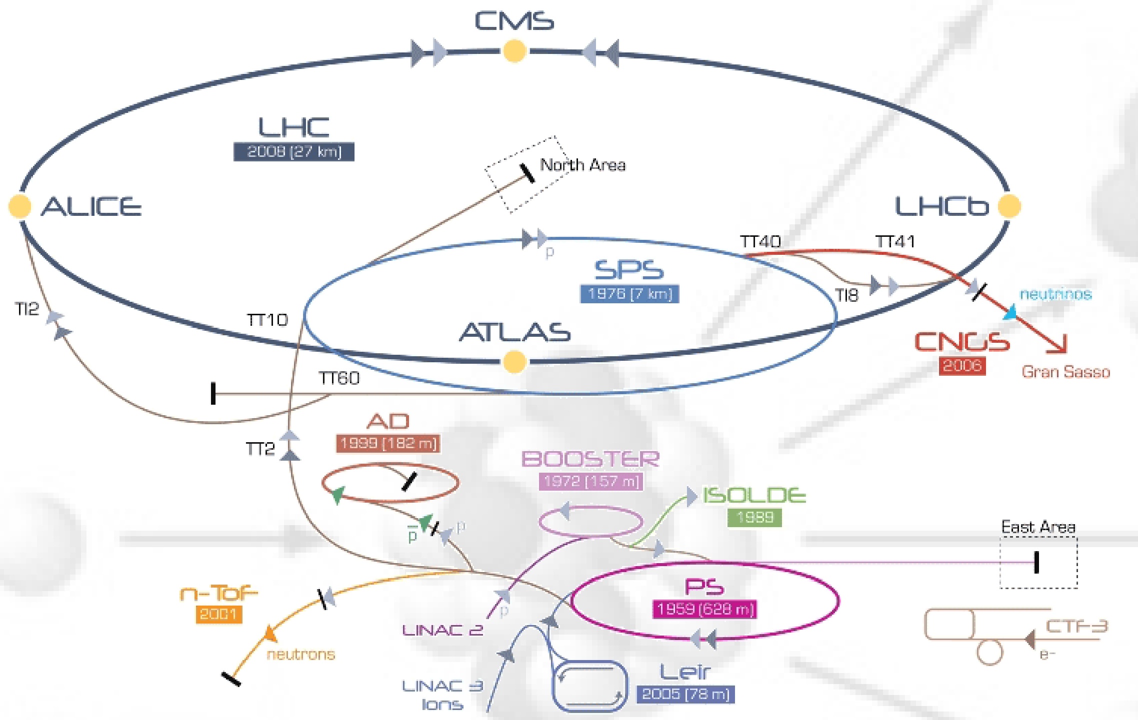
Monte Carlo Principles for Neutron Experiments

Alfredo Ferrari,
CERN, Geneva

NDRA 2016 - Summer School on Neutron Detectors and Related Applications

Riva del Garda, June 30th 2016

CERN: from low energies to LHC



- LINAC…4 (3-160 MeV)
- ..
- PS (20 GeV)
- ..
- SPS (400 GeV)
- LHC (6.5 TeV p, 2.5 TeV/n Pb ions, ultimately 7 TeV and 2.7 TeV/n)

- Energy deposition (quenching, damage)
- Radiation damage (electronics, insulation)
- Shielding
- Secondary beam line design
- Activation
- Residual dose rates (maintenance)
- Waste disposal
- Neutron cross section meas. (n_ToF)

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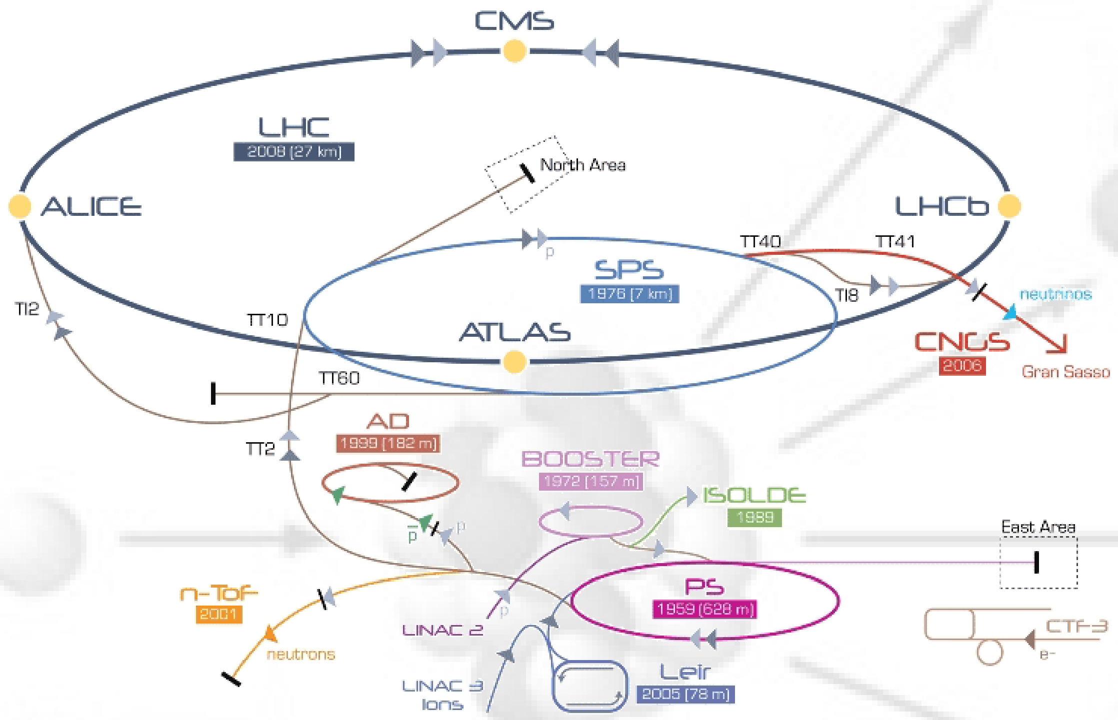

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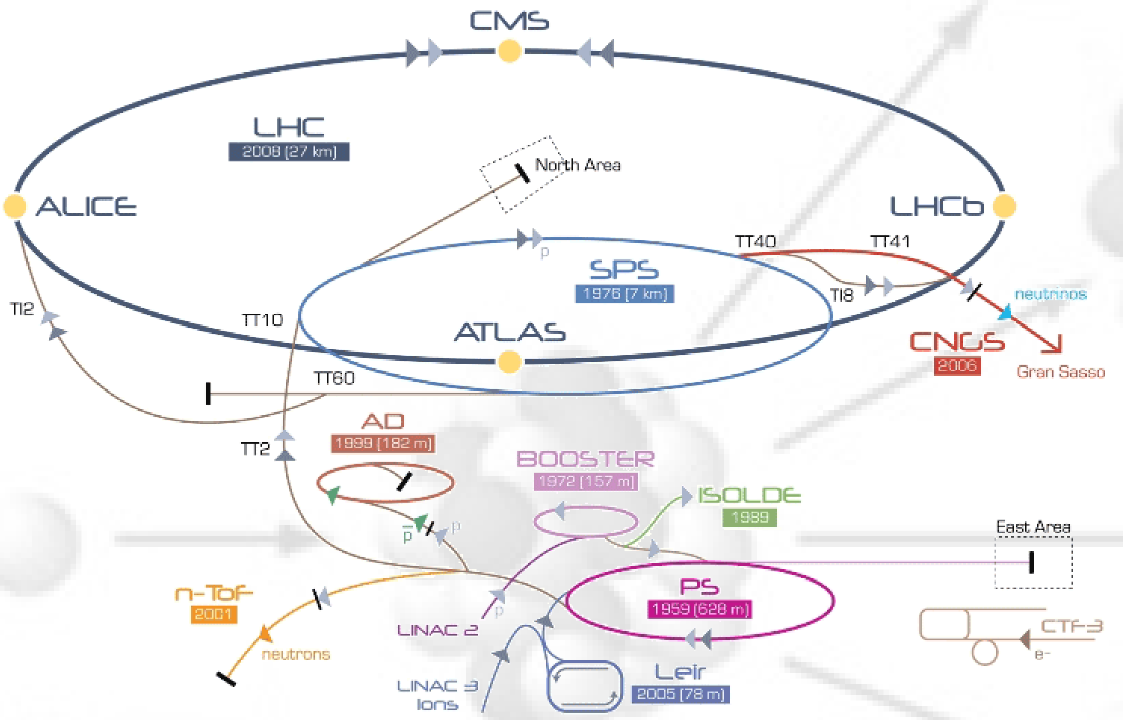

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All problems where neutrons play a critical (often dominant) role (treated with MC, FLUKA, calculations in collaboration between accelerator and RP groups, → my examples as well)

- Neutron cross section meas. (n_ToF)

Overview:

General Monte Carlo concepts:
- Phase space
- (The Boltzmann equation)
- Monte Carlo foundations
- (Simulation vs. integration)

(Sampling techniques)
- discrete
- by inversion
- by rejection

Particle Transport Monte Carlo
- Microscopic/Macroscopic
- Analog vs. biased Monte Carlo calculation
- Geometry, source term

Results and Errors:
- Statistical errors (single histories, batches)
- Figure of merit
- Estimators
- Common mistakes

Low and high energy neutron MC's:
- Evaluated data files
- Examples of evaluated cross sections
- High energy MC models
- caveats

Example with ^{3}He Bonner spheres
- Response functions
- Variations in cross sections/response functions
- Lead insert
- Pulse height distributions

Example with liquid scintillators
- Low energy pulse height distributions
- Well known "accident"
- High energy pulse height distributions

Short comments on simulations of:
- Activation detectors
- Fission detectors
- Capture detectors

Monte Carlo codes for n (very little!)

Phase space:

- Phase space: a concept of classical Statistical Mechanics
- Each Phase Space dimension corresponds to a particle degree of freedom
- 3 dimensions correspond to Position in (real) space: x, y, z
- 3 dimensions correspond to Momentum: p_x, p_y, p_z

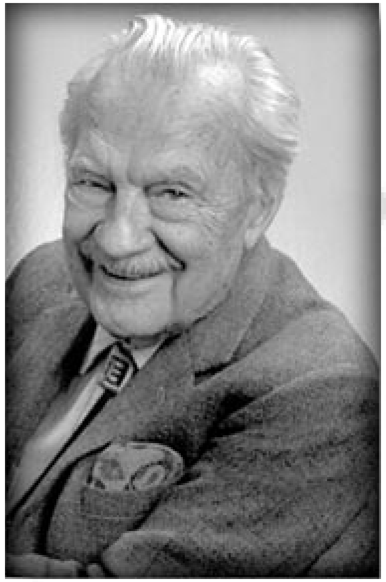
  (or Energy and direction: E, θ, φ)
- More dimensions may be envisaged, corresponding to other possible degrees of freedom, such as quantum numbers: spin etc
- Each particle is represented by a point in phase space
- Time can also be considered as a coordinate, or it can be considered as an independent variable: the variation of the other phase space coordinates as a function of time constitutes a particle "history"

The Boltzmann equation:

- All particle transport calculations are (explicit or implicit) attempts at solving the Boltzmann Equation
- It is a balance equation in phase space: at any phase-space-point, the increment of particle phase-space-density is equal to the sum of all "production terms" minus a sum of all "destruction terms"
- Production: Sources, "In-scattering", Particle Production, Decay
- Destruction: Absorption, "Out-scattering", Decay
- We can look for solutions of different type: at a number of (real or phase) space points, averages over (real or phase) space regions, projected on selected phase space hyper-planes, stationary or time-dependent

The Monte Carlo method:

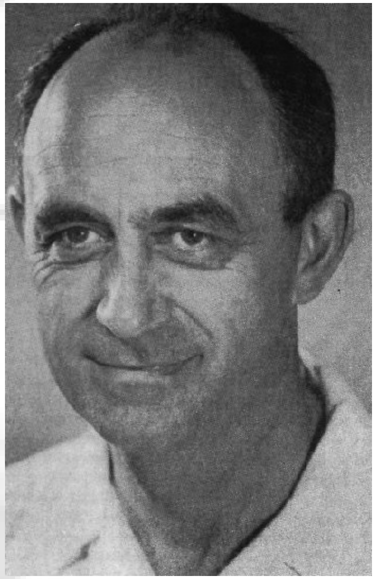
Invented in the late 40's by **John von Neumann**, **Stanislaw Ulam** and **Nicholas Metropolis** (who gave it its name), and independently by **Enrico Fermi**



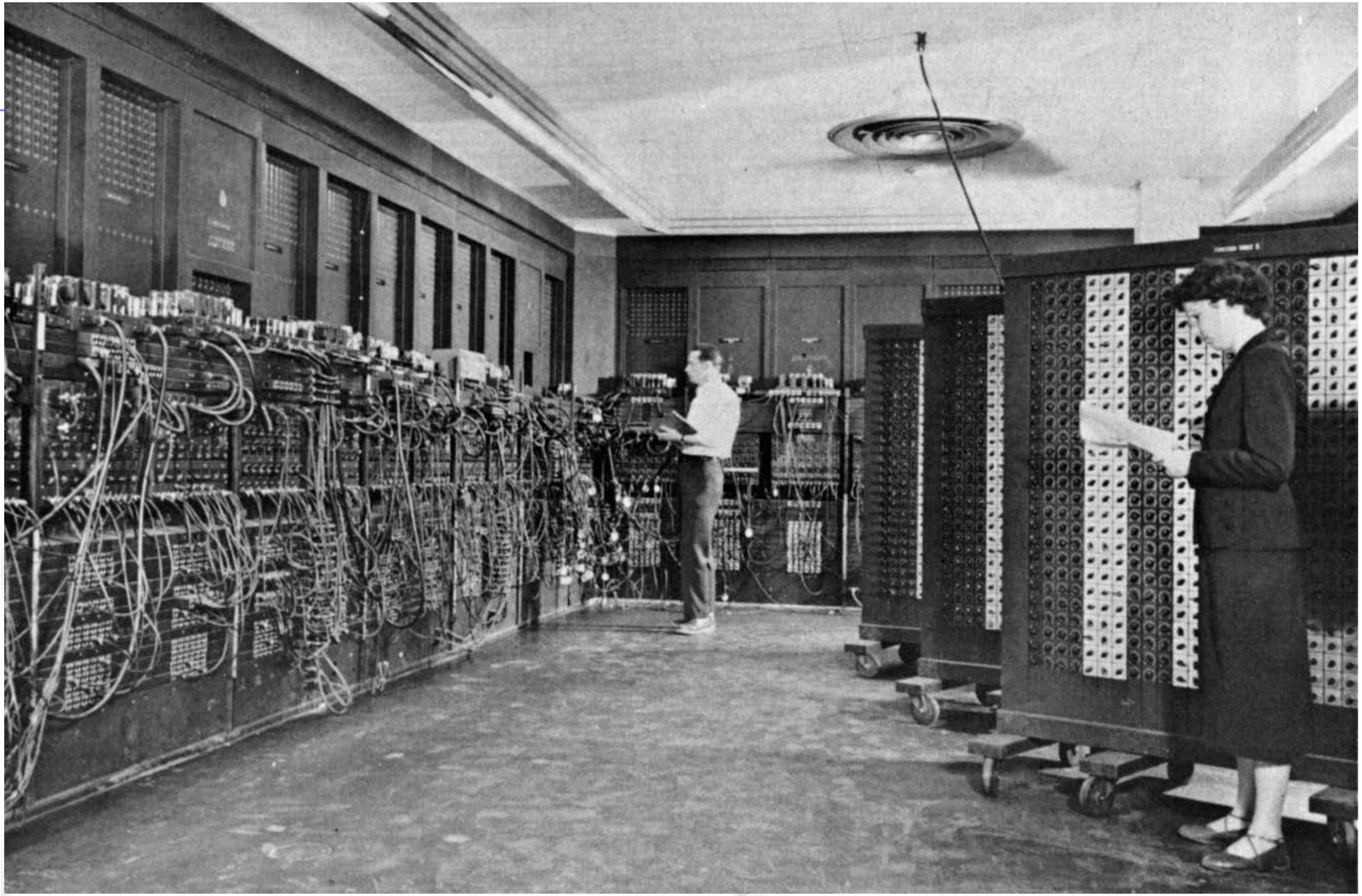
N. Metropolis

S. Ulam

J. von Neumann



E. Fermi



The ENIAC

Electronic Numerical Integrator And Computer

Monte Carlo mathematical foundation:

Several possible ways of defining Monte Carlo (MC):

- A mathematical method for Numerical Integration
  - Random sampling techniques
  - Convergence, variance reduction techniques…
- A computer simulation of a Physical Process
  - Physics
  - Tracking
  - Scoring…

Both are valid, depending on the problem one or the other can be more effective

MC Mathematical foundation

The Central Limit Theorem is the mathematical foundation of the Monte Carlo method. In words (mathematics in the backup slides):

Given any observable A, that can be expressed as the result of a convolution of random processes, the average value of A can be obtained by sampling many values of A according to the probability distributions of the random processes.

MC is indeed an integration method that allows to solve multi-dimensional integrals and/or integro-differential equations by sampling from a suitable stochastic distribution.

