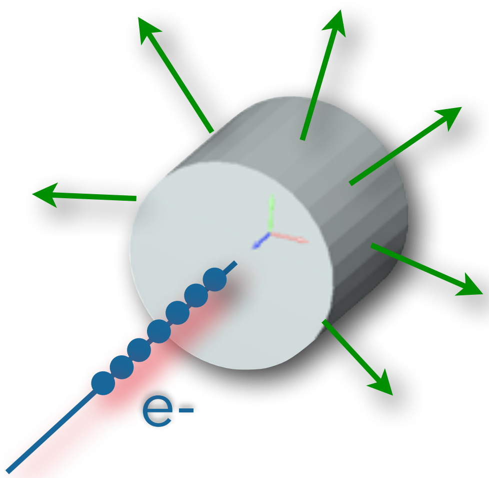


Unit test case: only EM +photo-nuclear in the target reducing the spurious dependencies

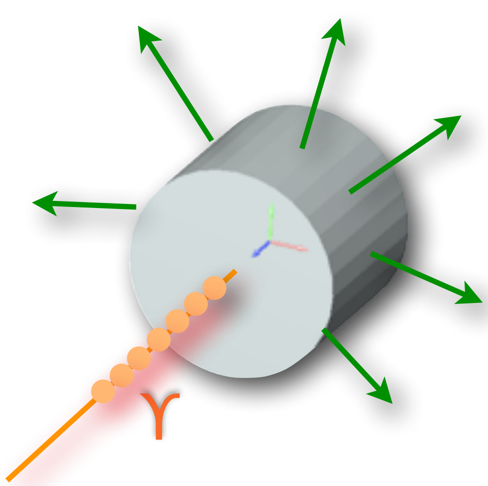
GEANT4 UNDERESTIMATES OF ABOUT 30% THE PHOTO NEUTRONS PRODUCED

NEUTRON SOURCE TERM ESTIMATION FROM BULK W: E- AND GAMMA

Tungsten case



510 MeV electrons	Physics Implemented	Neutron produced per SP	Proton produced per SP	Neutron escaping per SP	Proton escaping per SP
FLUKA	Precisio/Photonuc (+bias)	**0.22** ± 0.45%	1.44E-3 ±0.9%	**0.20** ± 0.45%	4.35E-5 ±3.6%
Geant4 "n@BTF"	QGS_BERT QGS_BERT_HP Shielding	**0.12** ±3%	1.74E-03 ±6%	**0.1** ±3%	6.5E-05 ±7%
Geant4 "Hadr-Extendend"	QGS_BERT QGS_BERT_HP Shielding	**0.13** ±3%	1.76E-03 ±6%	**0.1** ±3%	6.8E-05 ±7%

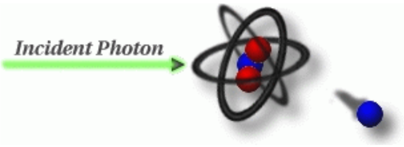


510 MeV gammas	Physics Implemented	Neutron produced per SP	Proton produced per SP	Neutron escaping per SP	Proton escaping per SP
FLUKA	Precisio/Photonuc (+bias)	**0.26** ±0.12%	2.77E-03 ±2%	**0.22** ±0.12%	1.82E-04 ±1.9%
Geant4	QGS_BERT QGS_BERT_HP Shielding	**0.15** ±3%	3.55E-03 ±6%	**0.12** ±3%	2.64E-04 ±7%

FLUKA simulations: 5E+4 primaries + biasing

Geant4 simulations: 5E+5 primaries

COMPARISON AND VALIDATION OF MC PREDICTIONS



Main goal:

In the frame of the "**Uncertainty Quantification**" **INFN project**, we want to individuate and possibly address the solution of some critical implementation in Geant4 (if any, after careful investigation) or eventually to promote an improvement of the photo-nuclear implementation inside the code itself.

Work approach and strategy:

- Rigorous **Statistical analysis carried out when experimental data are available** for all the nuclei and all the energy ranges (test of goodness of fit and possibly others, according the needs). The best would be to use independent experimental data , that are not used in the parametrisation.
- Since experimental data in high energy range (>150 MeV) are scarse, a special effort will be done to **identify possible significant differences in the theoretical models implemented**
- the **comparison among the results** obtained with independent codes **could highlight** special **needs** of adopting **conservative approach** for those cases potentially found not in agreement, **or**, in addition, **address experiments for benchmarking in upcoming high energy high brilliance facilities** (i.e. ELI)
- The **comparison of the photo-nuclear cross sections**, for all the cases in which we are interested, represents **only the initial part** of the work (still in progress). T**he complete analysis will foresee to compare the secondary particles and the final state** (typology, energy dependence, angular cross section, etc) as well

GOING MORE IN DETAIL OF PHYSICS IMPLEMENTATION IN FLUKA, MCNP, GEANT4

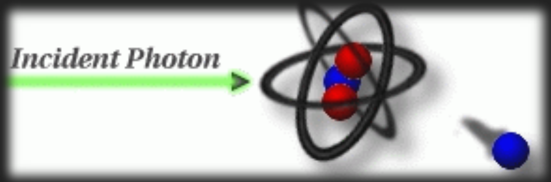
STEP1: Analysis of the implemented photo-nuclear cross sections.