The precision of MC estimator depends on the number of samples:

$$\sigma \propto \frac{1}{\sqrt{N}}$$

A typical particle transport Monte Carlo problem is a 7-D problem!
x, y, z, p_x, p_y, p_z and t !!

Analog Monte Carlo:

In an analog Monte Carlo calculation ("honest" simulation), not only the mean of the contributions converges to the mean of the real distribution,

$$\lim_{N\to\infty} S_N = \lim_{N\to\infty} \frac{\sum_{i=1}^{N} A(x_{i,}y_i,z_i,...)\,f'(x_{i,}y_i,z_i,...)\,g'(x_{i,}y_i,z_i,...)\,h'(x_{i,}y_i,z_i,...)}{N} = \overline{A}$$

but also the variance and all moments of higher order

$$\overline{\mu}^{m} = \int_x\int_y\int_z ...\int \left[A(x,y,z,...) - \overline{A}\right]^m f'(x,y,z,...)\,g'(x,y,z,...)\,h'(x,y,z,...)\,dx\,dy\,dz...$$

converge as well:

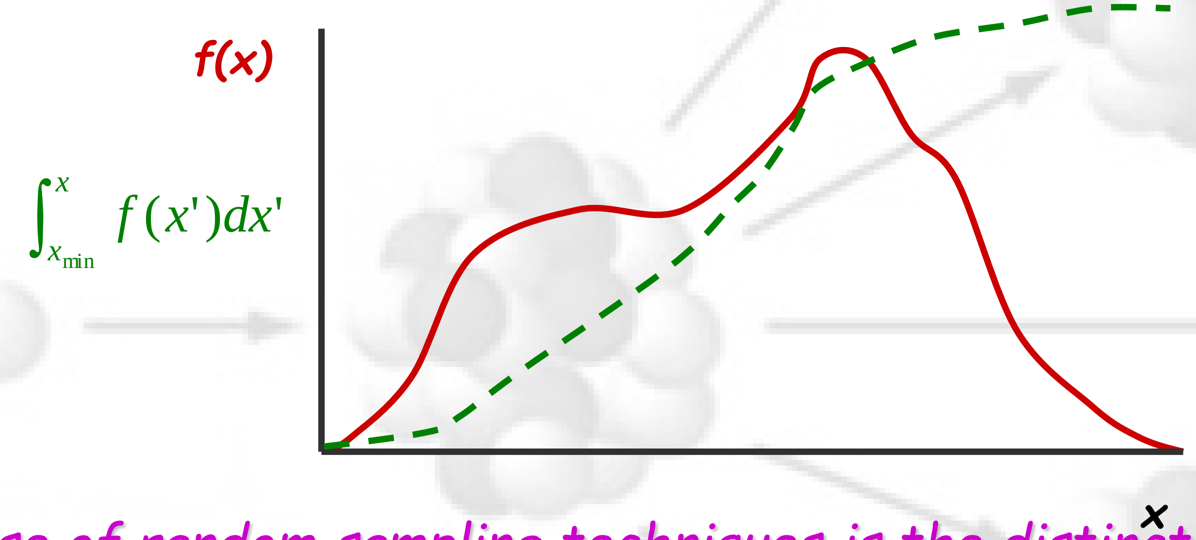
$$\lim_{N\to\infty}\left[\frac{\sum_{i=1}^{N}\left(A_i - S_n\right)^m}{N}\right] = \overline{\mu}^{m}$$

and fluctuations and correlations are faithfully reproduced

Random Sampling: the key to Monte Carlo!

The central problem of the Monte Carlo method:

Given a Probability Density Function (pdf), f(x), generate a sequence of x's distributed according to f(x) (x can be multi-dimensional)



The use of random sampling techniques is the distinctive feature of Monte Carlo

The use of Monte Carlo to solve the integral Boltzmann transport equation consists of:

- Description and random sampling of the source term
- Random sampling of the outcome of physical events
- Geometry and material description of the problem

(Pseudo) Random numbers:

- Basis for all Monte Carlo integrations are random numbers, *i.e.* values of a variable distributed according to a pdf (probability distribution function).
- In real world: the random outcome of a physical process
- In computer world: pseudo-random numbers
- The basic pdf is the uniform distribution:

$$f(\xi) = 1 \qquad 0 \leq \xi < 1$$

- Pseudo-random numbers are sequences that reproduce the uniform distribution, constructed from mathematical algorithms.
- All computers provide a pseudo-random number generator (or even several of them). In most computer languages (e.g., Fortran 90, C, C++) a PRNG is even available as an intrinsic routine ***(don't use them!)***
- Random numbers can be used to sample from whichever distribution through a variety of techniques (inversion, rejection, etc, see backup slides)

Particle transport Monte Carlo:

Assumptions:

- Static, homogeneous, isotropic, and amorphous media (and geometry)
- Markovian process: the fate of a particle depends only on its actual properties, not on previous events or histories
- Particles do not interact with each other
- Particles interact with individual atoms/nuclei/molecules (invalid at low energies)
- Material properties are not affected by particle reactions

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⇓

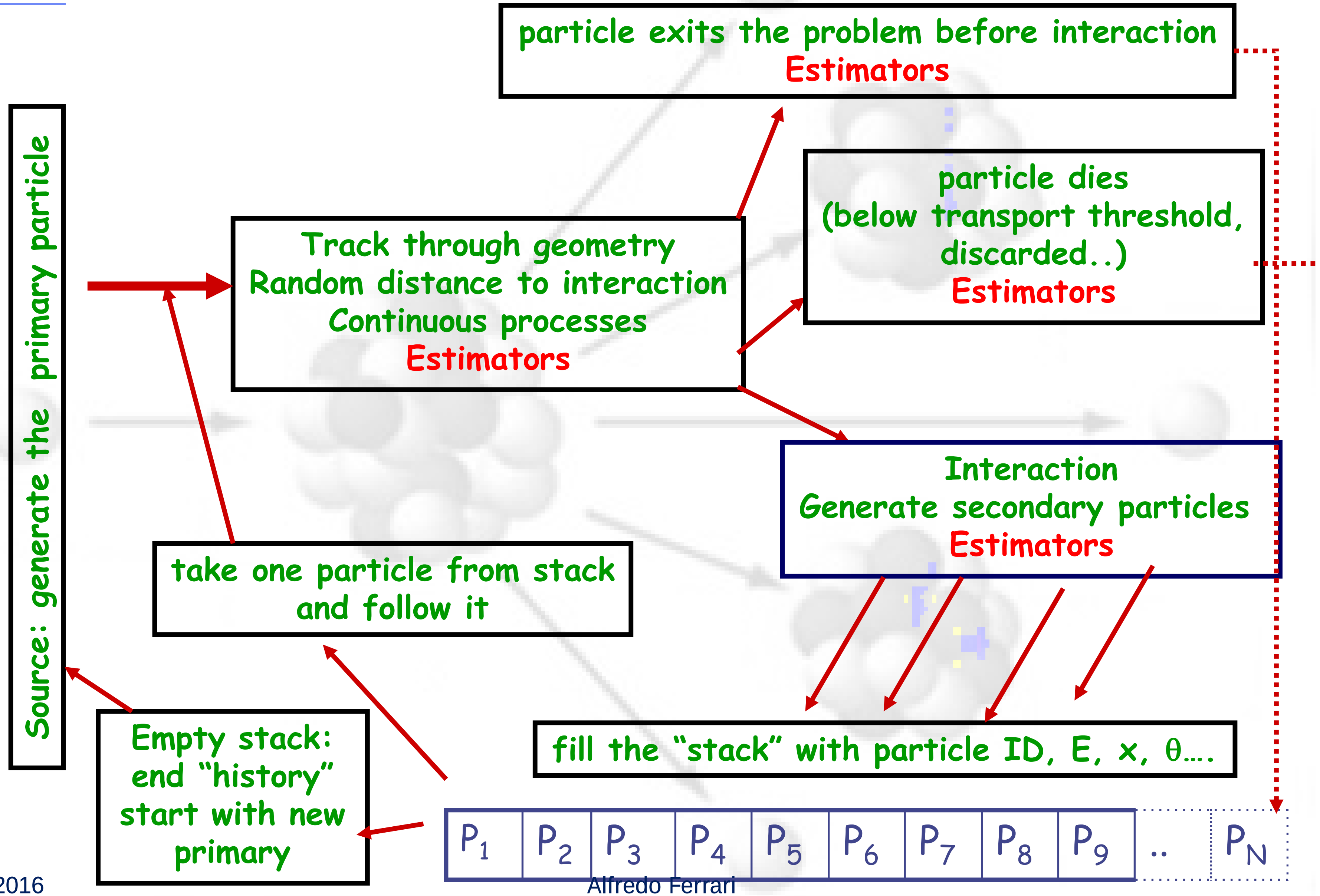
The superposition principle can be used

Particle transport Monte Carlo:

Application of Monte Carlo to particle transport and interaction:

- Each particle is followed on its path through matter.
- At each step the occurrence and outcome of interactions are decided by random selection from the appropriate probability distributions.
- All the secondaries issued from the same primary are transported before a new history is started.
- The accuracy and reliability of a Monte Carlo depends on the models or data on which the pdf's are based
- Statistical precision of results depends on the number of "histories"
- Statistical convergence can be accelerated by "biasing" techniques.

Practical implementations



Reaction Rate and Cross Section (1/2)

- Mean free path λ*[cm]*: the average distance travelled by a particle in a material before an interaction. Macroscopic cross section $\Sigma=\lambda^{-1}$: probability of interaction per unit distance. Both λ and Σ depend on the material and on the particle type and energy.
- Over a track length $\mathrm{d}l$ the probability of interaction will be: $\mathrm{d}R = \mathrm{d}l\,\Sigma$ and the corresponding reaction rate: $\dot{R} = \mathrm{d}l/\mathrm{d}t\,\Sigma = v\Sigma$, where v is the particle velocity.
- $n(\mathbf{r},v)=dN/dV$ $[cm^{-3}]$: density of particles with velocity $v=dl/dt$ $[cm/s]$, at a position $\mathbf{r}$. The reaction rate inside the volume element $\mathrm{d}V$ will be: $\mathrm{d}\dot{R}/\mathrm{d}V = n(\mathbf{r},v)v\Sigma$
- The quantity $\dot{\Phi}(\mathbf{r},v) = n(\mathbf{r},v)v$ is called ***fluence rate*** or ***flux density*** and has dimensions $[cm^{-3}\ cm\ s^{-1}]=[cm^{-2}\ s^{-1}]$, its time integral $\Phi(\mathbf{r},v) = n(\mathbf{r},v)\mathrm{d}l$ is the ***fluence*** $[cm^{-2}]$
- Fluence is measured in particles per cm^2 but in reality it describes the ***density of particle tracks***
- The number of reactions inside a volume V is given by the formula: $R = \Sigma\Phi V$ (where the product $\Sigma\,\Phi$ is integrated over energy or velocity)

Reaction Rate and Cross Section (2/2)

- Dividing the macroscopic cross section by n_0, the number of atoms per unit volume, one obtains the microscopic cross section: $\sigma[barn=10^{-24}cm^2]$

$$\frac{\text{probability/cm}}{\text{atoms/cm}^3} = \frac{\text{probability} \times \text{cm}^2}{\text{atom}} = \text{atom effective area}$$

  i.e., the area of an atom weighted with the probability of interaction (hence the name "cross section");

- But it can also be understood as the probability of interaction per unit length, with the length measured in atoms/cm^2 (the number of atoms contained in a cylinder with a 1 cm^2 base).
- In this way, both microscopic and macroscopic cross section are shown to have a similar physical meaning of "probability of interaction per unit length", with length measured in different units. Thus, the number of interaction can be obtained by both by multiplying by the corresponding particle track-length.

Fluence estimation (1/2)

- Track length estimator:

$$\dot{\Phi}(v)\,dt = n(v)\,v\,dt = \frac{dn(v)}{dV}\frac{dl(v)}{dt}dt = \lim_{\Delta V \to 0} \frac{\sum_i l_i(v)}{\Delta V}$$

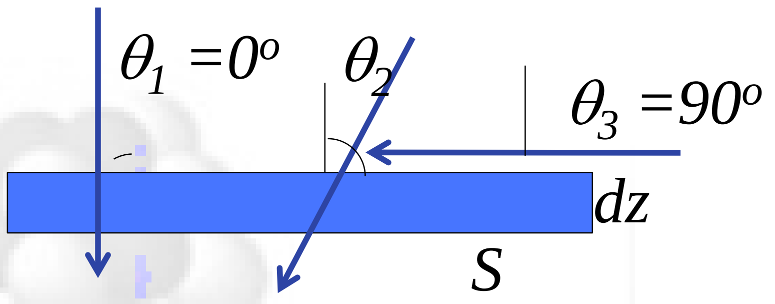
- Collision density estimator:

$$\dot{\Phi}(v) = \frac{\dot{R}(v)}{\sigma(v)\,n_o \Delta V} = \frac{\dot{R}(v)}{\Sigma(v)\Delta V} = \frac{\dot{R}(v)\lambda(v)}{\Delta V}$$

Fluence estimation (2/2)

Surface crossing estimator:

- Imagine a surface having an infinitesimal thickness dz
  A particle incident with an angle θ with respect to the normal of the surface S will travel a segment $dz/cos\theta$.



- Therefore, we can calculate an average surface fluence by adding $dz/cos\,\theta$ for each particle crossing the surface, and dividing by the volume $S\,dz$:

$$\Phi = \lim_{dz \to 0} \frac{\sum_i \frac{dz}{\cos\theta_i}}{S\,dz} = \frac{1}{S} \sum_i \frac{1}{\cos\theta_i}$$

- While the current J ***counts*** the number of particles crossing the surface divided by the surface: $J = dN/dS$

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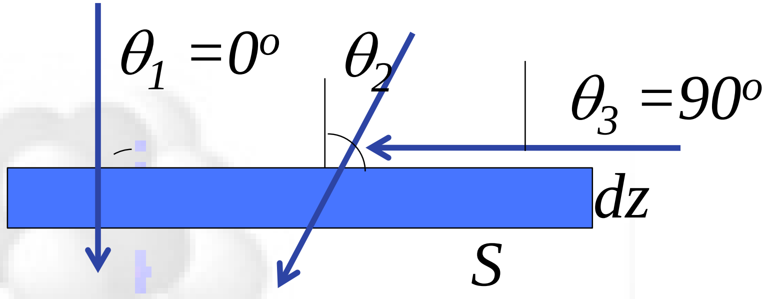

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- While the current J ***counts*** the number of particles crossing the surface divided by the surface: $$J = dN/dS$$

> The fluence is ***independent*** from the orientation of surface S,
> while the current is ***NOT***!
> Fluence is a property of the radiation field
> In an isotropic field can be easily seen that on a flat surface $J = \Phi/2$

Neutron simulations: two different "worlds"

Evaluated data files (E_{max}=20-150/200 MeV)

- Based on expert "evaluations" of available exp. data, often complemented by models
- "High" energy (> 20 MeV) evaluations based on complex (non MC) nuclear models, **(GNASH, Talys, Empire)** whose reliability becomes more and more unproven with increasing energy

Pros:

- ✓ E < 20 MeV: as good as our best knowledge
- ✓ Standard formats/processing tools available
- ✓ Little CPU (… but memory hungry)
- ✓ No real alternative below 20 MeV

Cons:

- No correlations!!
- Slow and complex to update when new data/improved models
- Sometimes incomplete or inconsistent

(MC) Models: 10-20 MeV - E_{max} up to TeV's

- MC nuclear models aimed at the description of particle production spectra by whichever projectile
- A large variety available (not necessarily all good)

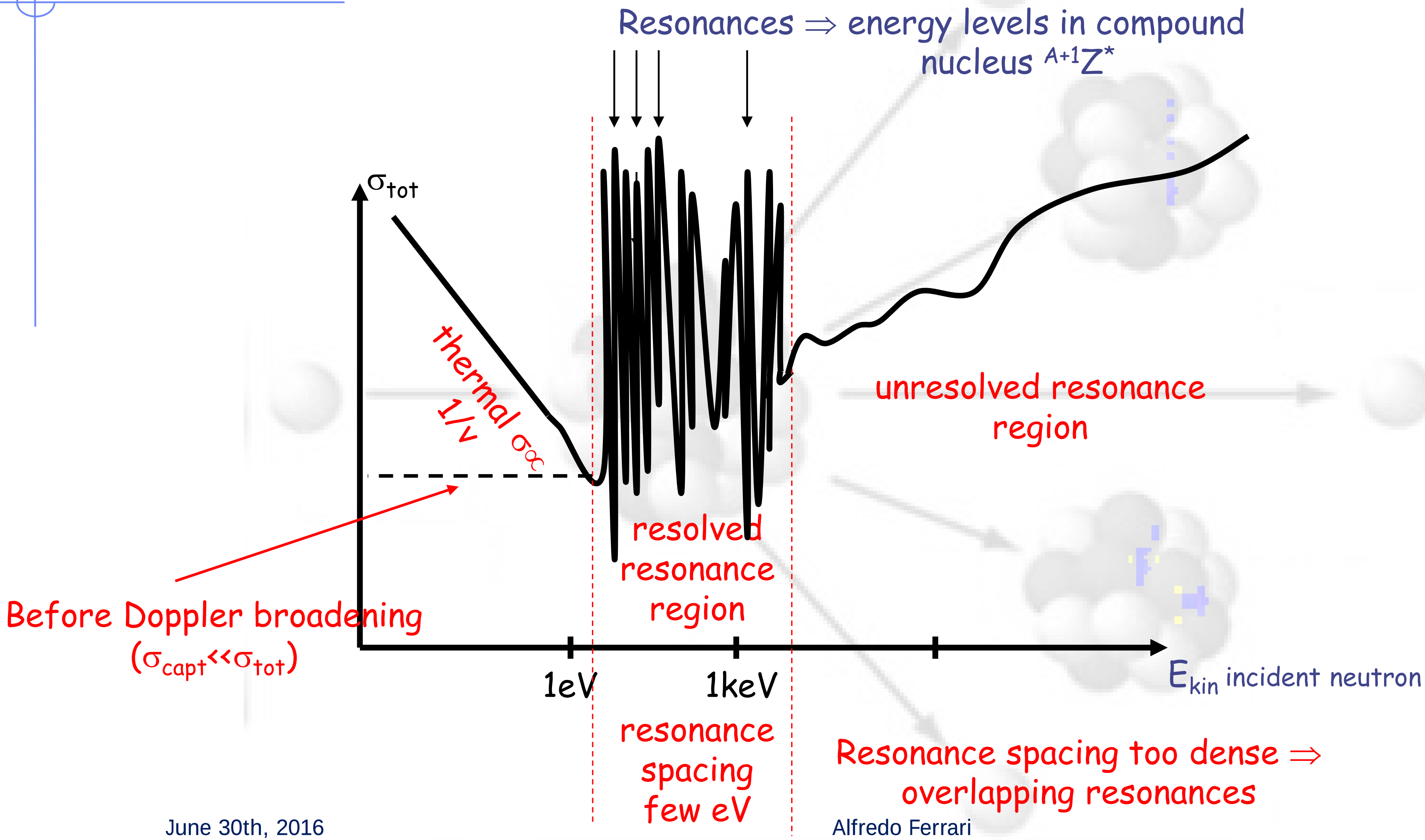
Pros:

- ✓ Work for all proj/energies/targets
- ✓ They produce (at least the good ones) fully correlated physical events (eg conservation laws fulfilled event-by-event)
- ✓ Easy to update, just update the code and run again

Cons:

- As good as the physics inside, sometimes good for most apps, horrible for a few
- Not really usable below 10-20 MeV (or even higher for many)

Typical neutron cross section



Evaluated Nuclear Data Files

- Evaluated nuclear data files (ENDF/B, JEFF, JENDL...), ENDF format
  - typically provide neutron σ (cross sections) and secondary particles (sometimes only neutrons) inclusive distributions for E < 20MeV for all channels. Recent evaluations include data up to 150/200 MeV for a few isotopes
  - σ are stored as continuum + resonance parameters

Point-wise and Group-wise cross sections

- In neutron transport codes in general two approaches are used: point-wise ("continuous" cross sections) and group-wise transport
- Point-wise follows cross section precisely but it can be time and memory consuming
- Group approach is often used in neutron transport codes because it is fast and gives good results for most application (eg shielding, reactor criticality) and it is suitable for discrete ordinates codes and adjoint calculations, however there are applications where pointwise is required (particularly when the energy mesh is comparable with resonance spacing)

Complex programs (NJOY, PREPRO...) convert ENDF files to point-wise or group-wise cross sections, including Doppler broadening, possibly $S(\alpha,\beta)$* treatment for chemical bounds in the thermal region etc.

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Point-wise and Group-wise cross sections

- In ne... cross secti...
- Point...

** S(α,β) treatment is NOT specific to any code, the data for it, if available, are in the evaluated data files, and they are "processed" if asked for by Njoy or similar codes when preparing cross section files for MCNP, FLUKA etc*

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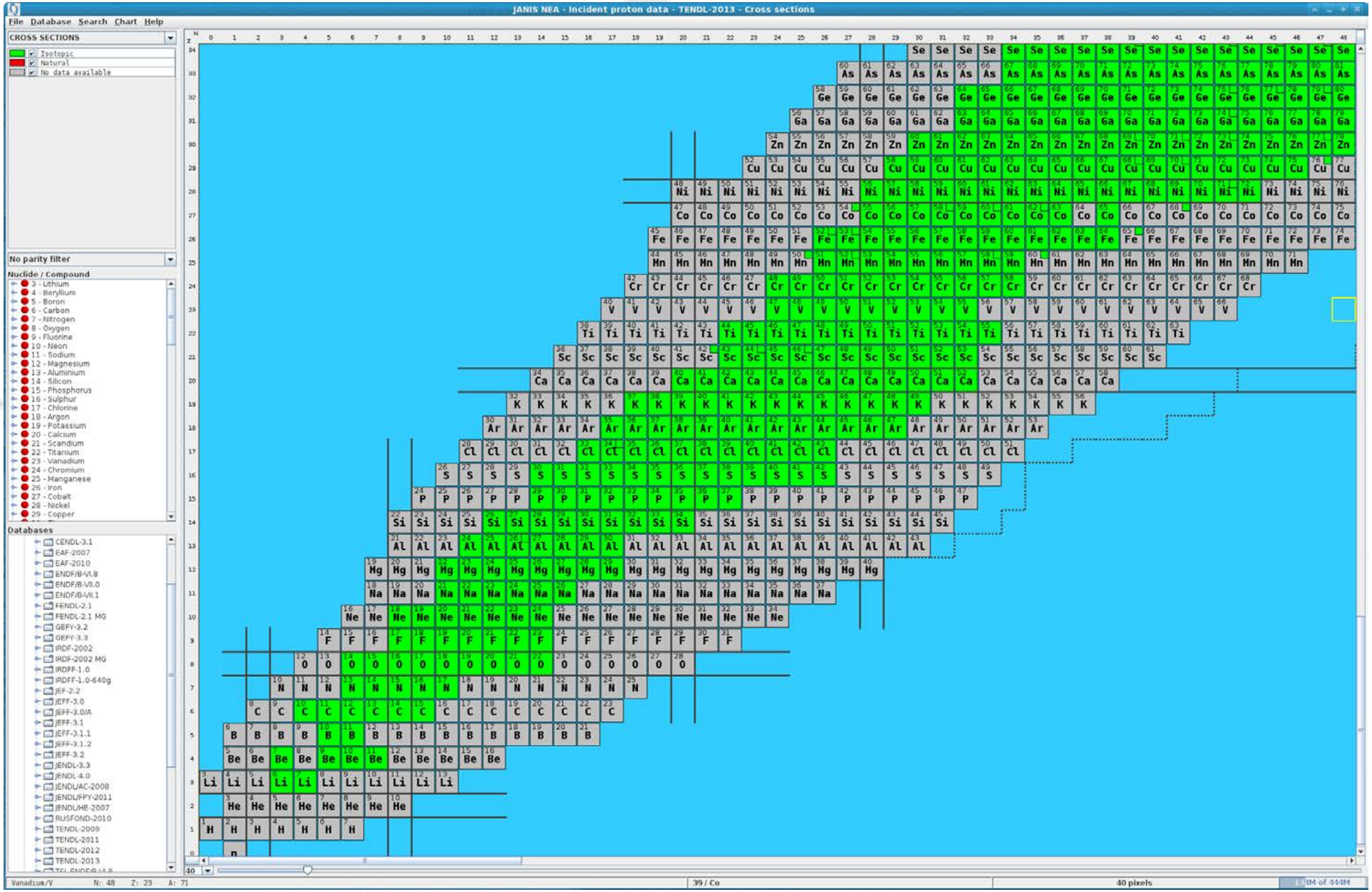
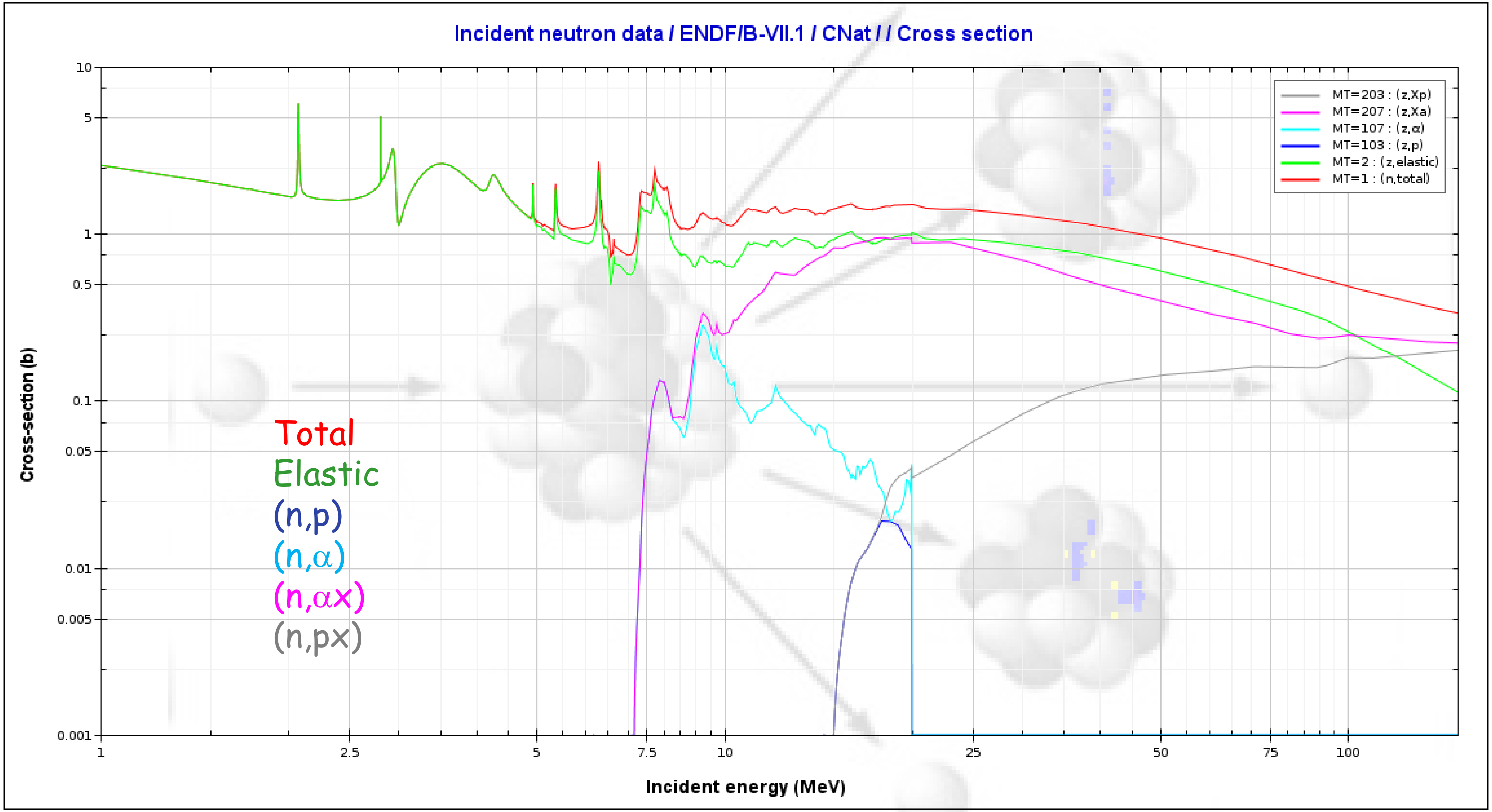
Some examples (eg from http://www.oecd-nea.org/janis/):

ENDF/B-7.1: US
JENDL-4.0: Japan
JEFF-3.1.2: Europe
...
TENDL-2009/15:
Model (TALYS)

Some of them include data for incident charged particles as well, and/or evaluations up to 150/200 MeV for some isotopes