- As initial analysis: we focus on σ(γ,abs): the total photo-absorbtion XS

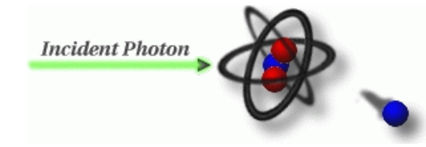
$$\begin{aligned}\sigma(\gamma,abs) &= \sigma(\gamma,sn)+\sigma(\gamma,p)+\sigma(\gamma,2p)+\cdots+\\ &+ \sigma(\gamma,d)+\sigma(\gamma,dp)+\cdots+\sigma(\gamma,\alpha)+\cdots\end{aligned}$$

- In case of heavy nuclei:

$$\sigma(\gamma,abs)\cong\sigma(\gamma,sn)$$



Photonuclear Cross Sections in Fluka



Taking advantage from:

- the new IAEA Photonuclear Data Library for 164 isotopes (2000)
- other evaluated data from various Laboratories (ORNL, LANL, CNDC, JAERI, KAERI, MSU)
- many experimental data made available via the EXFOR database

Important upgrade for the photonuclear physics was done in 2005: the Fluka Library was updated and completed:

At present a total cross section data for 190 nuclides have been inserted

190 nuclides data are tabulated :

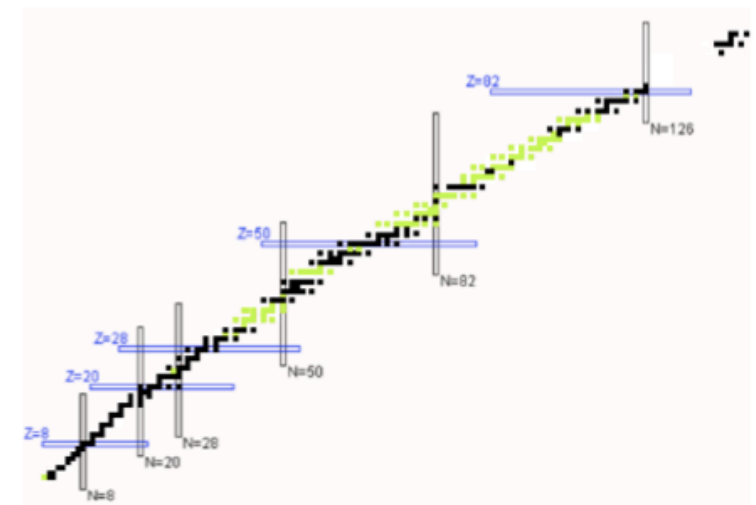


FIGURE 12. The 190 nuclides of the FLUKA GDR total cross section library (black squares). The grey squares indicate the stable nuclides not included in the library

If experimental cross sections are not available then Lorentz fits of the existing data are used:

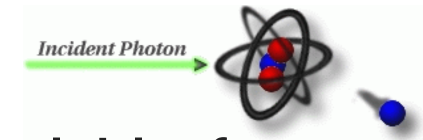
- **If Z>29 then Lorentz parametrization is used (with published Lorentz parameters as peak energy, peak height, width) if they exist.** They are all those reported in the Atlas of Dietrich and Berman Atomic Data and Nuclear Data Tables 38, 199 (1988), except Pr, Au and Pb, for which we have used the parameters published in Berman et al., Phys. Rev. C36, 1286 (1987). otherwise
- **Lorentz parametrization with parametrized Lorentz parameters.** (it sounds funny, but Berman and Fultz (Rev. Mod. Phys. 47, 713 (1975) have published some general formulas giving the 3 Lorentz parameters as a function of A and Z.)