Carbon from ENDF/B-VII.1



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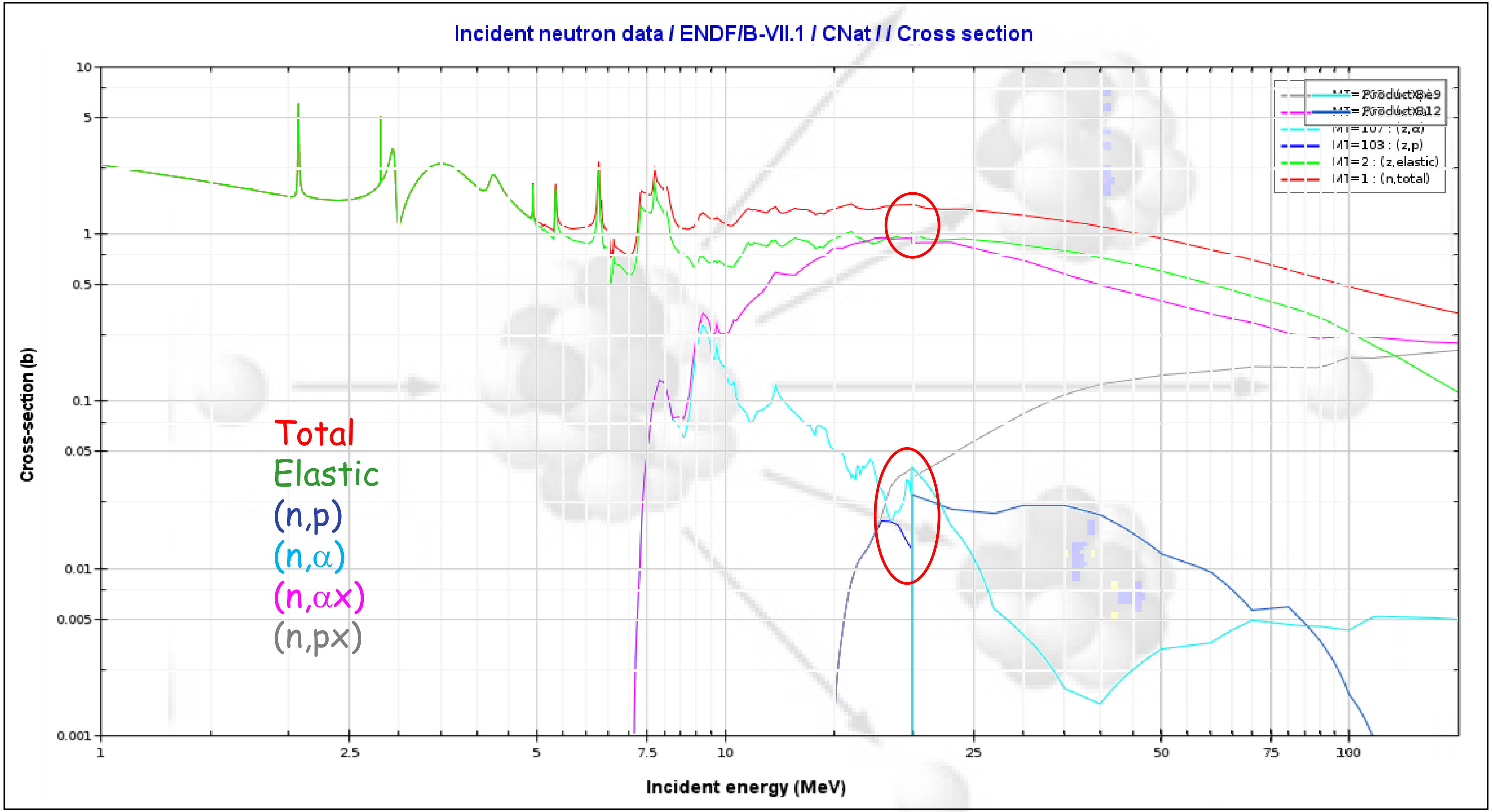
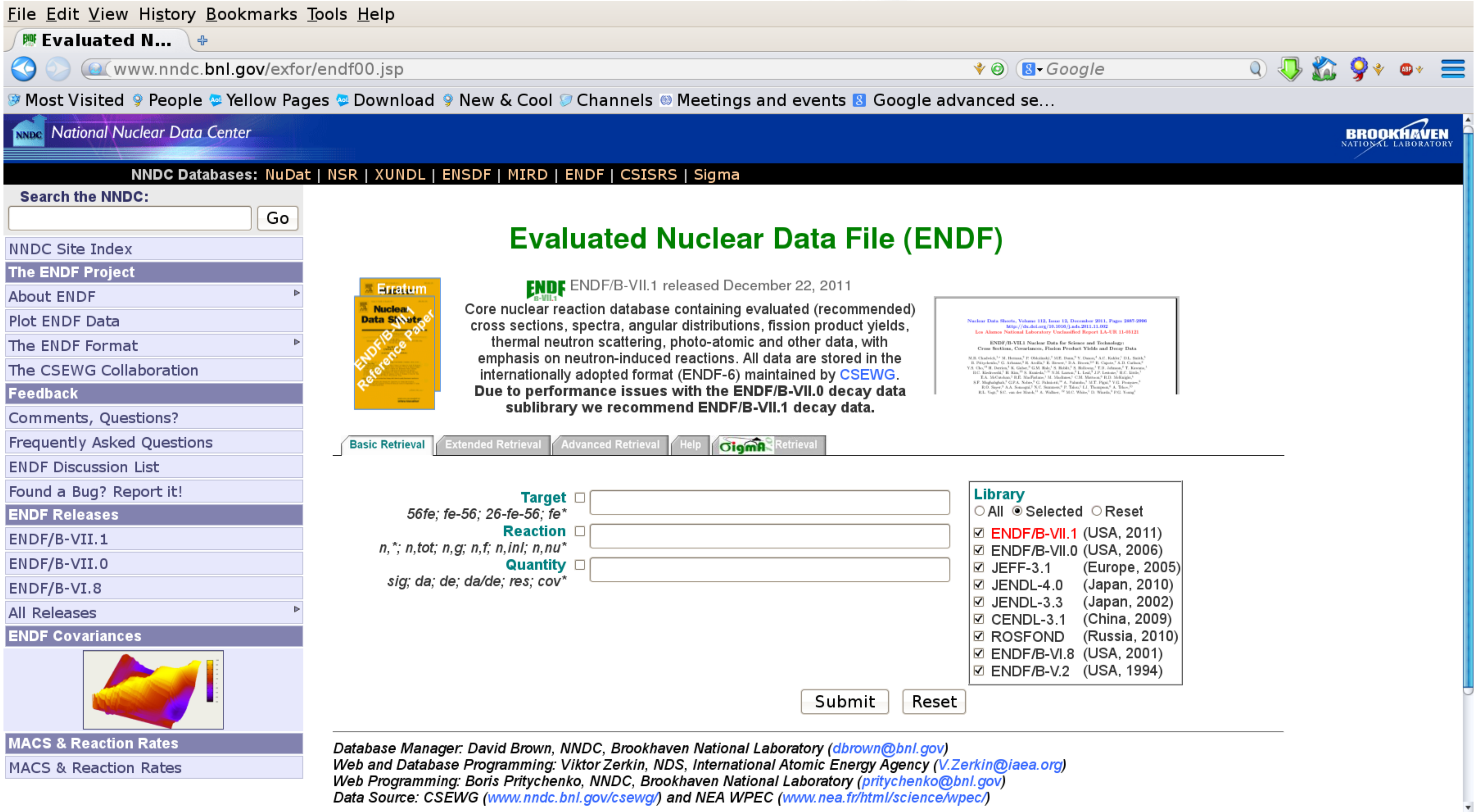
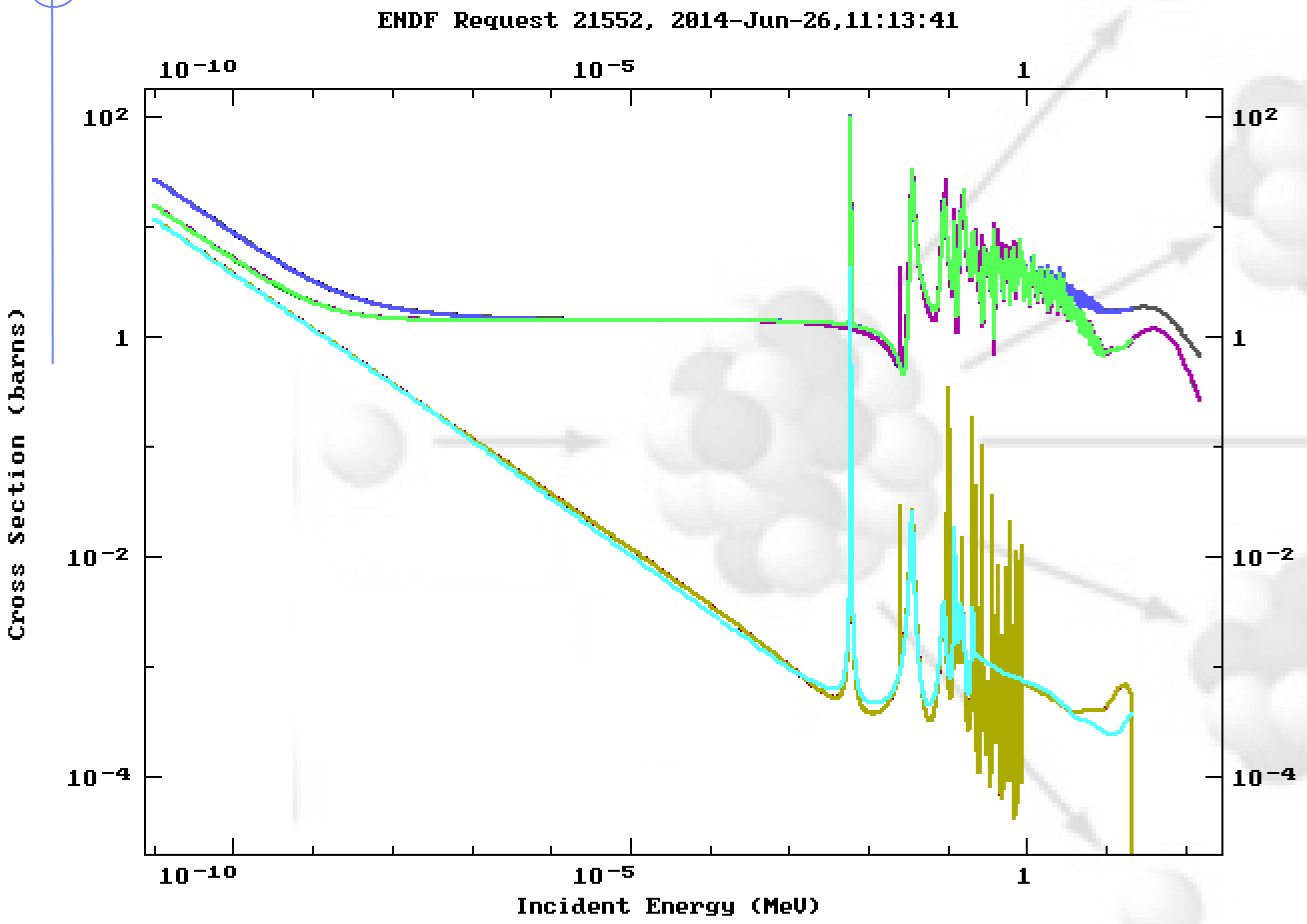
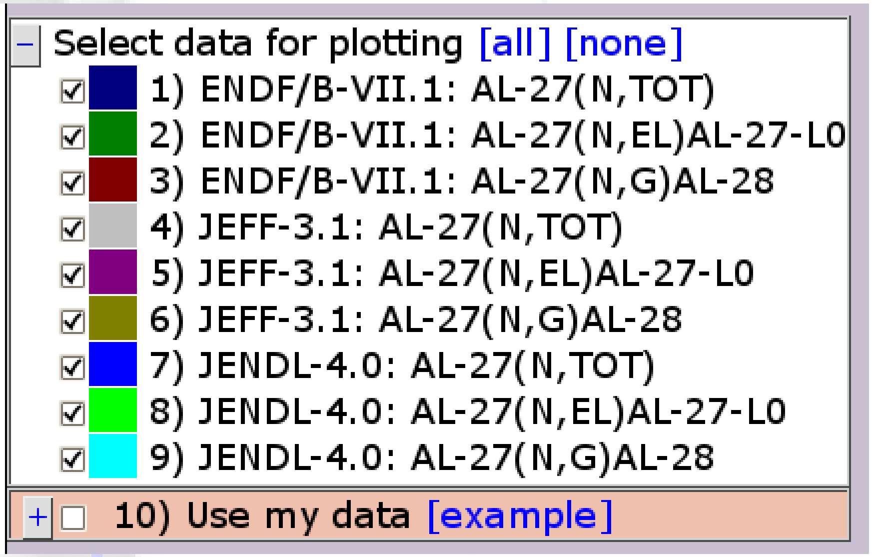


… or from http://www.nndc.bnl.gov :



^{27}Al (evaluated) cross sections:





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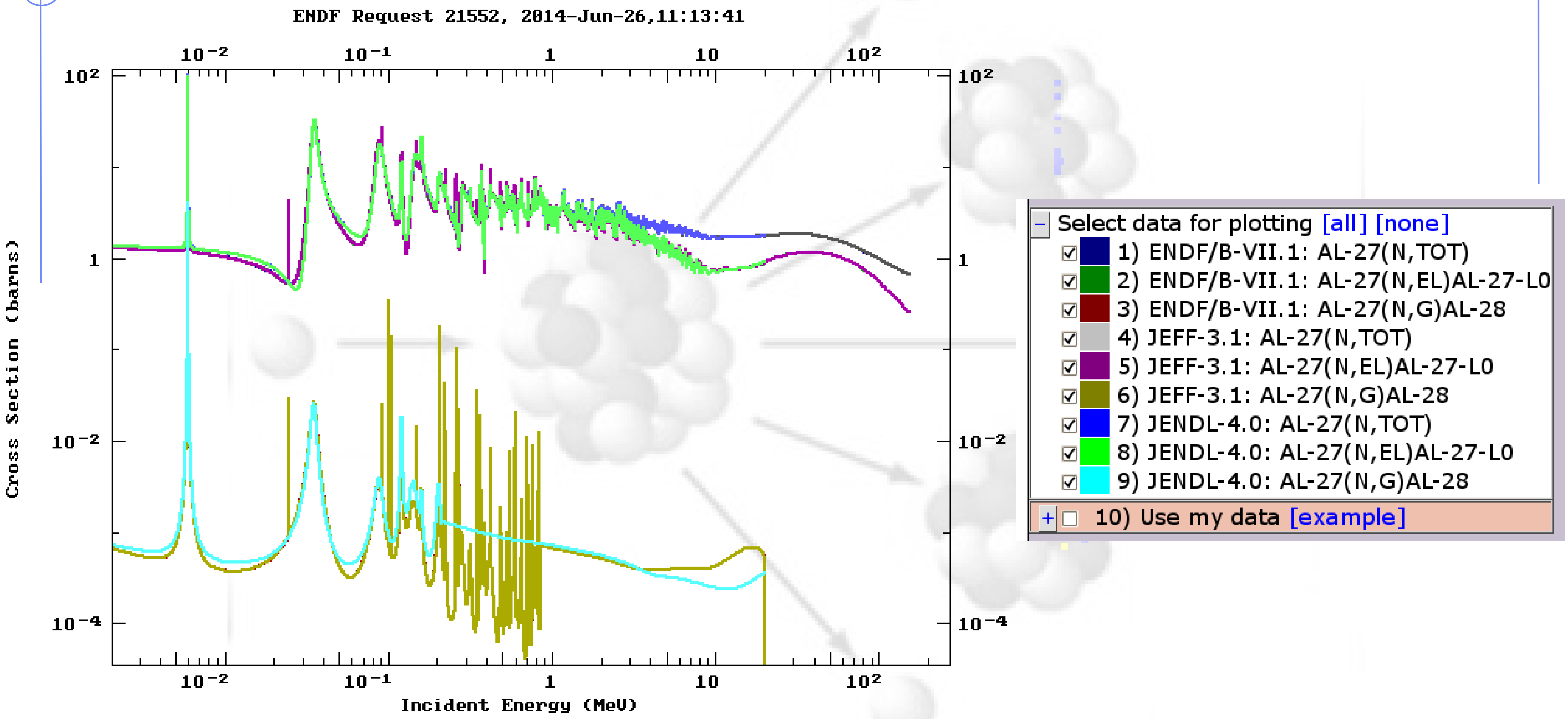

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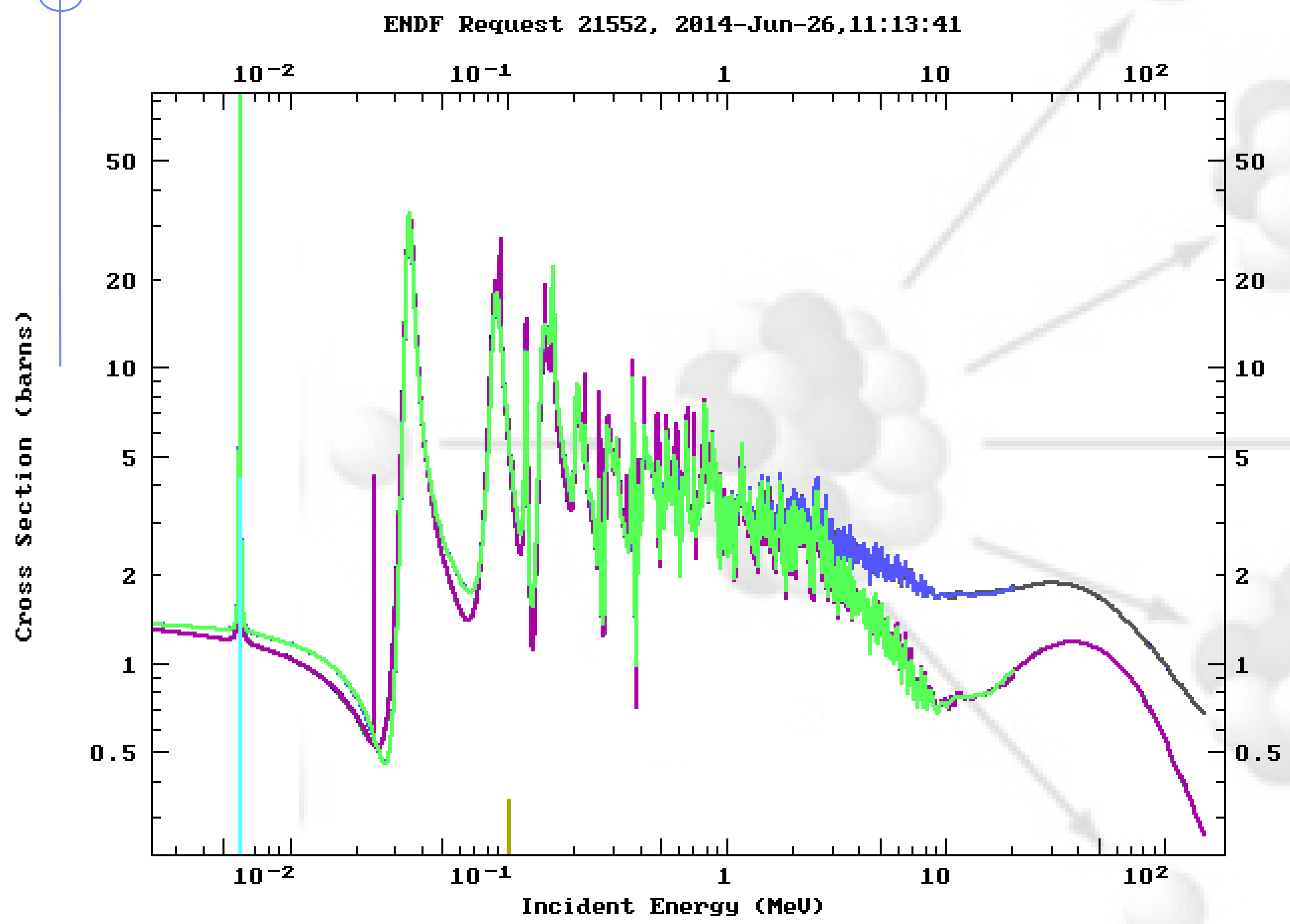
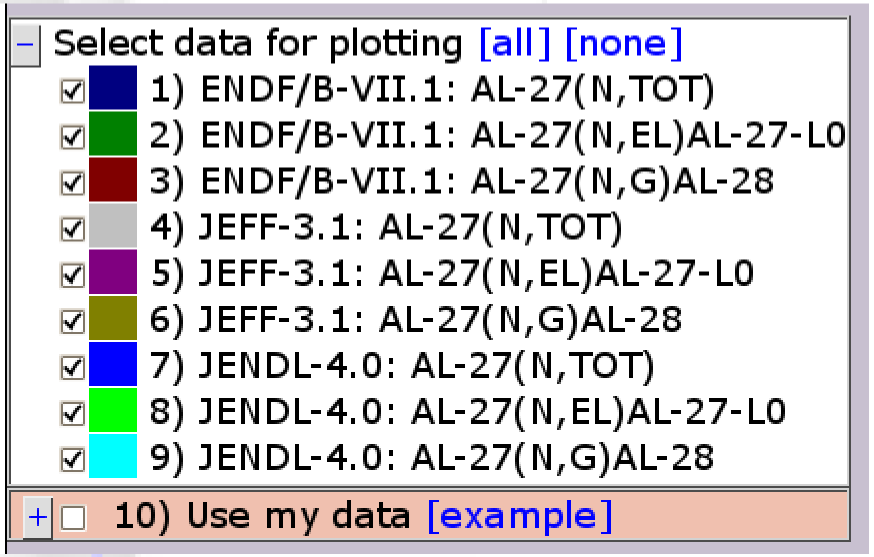
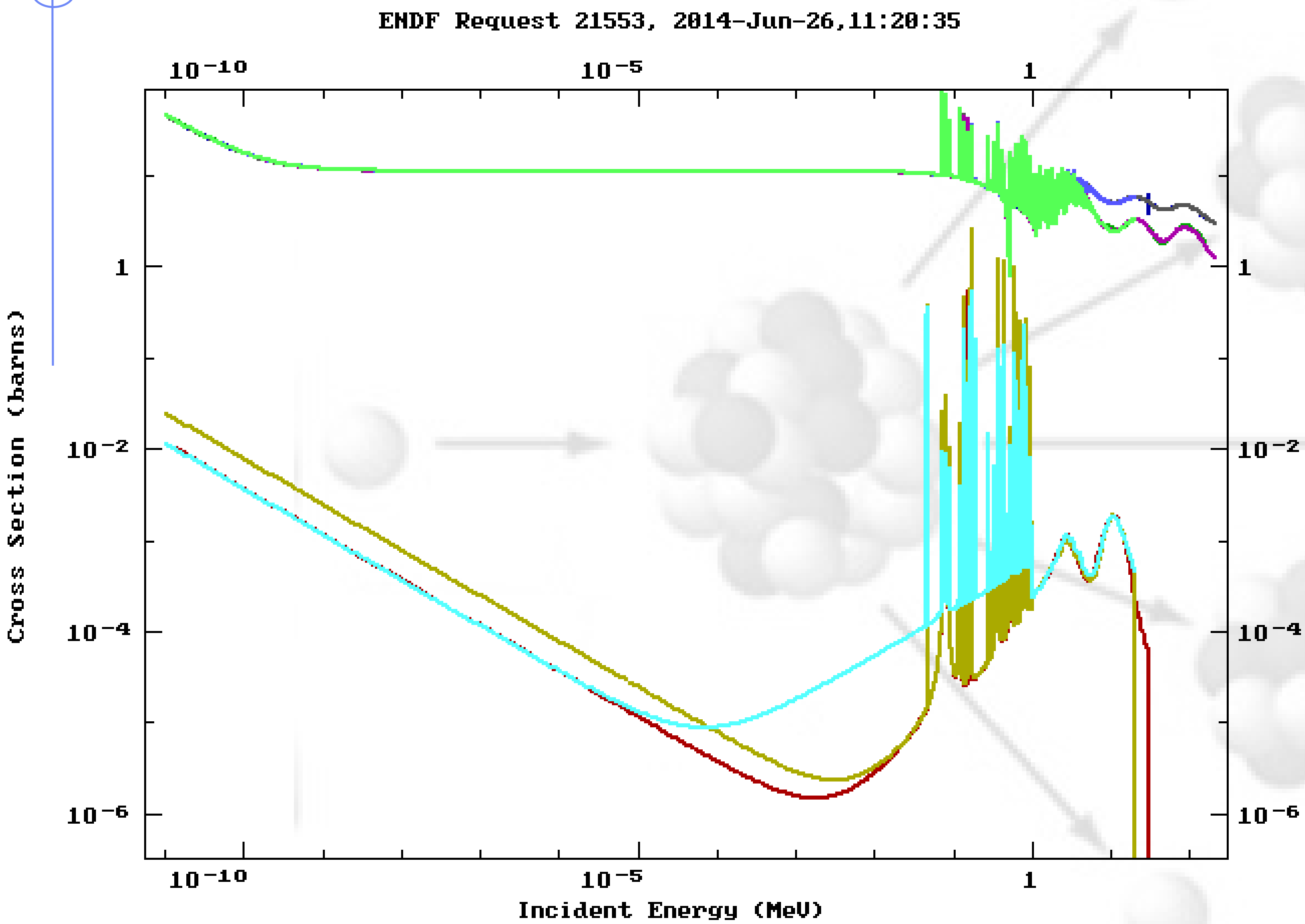
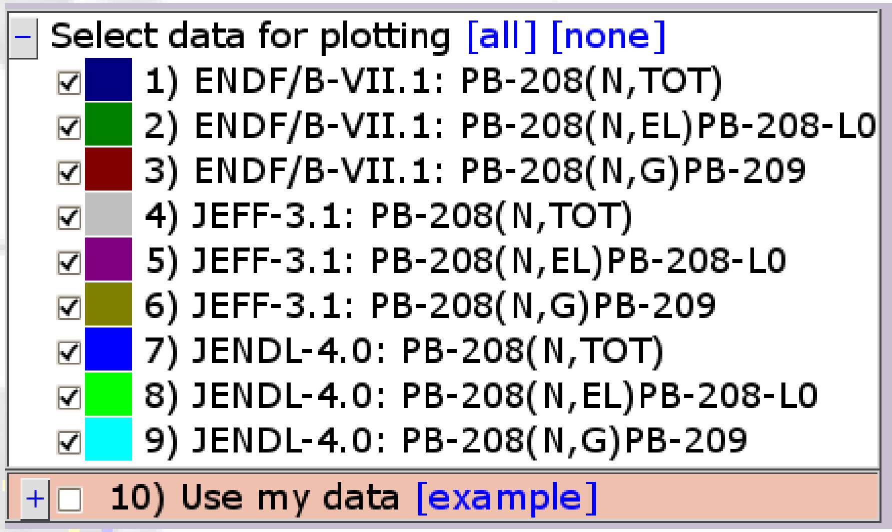