REFERENCE:

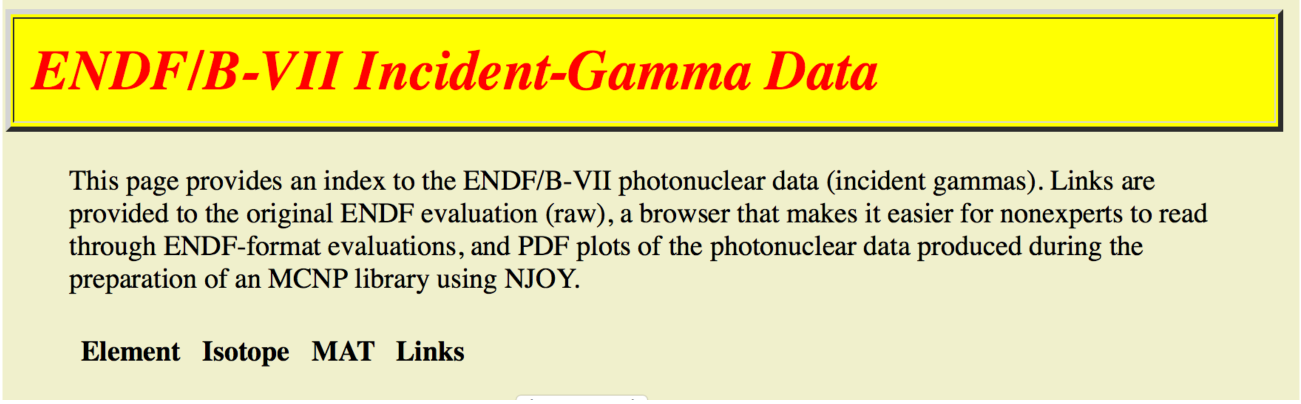
A. Fassò, A. Ferrari, P.R. Sala – Photonuclear Reactions in FLUKA: Cross Sections and Interaction Models – *AIP Conf. Proc. 769 (2005) pp.1303-1306*

MCNP: PHOTO-NUCLEAR CROSS SECTION IMPLEMENTATION

[ref]: LA-UR-13-22934: [*https://mcnp.lanl.gov/pdf_files/la-ur-13-22934.pdf*](https://mcnp.lanl.gov/pdf_files/la-ur-13-22934.pdf)



- **Photonuclear data, including Nuclear Resonance Fluorescence (NRF), is available for 157 specific isotopes up to 150 MeV in the endf7u library,**
- **Photo-nuclear from 1.0 to 150.0 MeV in tabular range.**
- **Above the respective energy for the above reactions and for all nuclides that have no data, interactions are based on theoretical models with empirical corrections.**
- **Photo-nuclear reactions are not active in calculations by default.**
- The photo-nuclear physics implementation in MCNP had **an important upgrade in 2005,** when new physics packages for photons with energies from 5 MeV to about 2 GeV have been added.
- The added models compliment the existing photo-nuclear data, on the base of the **"mix and match"** capability (available with MCNPX2.5.b , November 2002), according to which **table data are used when available, otherwise physics models are applied**
- **The photo-nuclear data files, with the .70u designation, are the latest ENDF/VII issued libraries, as reported in** https://t2.lanl.gov/nis/data/endf/endfvii-g.html

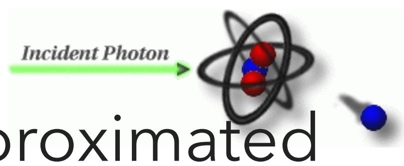

ENDF/B-VII Incident-Gamma Data

This page provides an index to the ENDF/B-VII photonuclear data (incident gammas). Links are provided to the original ENDF evaluation (raw), a browser that makes it easier for nonexperts to read through ENDF-format evaluations, and PDF plots of the photonuclear data produced during the preparation of an MCNP library using NJOY.

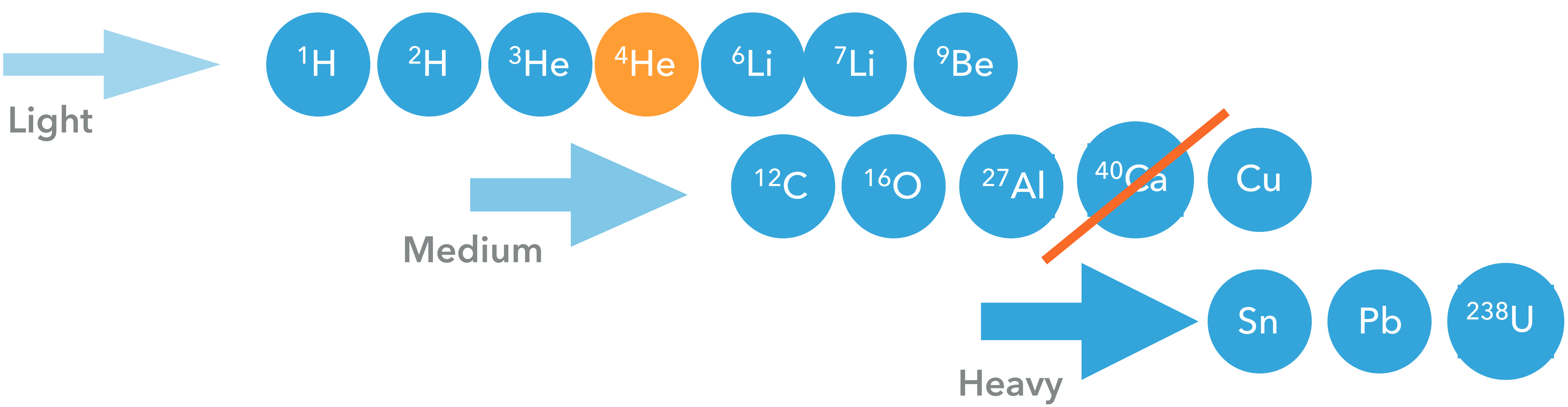
Element	Isotope	MAT	Links

GEANT4: PHOTONUCLEAR CROSS SECTION IMPLEMENTATION

[ref]: J.P.Wellisch, M.Kossov, P. Degtyarenko "Electro and gamma physics in Geant4 "



- Photonuclear interaction cross sections in Geant4 database are approximated for ALL NUCLEI and ALL ENERGIES (from hadron production threshold to about 40 TeV).
- The Geant4 database is made of **parametrised cross sections for 49 nuclei**
- The cross section parametrisation in the different energy range is expressed as function of: Atomic mass "A," energy "e" and several other parameters (ci,pi,si,..) that are calculated for a list of selected 14 nuclei and interpolated for all the other nuclei
- Currently the following 14 nuclei are used in the parametrization and extrapolation to high energy:



COMPLETE LIST OF CROSS SECTION DATA SET IN GEANT4