^{208}Pb (evaluated) cross sections:





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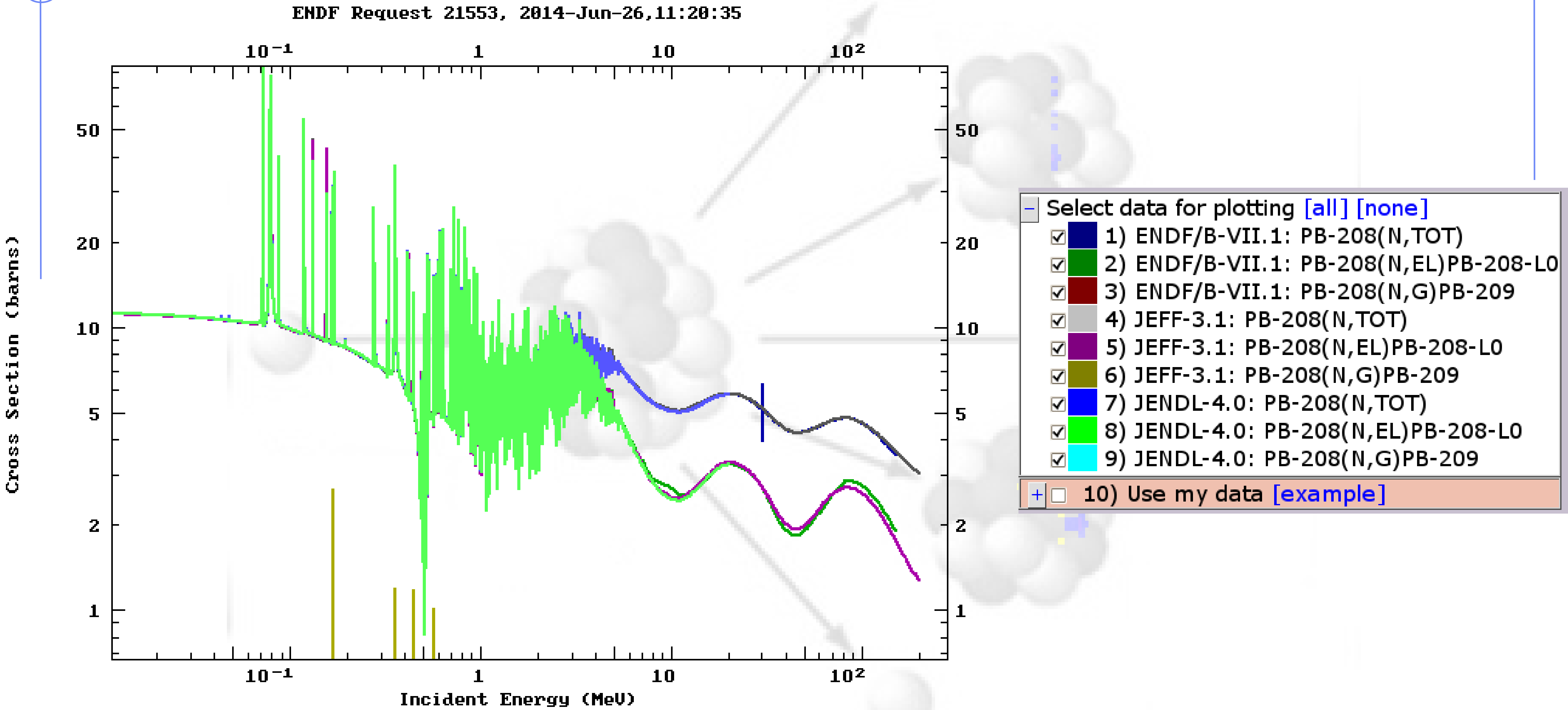
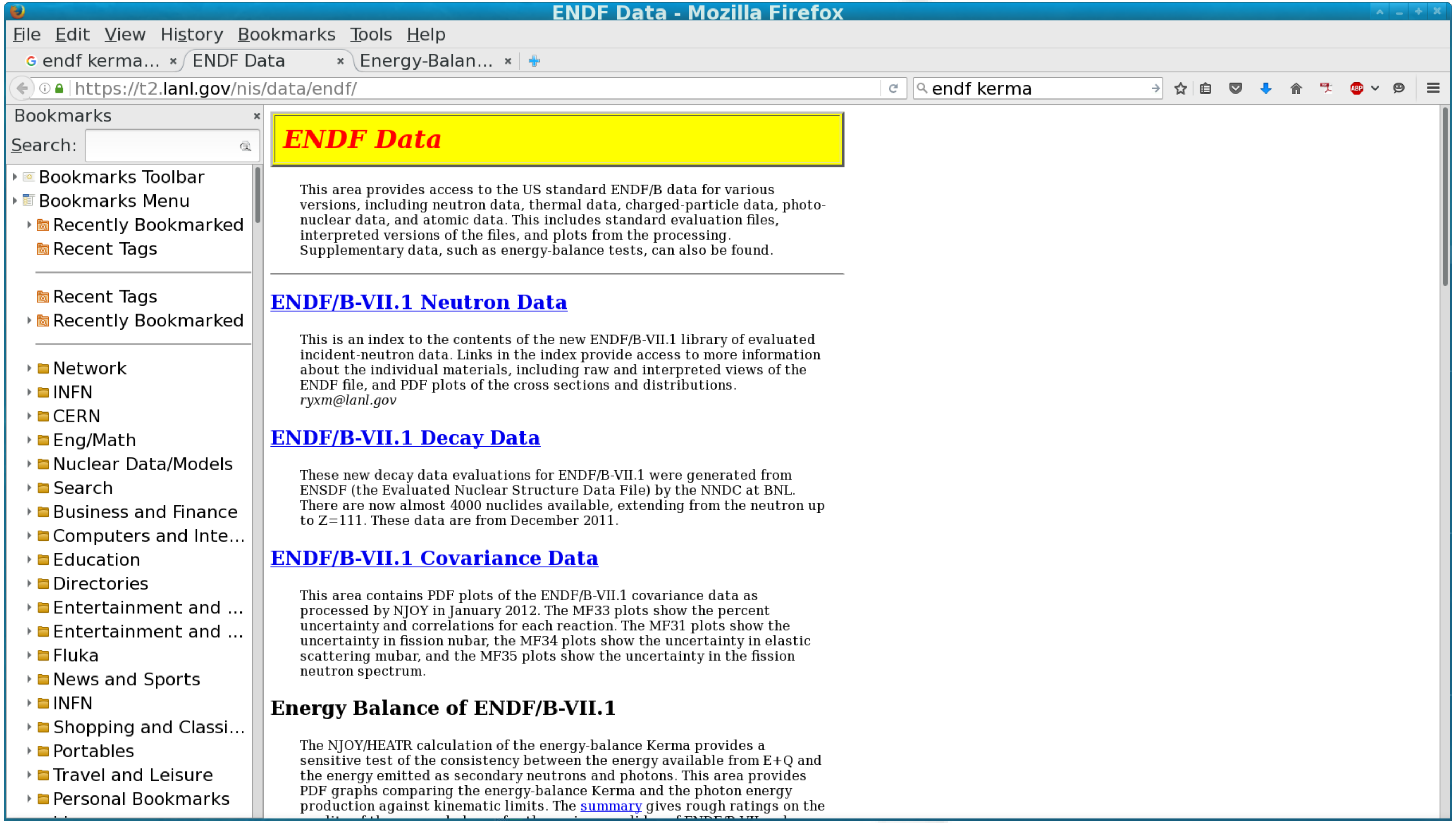


Be careful! For example for ENDF/B-VII.1



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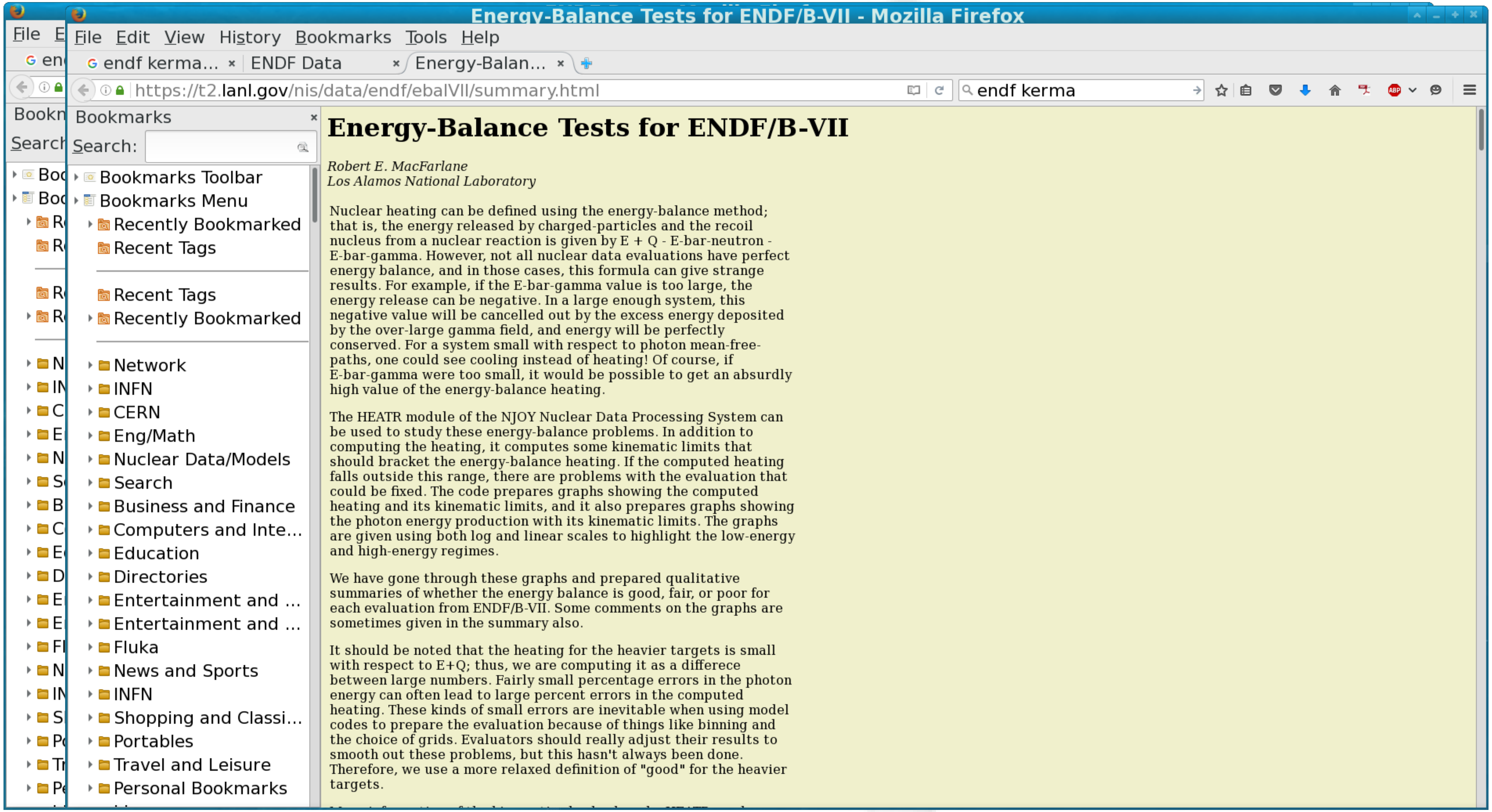