[ref]: M.V. Kossov "Approximation of photo nuclear interaction cross-section" EPJ A.14, 2002

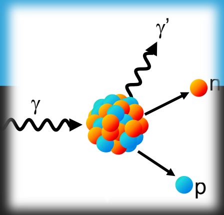
2H	4He	6Li	7Li	9Be	12C
14N	15N	16O	19F	23Na	24Mg
27Al	28Si	32S	34S	40C	40Ar
54Fe	58Ni	59Co	63.5**Cu**	65.4**Zn**	76Se
82Se	107.8Ag	112.4**Cd**	118.7**Sn**	126.8**I**	154Sm
156Gd	159Tb	165Ho	168Er	174Yb	178Hf
181Ta	184W	186W	197Au	204.4**Tl**	207.2**Pb**
209Bi	232Th	235U	238U	239Pu	

Blu boxes are natural element. The isotopes in the green circles are not documented in the Kossov reference work.

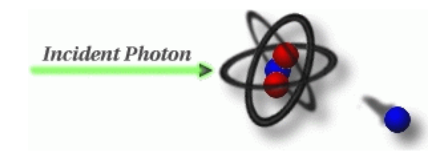
The photo-absorbption cross sections for the isotopes and elements in the red circles have been analysed and compared to,respectively: a) IAEA recommended, b) FLUKA implemented, c) the MCNP used.

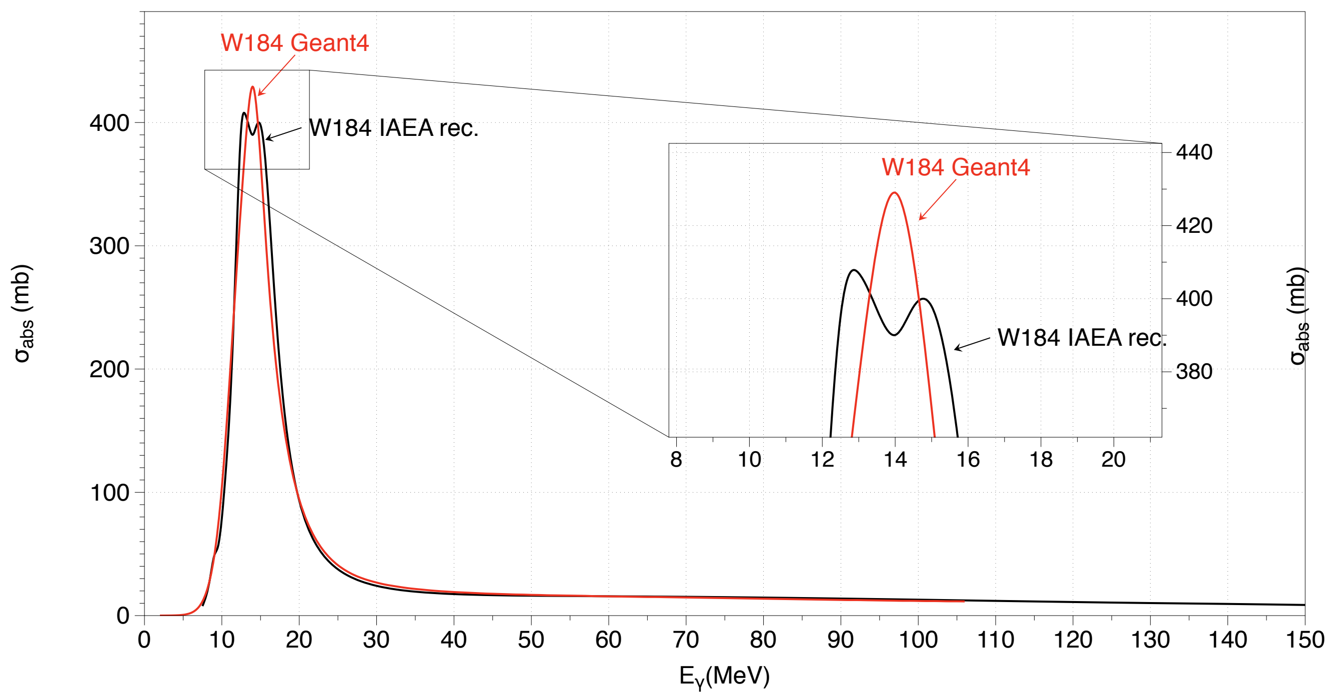
STATISTICAL TESTS OF COMPARISON AMONG IMPLEMENTED CROSS SECTIONS IN THE CODE AND THE THE IAEA RECOMMENDED ONES:

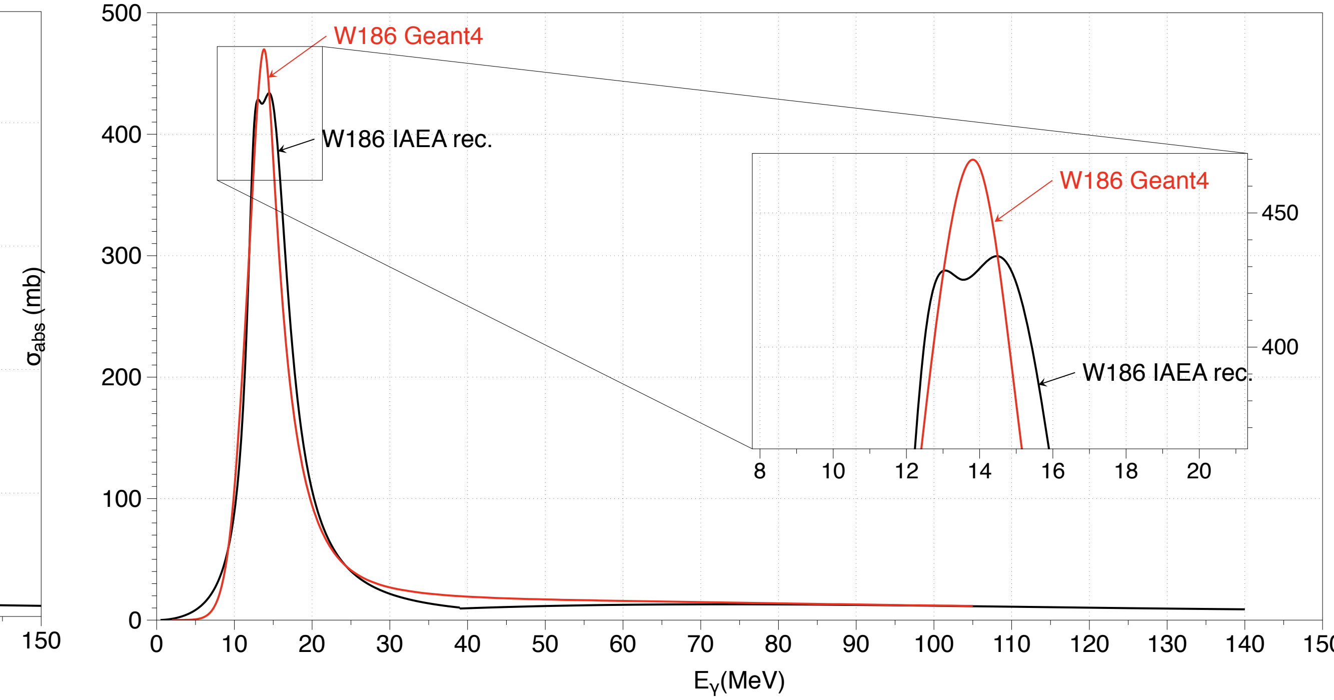
SOME PRELIMINARY RESULTS



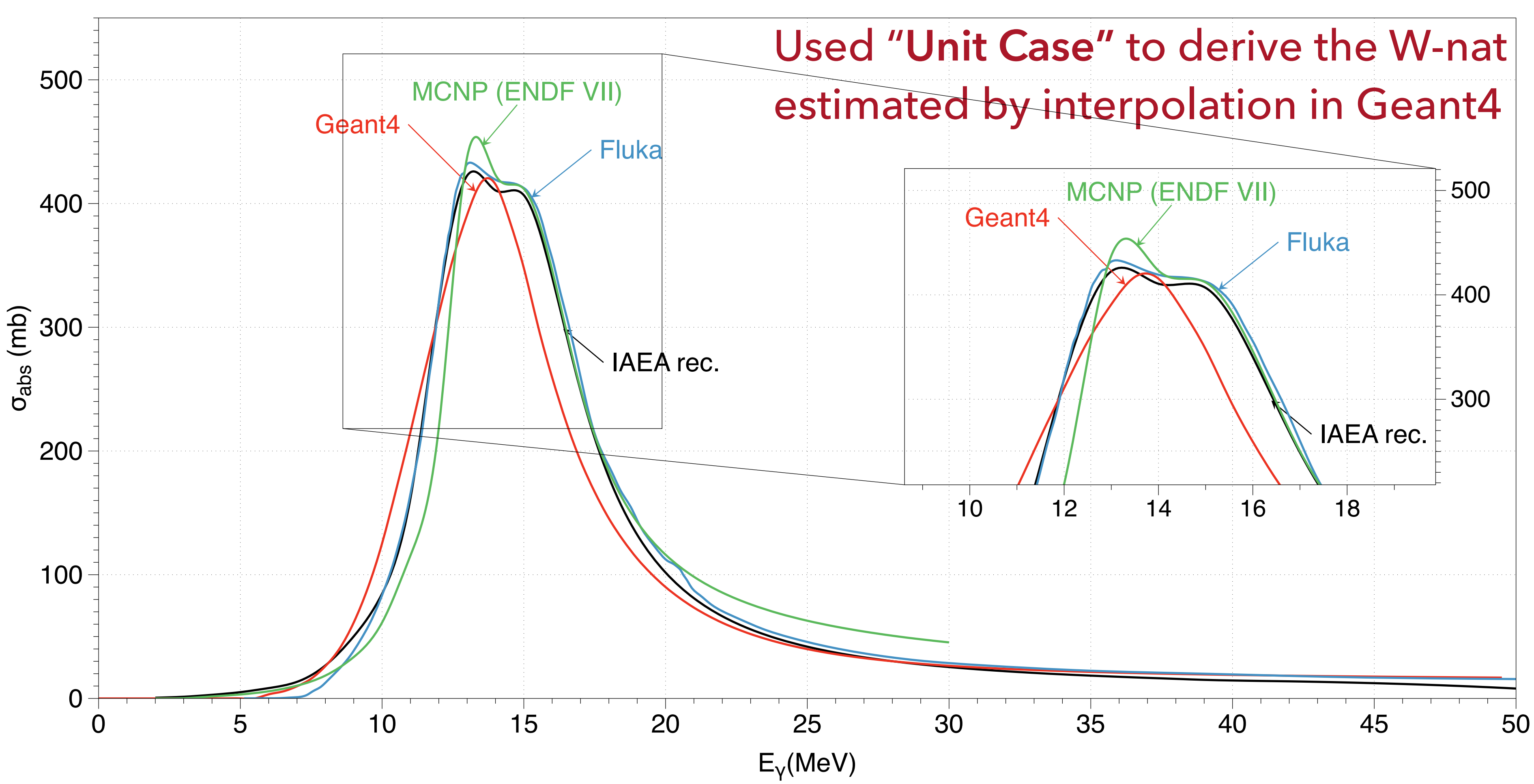
W184,W186, W: XS COMPARISON







W-NAT (IAEA RECOM., GEANT4, FLUKA, MCNP)