Energy-Balance Tests for ENDF/B-VII

Robert E. MacFarlane
Los Alamos National Laboratory

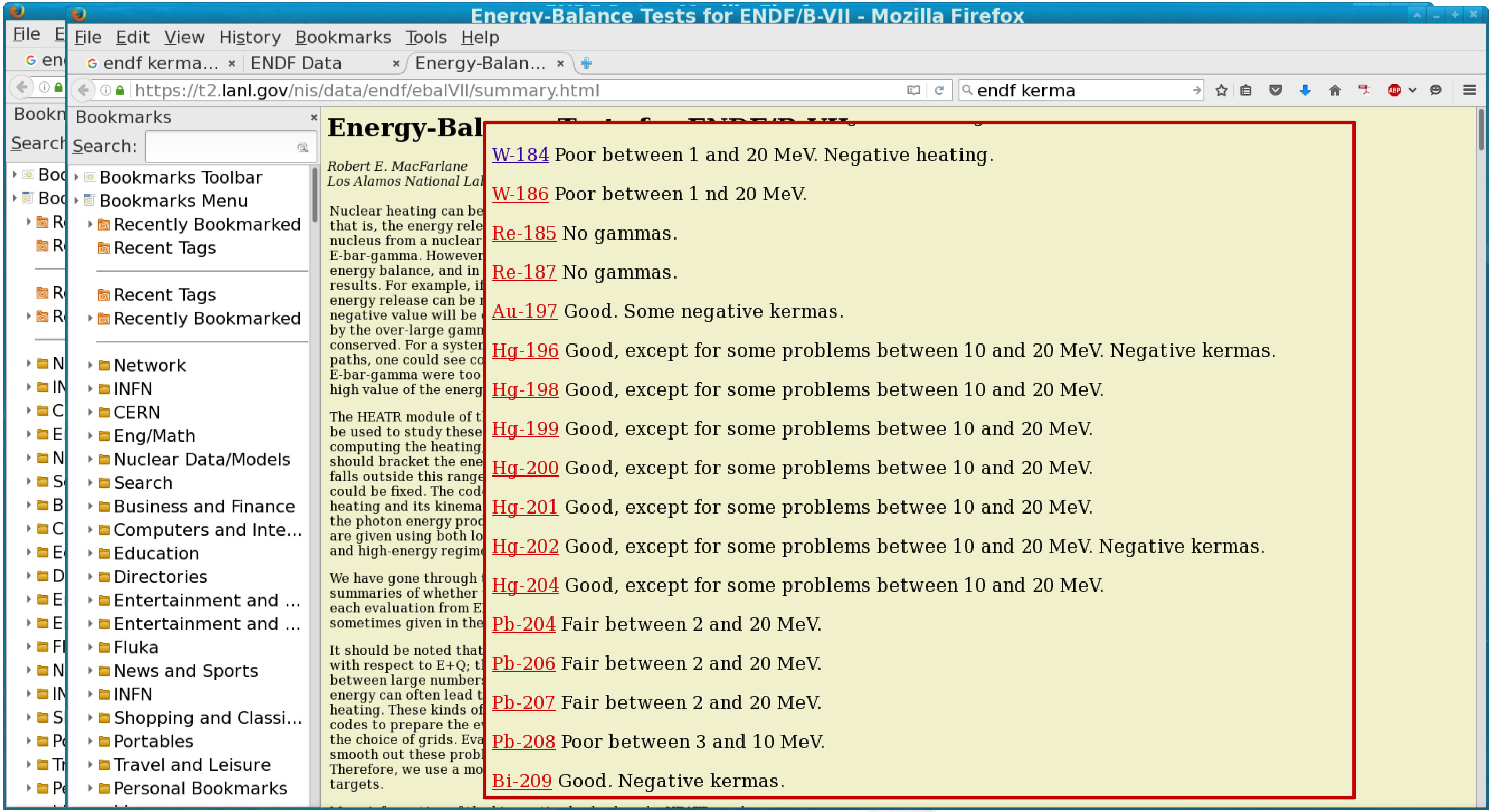
Nuclear heating can be defined using the energy-balance method; that is, the energy released by charged-particles and the recoil nucleus from a nuclear reaction is given by E + Q - E-bar-neutron - E-bar-gamma. However, not all nuclear data evaluations have perfect energy balance, and in those cases, this formula can give strange results. For example, if the E-bar-gamma value is too large, the energy release can be negative. In a large enough system, this negative value will be cancelled out by the excess energy deposited by the over-large gamma field, and energy will be perfectly conserved. For a system small with respect to photon mean-free-paths, one could see cooling instead of heating! Of course, if E-bar-gamma were too small, it would be possible to get an absurdly high value of the energy-balance heating.

The HEATR module of the NJOY Nuclear Data Processing System can be used to study these energy-balance problems. In addition to computing the heating, it computes some kinematic limits that should bracket the energy-balance heating. If the computed heating falls outside this range, there are problems with the evaluation that could be fixed. The code prepares graphs showing the computed heating and its kinematic limits, and it also prepares graphs showing the photon energy production with its kinematic limits. The graphs are given using both log and linear scales to highlight the low-energy and high-energy regimes.

We have gone through these graphs and prepared qualitative summaries of whether the energy balance is good, fair, or poor for each evaluation from ENDF/B-VII. Some comments on the graphs are sometimes given in the summary also.

It should be noted that the heating for the heavier targets is small with respect to E+Q; thus, we are computing it as a difference between large numbers. Fairly small percentage errors in the photon energy can often lead to large percent errors in the computed heating. These kinds of small errors are inevitable when using model codes to prepare the evaluation because of things like binning and the choice of grids. Evaluators should really adjust their results to smooth out these problems, but this hasn't always been done. Therefore, we use a more relaxed definition of "good" for the heavier targets.

Be careful! For example for ENDF/B-VII.1



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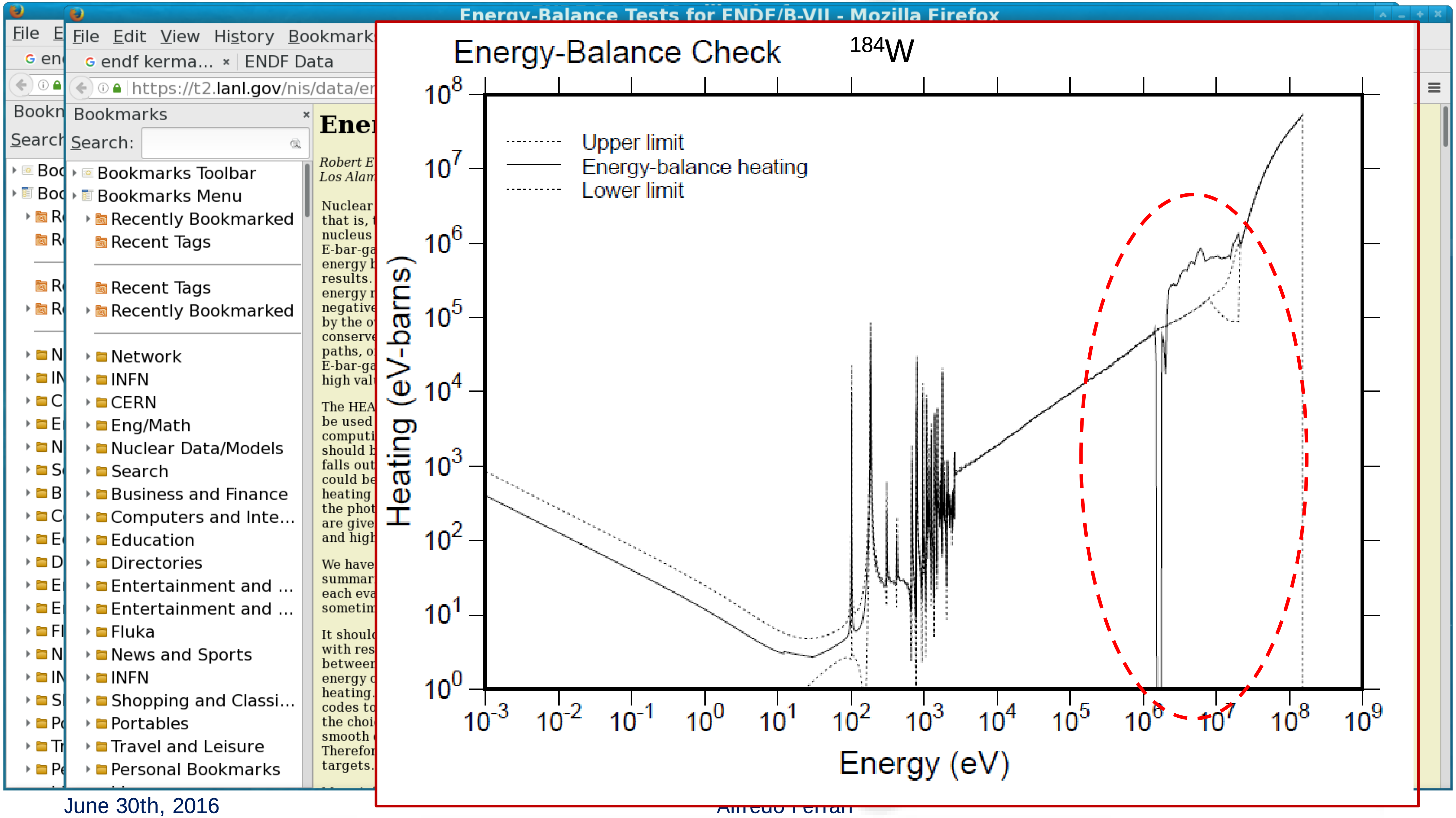

… an example of a qui-pro-quo:

In a recent meeting dealing with the design of a new target for the n_ToF facility at CERN, the engineering team proposed to move ***from pure Pb to Pb with 4% Sb*** for mechanical reasons. One of the main concerns is to keep as low as possible the γ background from the target, but assurances were given that MC simulations including the 4% Sb did not show any increase in the γ background despite the non negligible Sb capture cross section

A quick check after the meeting showed that the ENDF/B (and JENDL, JEFF etc) evaluated data files, surprise surprise…

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Sn-120 No gammas.

Sn-122 No gammas.

Sn-123 No gammas.

Sn-124 No gammas.

Sn-125 Good, except for a big, sharp glitch at 6 MeV. Negative kermas. Comes from a bad photon yield (1.565e6!) at the threshold in MF=6/MT=16.

Sn-126 No gammas.

Sb-121 No gammas.

Sb-123 No gammas.

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Sb-125 No gammas.

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Indeed the calculation could have not shown any increase in γ background because the relevant data do not exist!! Unfortunately in real life Sb isotopes do capture emitting γ's

Evaluated data files: the correlation issue

Evaluated data files contain ***uncorrelated*** information, as a consequence:

- Gamma ray cascades (eg following capture) are ***uncorrelated*** → their energies sum up to the Q_{capt} only ***on average*** and not event-by-event
- All reactions like (n,n'), (n,2n), (n,p) etc which emit gammas don't have the correlation between the outgoing particles energies and angles, and the gammas
- All reactions like (n,2n), (n,3n), (n,np) etc don't have the correlations among the emitted particles → ***energy and momentum are conserved only on average*** and not event-by-event

… in summary no way to produce fully correlated, energy/momentum and quantum number conserving events from evaluated nuclear data files, → no coincidence-like calculations can be done, on top…

- … often codes do not correlate even when it is partially possible (eg emitting capture gammas when the neutron is captured, trying to correlate (n,n') etc)
- … and often they do not explicitly produce charged particles (at least below 20 MeV)
- … often the information is incomplete (no γ prod.) and/or inconsistent (eg. kermas…)

A recent attempt to "correlate" inclusive σ data:

Nuclear Instruments and Methods in Physics Research A 763 (2014) 575–590

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Development of a reaction ejectile sampling algorithm to recover kinematic correlations from inclusive cross-section data in Monte-Carlo particle transport simulations

T. Ogawa [a,*], T. Sato [a], S. Hashimoto [a], K. Niita [b]

[a] *Research Group for Radiation Protection, Environment and Radiation Sciences Unit, Nuclear Science and Engineering Center, Japan Atomic Energy Agency, Shirakata-Shirane, Tokai, Ibaraki 319-1195, Japan*

[b] *Research Organization for Information Science and Technology, Shirakata-shirane, Tokai, Ibaraki 319-1188, Japan*

A R T I C L E I N F O

Article history:
Received 5 March 2014
Received in revised form
9 May 2014
Accepted 18 June 2014
Available online 10 July 2014

A B S T R A C T

A new phenomenological approach is developed to reproduce the stochastic distributions of secondary particle energy and angle with conservation of momentum and energy in reactions ejecting more than one ejectiles using inclusive cross-section data. The summation of energy and momentum in each reaction is generally not conserved in Monte-Carlo particle transport simulation based on the inclusive cross-sections because the particle correlations are lost in the inclusive cross-section data. However, the

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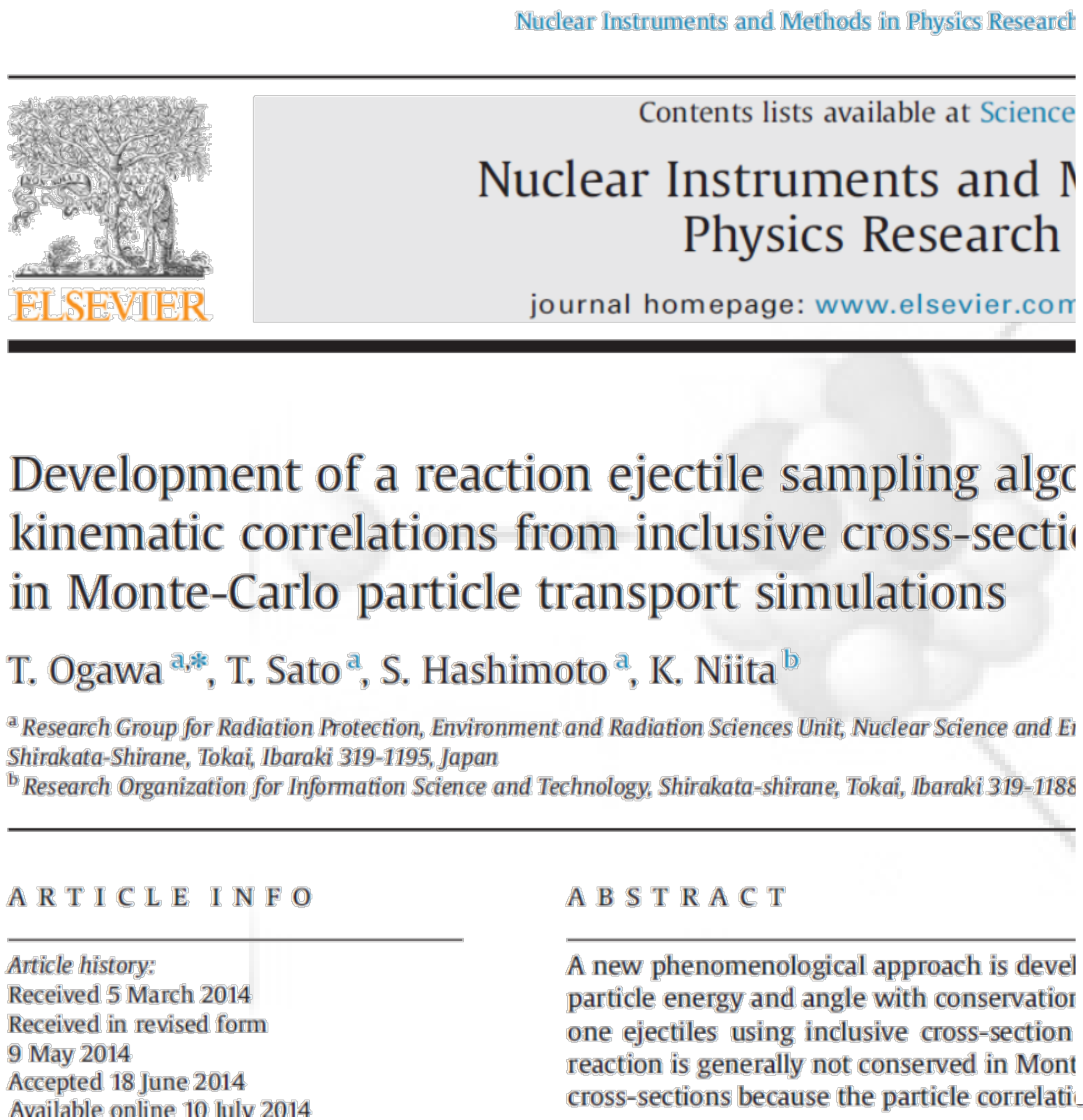

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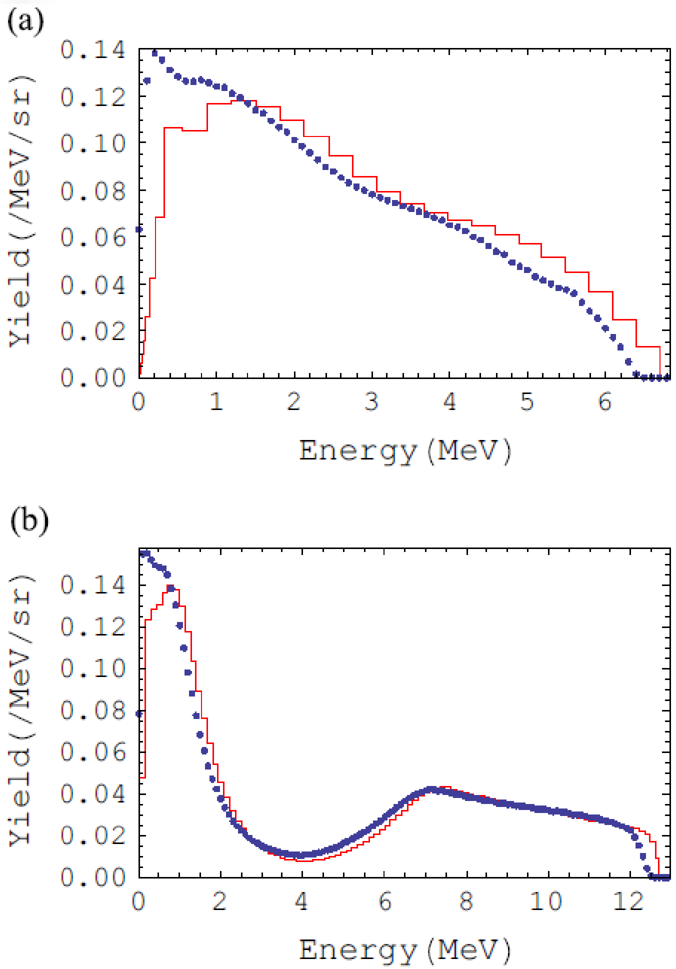

Fig. 19. Angle-integrated secondary neutron energy spectra by 20 MeV neutrons calculated using RAKIC. The line represents the cross-section data taken from JENDL-4.0. (a) ^{54}Fe(n,2n) reaction and (b) ^{150}Nd(n,2n) reaction.