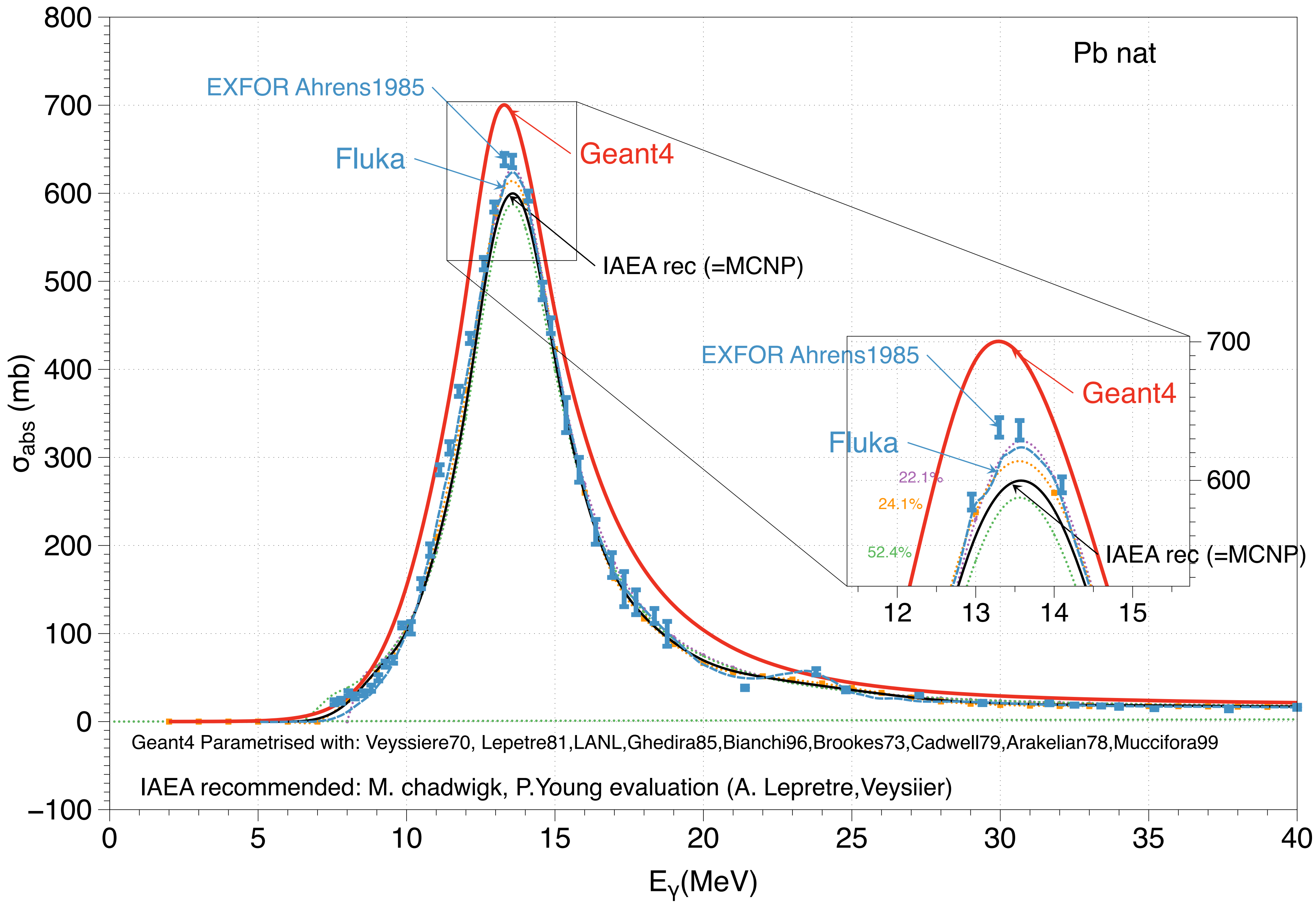


Kolmogorov-Smirnoff Test (significance level alpha=0.01);

The null hypothesis: data vectors Geant4 and IAEA are from populations with the same distribution at the 1% significance level;

Result: Rejected

PB-NAT: XS COMPARISON



Kolmogorov-Smirnoff Test (significance level alpha=0.01):

Null hypothesis: **Geant4 estimates the recommended IAEA distribution;**

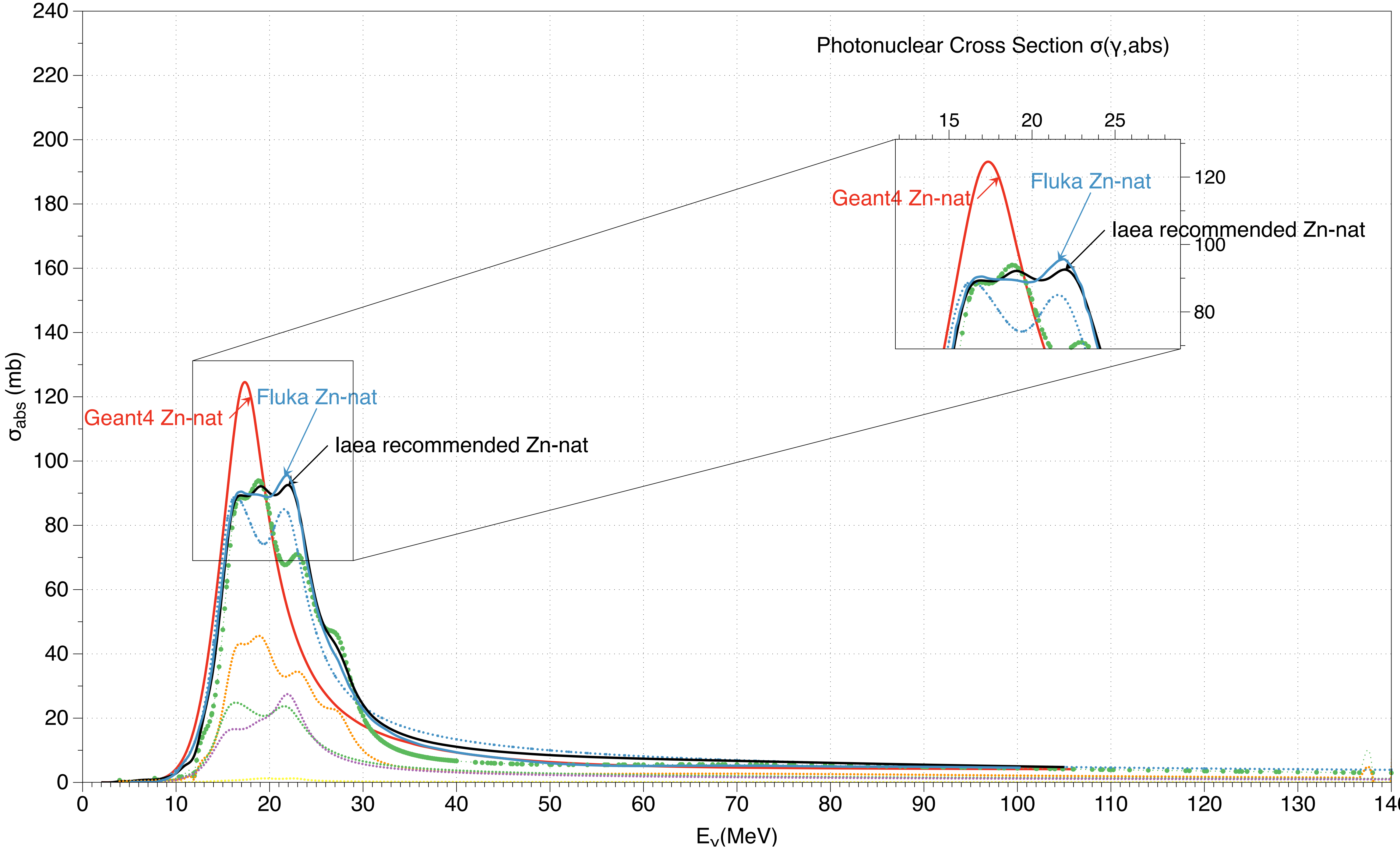
Result: Rejected (p=2.3E-3)

Kolmogorov-Smirnoff test IAEA-Exp data (with which FLUKA complies) with significance level alpha=0.01:

Null Hypothesis: that is **IAEA (and FLUKA) estimates the real experimental distribution**

Result: Not rejected

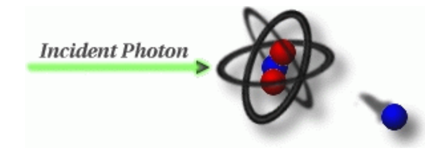
ZN-NAT CASE



Kolmogorov-Smirnoff Test (significance level alpha=0.01).

Null hypothesis: Geant4 estimates the recommended IAEA distribution.

Result: Rejected



CONCLUSION & FUTURE PLAN

- **Increasing interest in obtaining accurate estimations with MC codes**, **especially in high energy range (mainly for dosimetric purposes and/or radiation shielding design)**
- **In case of lack of experimental data, the comparison among the results obtained with independent codes**, even if not appropriate to validare the simulation observables, **could highlight special needs** of adopting conservative approach for those cases potentially found not in agreement or, in addition, **address experiments for benchmarking purposes in the future high-energy neutron calibration fields or high brilliance gamma source**, as eventually they are going to be provided for neutron metrology purposes
- The analysis is in progress and first we will **focus on materials that are widely used in high energy accelerator context (lead, tungsten, copper, etc)**: validation of predictions with accurate statistical tests (when experimental values are available), first on the cross section (process) and after on the secondary particles produced (energy spectra, angular distribution)
- At this stage of the analysis and **for the specific cases examined**, **Fluka and MCNP show to be more "reliable" with respect to Geant4 for photo-nuclear predictions. Anyway, in Fluka, original cross section database, contrarily to Geant4 and MCNP, is not accessible directly by the user**!!

THANK YOU FOR YOUR ATTENTION!