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Nuclear Instruments and Methods in Physics Research A

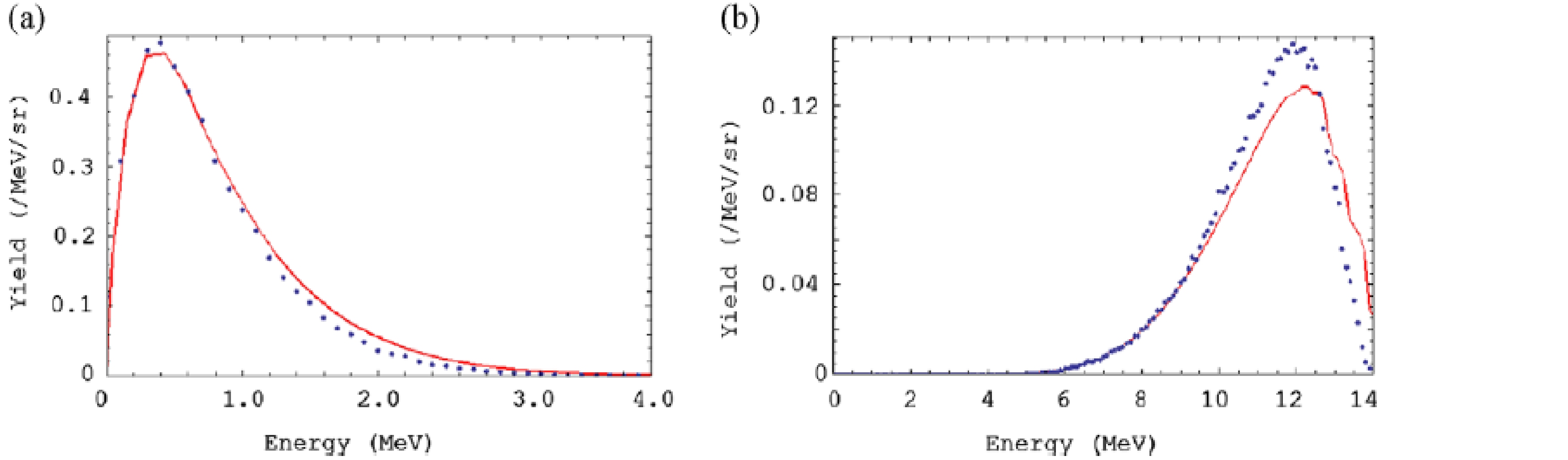

Fig. 31. Secondary particle energy spectra of ^{197}Au(n,np) reactions by 20 MeV neutrons integrated over the whole solid angle. The line represents the original cross-section of JENDL 4.0. (a) Neutron and (b) proton.

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Monte Carlo Flavors –I

Microscopic Analog Monte Carlo

- Uses theoretical models to describe physical processes whenever possible
- Samples from actual physical phase space distributions
- Predicts average quantities and all statistical moments of any order
- Preserves correlations (provided the physics is correct, of course!)
- Reproduces fluctuations (provided. . . see above)
- Is (almost) safe and (sometimes) can be used as a “black box" (idem)

But:

- Can be inefficient and converge slowly
- Can fail to predict contributions due to rare events
- Often (neutronics the most striking example!) the information to preserve correlations is simply not there!

Monte Carlo Flavors –II

Biased or Inclusive Monte Carlo

- Uses theoretical models to describe physical processes whenever possible
- samples from artificial and/or inclusive distributions, can apply a weight to the particles to correct for the bias (*similar to an integration by a change of variable*)
- predicts average quantities, but not the higher moments (on the contrary, biased calculation goal is to *minimize* the second moment!)
- Biasing if proper applied $\rightarrow$ same mean with smaller variance → faster convergence
- allows sometimes to obtain acceptable statistics where an analog Monte Carlo would take years of CPU time to converge

But:

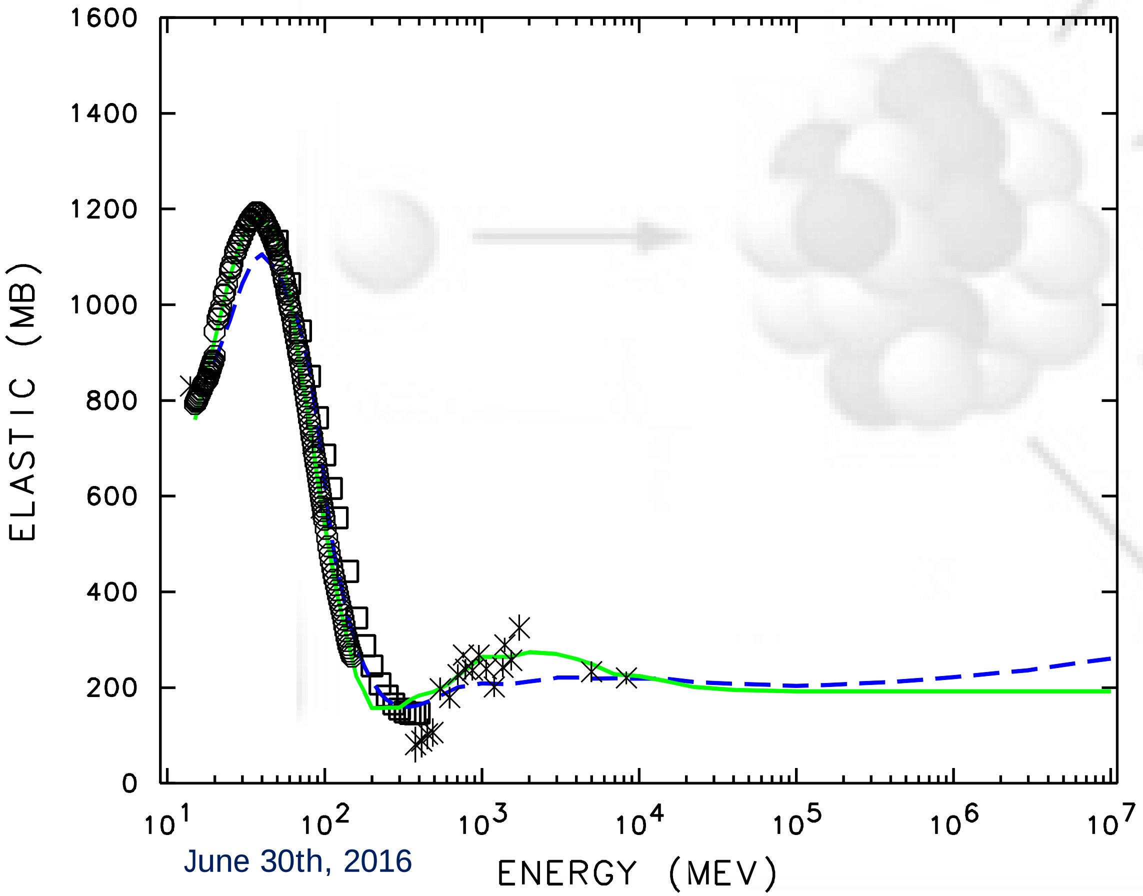
- cannot reproduce correlations and fluctuations
- ONLY privileged observables converge faster (*some regions of phase space are sampled more than others*).

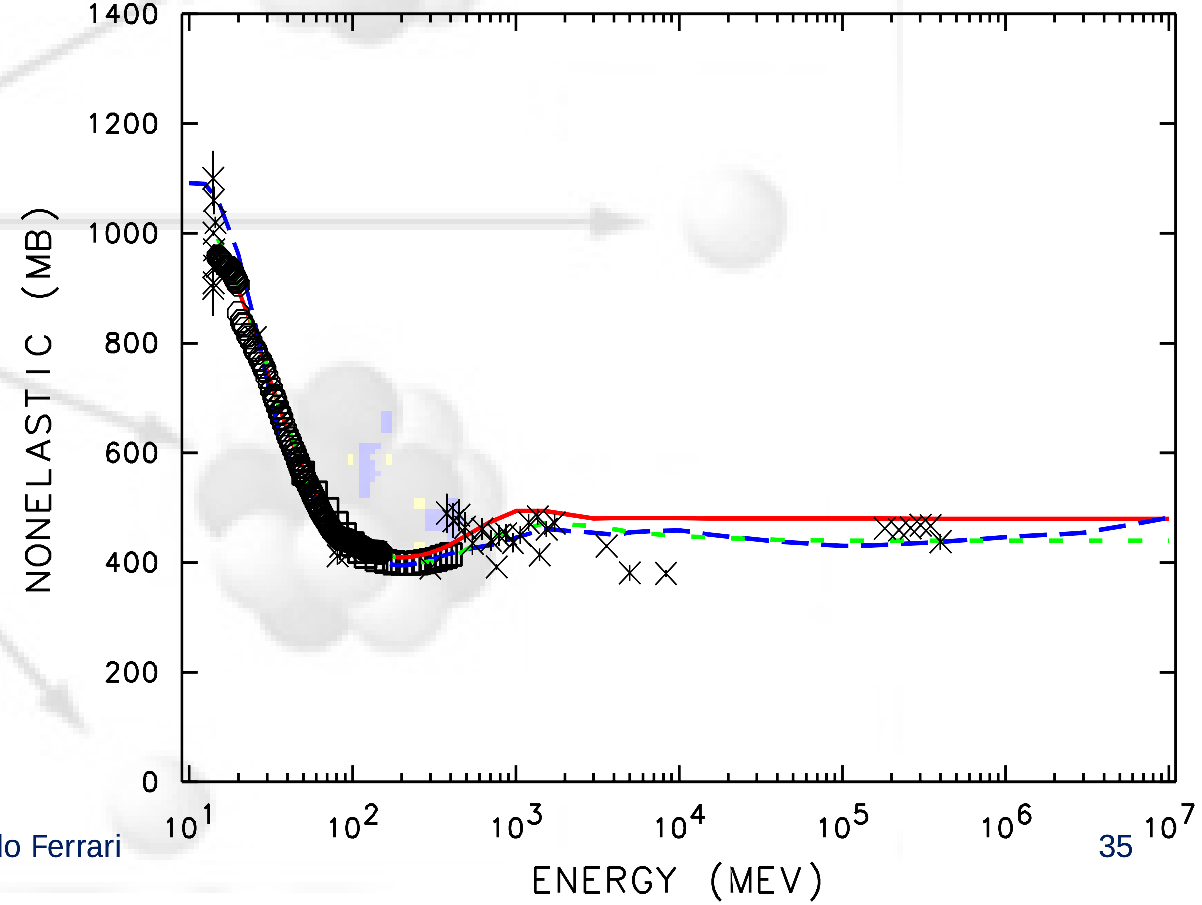
"High" (> 20/150 MeV) energy MC nuclear models:

- A large variety exists…
- Most (but not all) are based on similar physics concepts (shortly presented in the following)
- Ranges of validity can vary a lot:
  - Projectile energy range
  - Supported projectiles
  - Targets
  - Reliable outputs (spectra, residuals, γ's…)
- … for many problems one has to use them…
- … the good thing is that (good) models fully conserve correlations on an event-by-event basis …
- … the bad thing(s), too many to list!

Example of σ_{non}, σ_{el} for ^{27}Al:

Experimental (X's), optical model (open square), and curves from various codes (colored lines), for the elastic (below left) and non elastic (below right) neutron cross section on ^{27}Al at energies above 10 MeV





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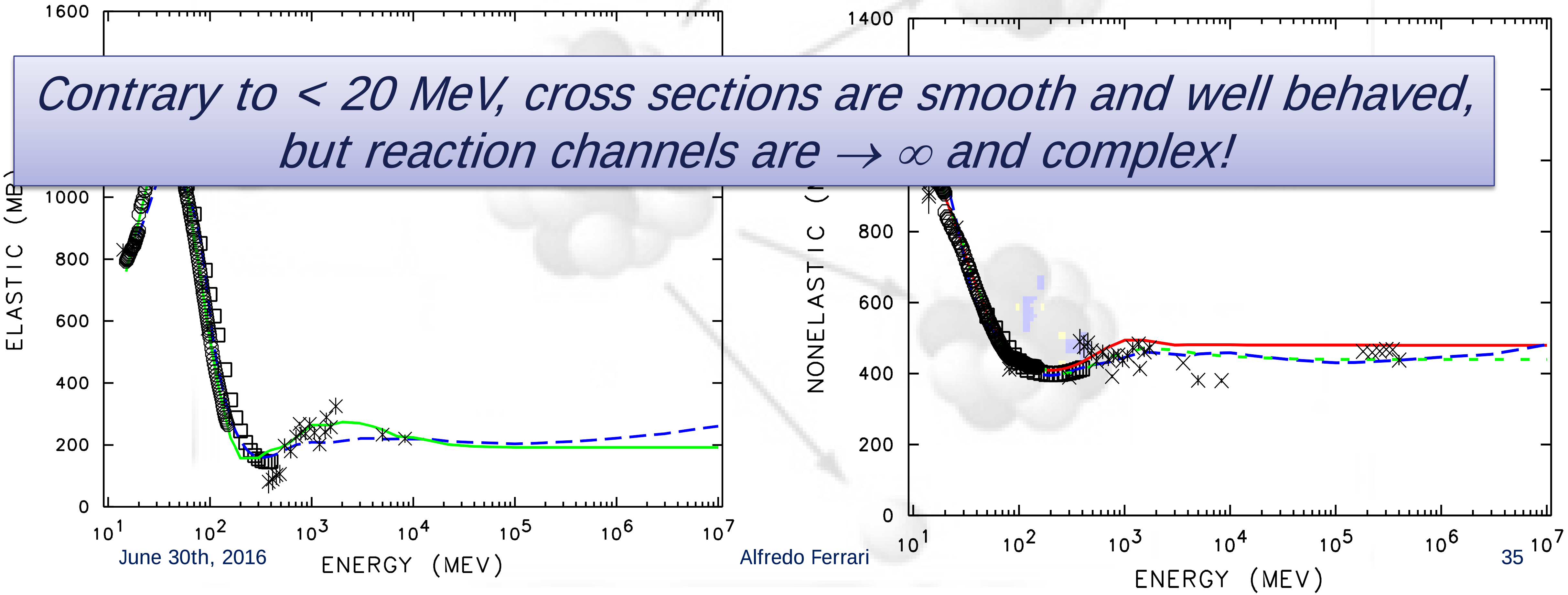
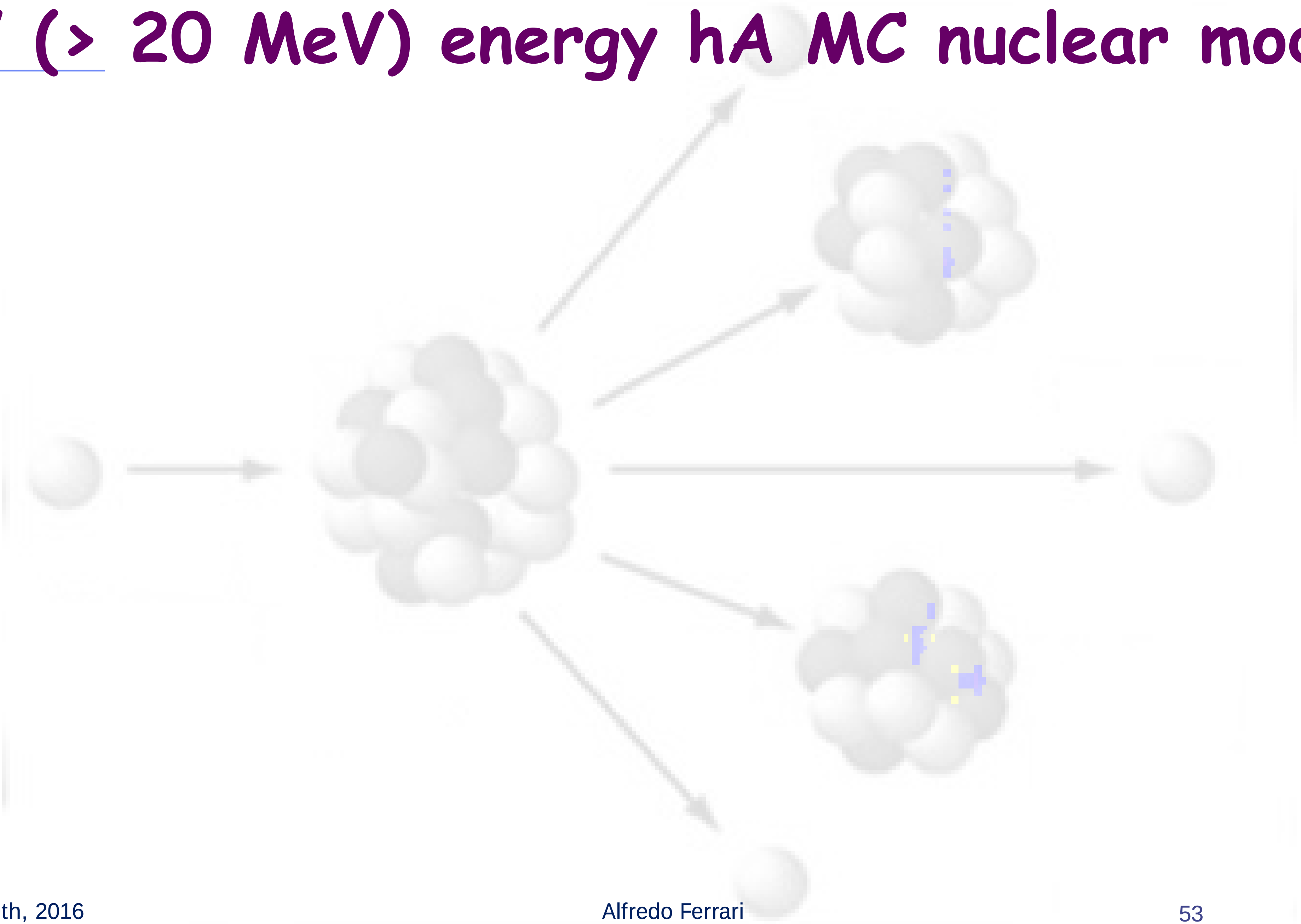


Contrary to < 20 MeV, cross sections are smooth and well behaved, but reaction channels are → ∞ and complex!

"High" (> 20 MeV) energy hA MC nuclear models:



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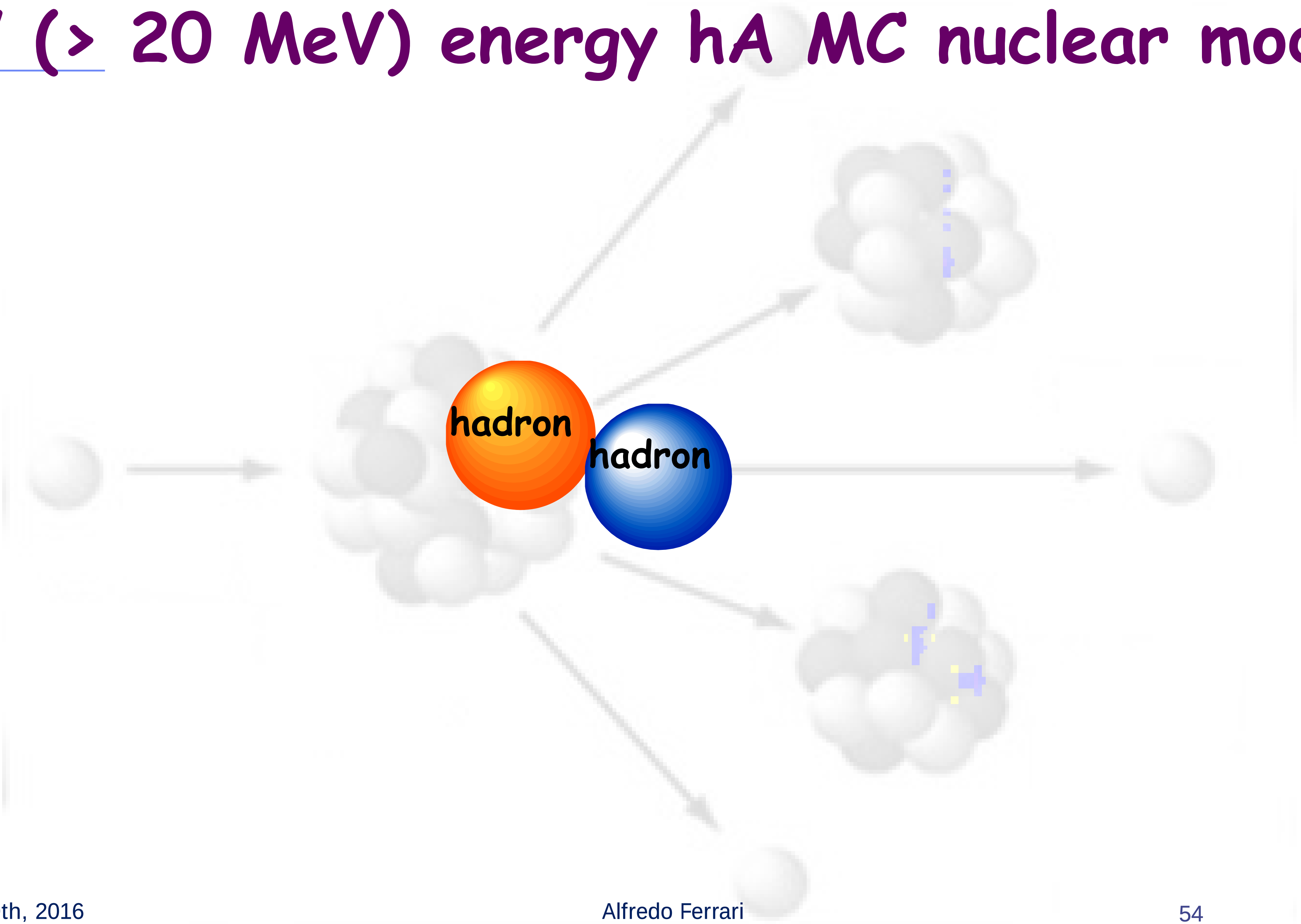

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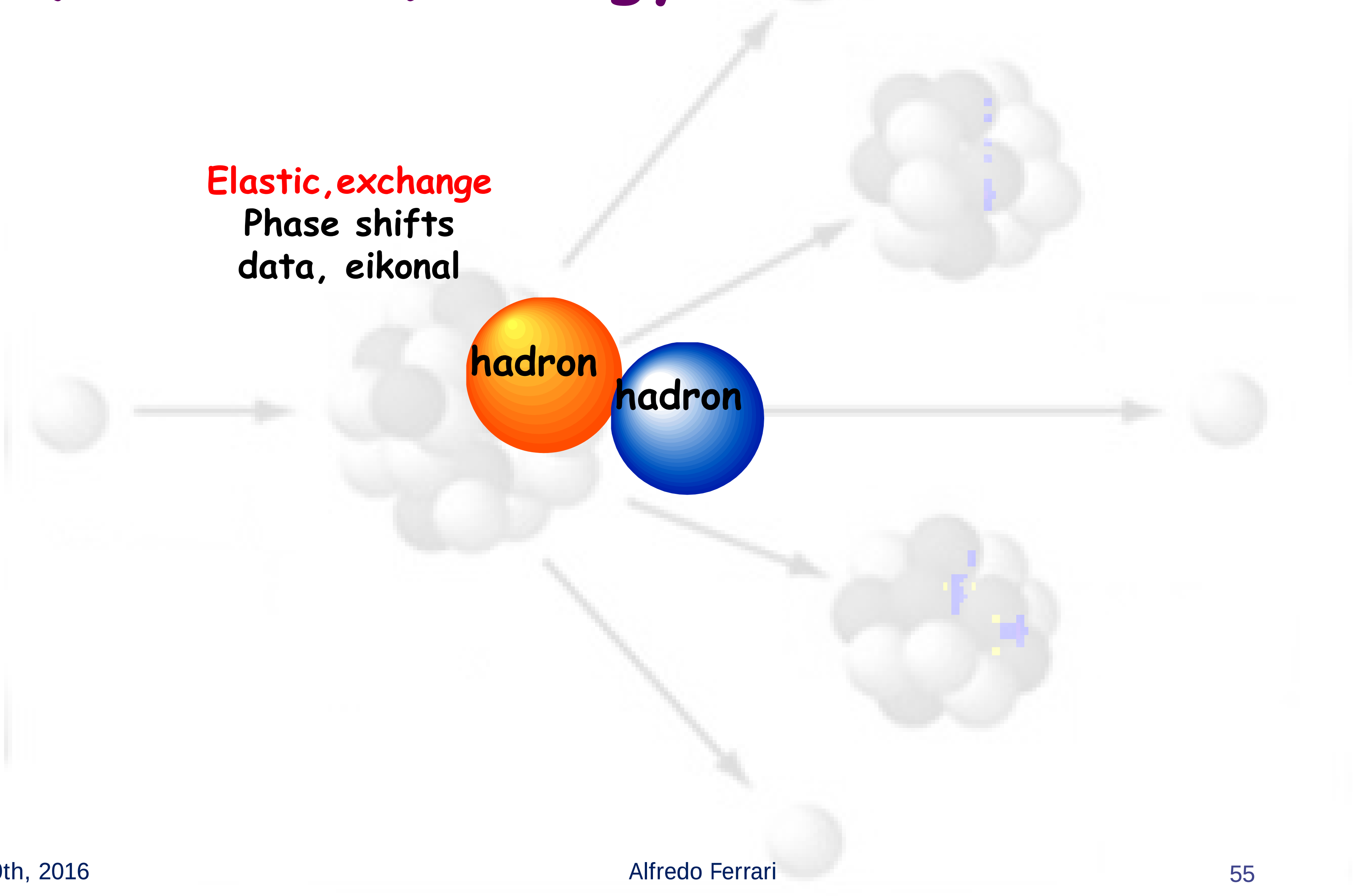

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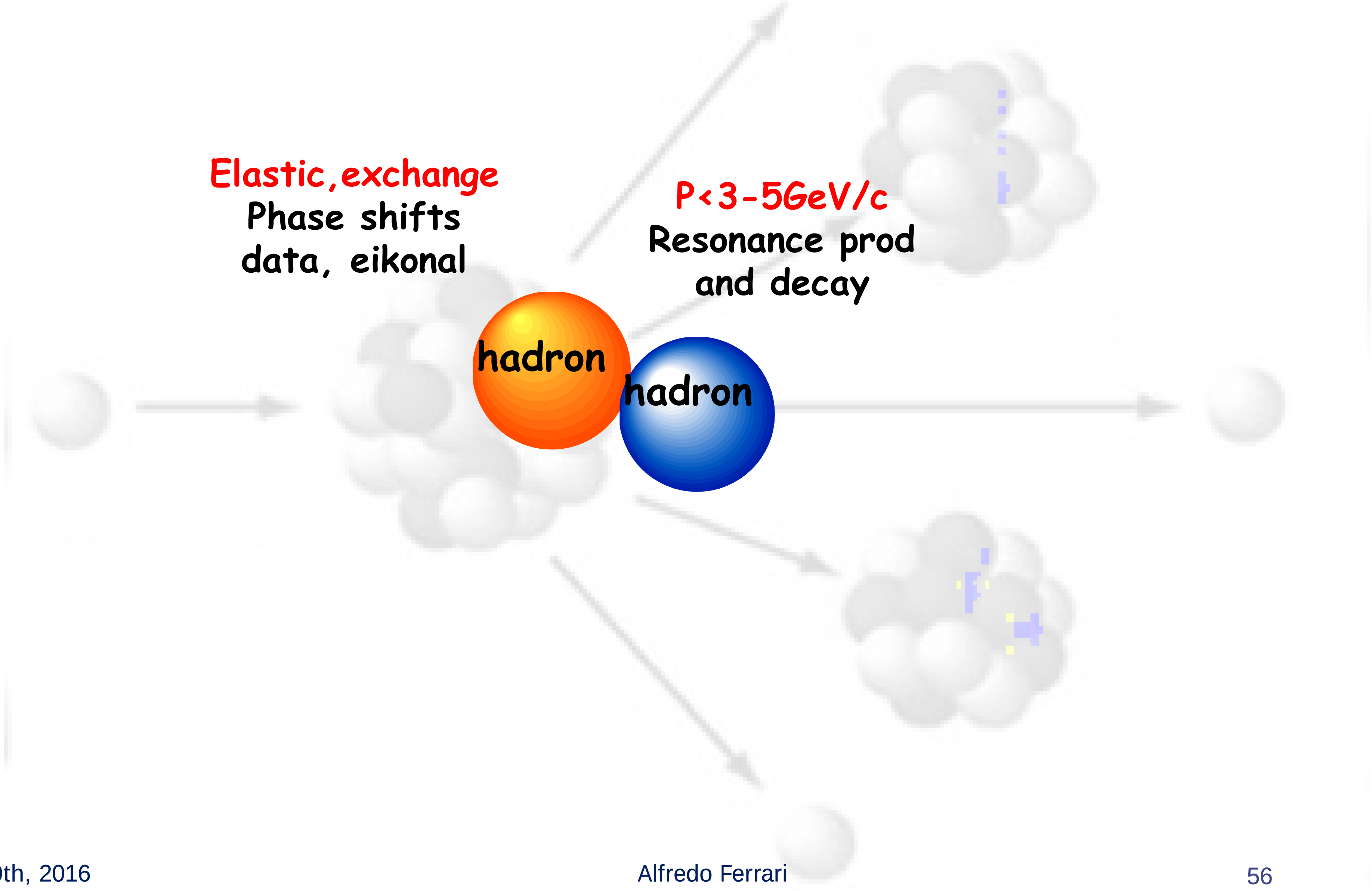

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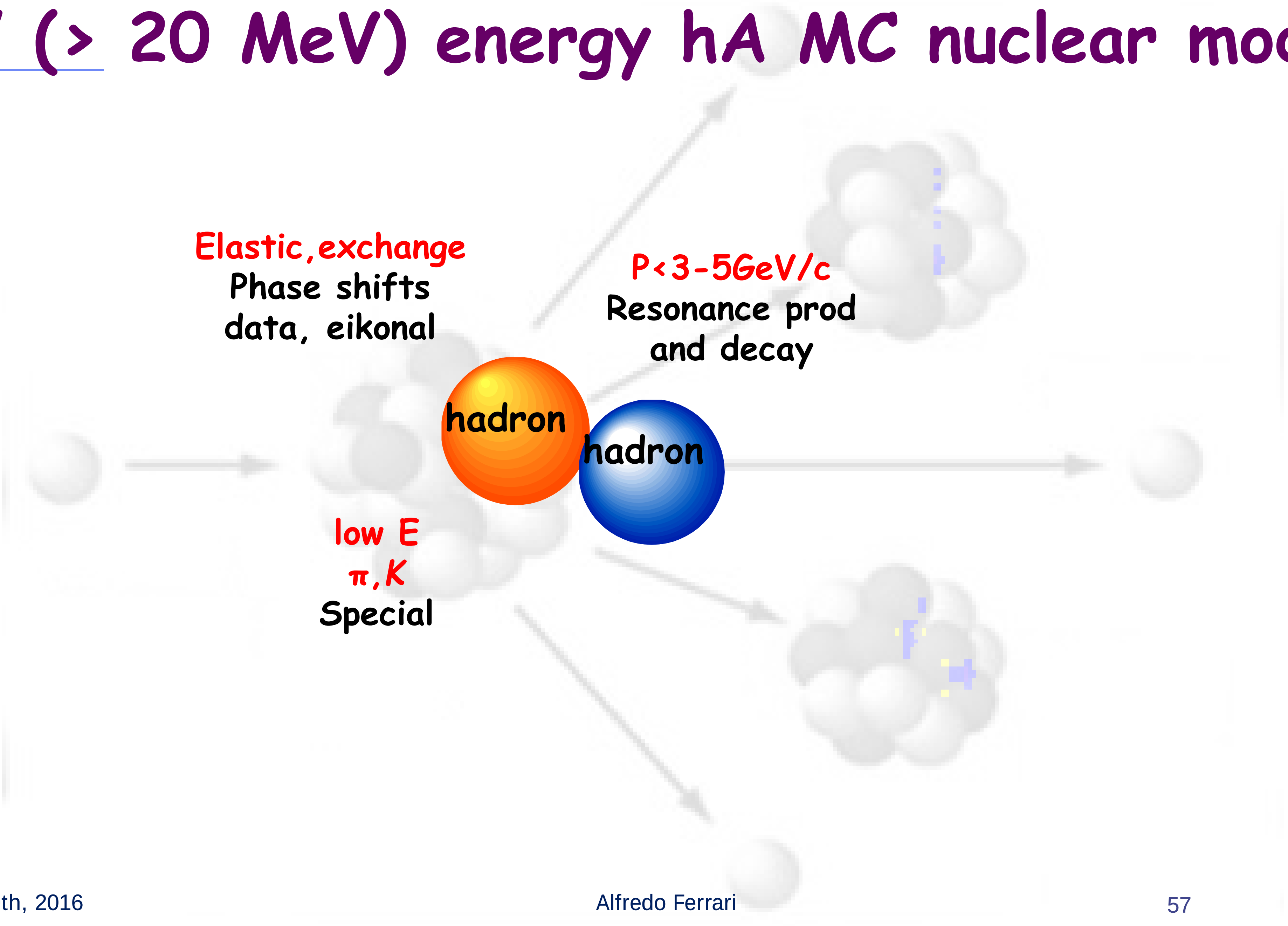

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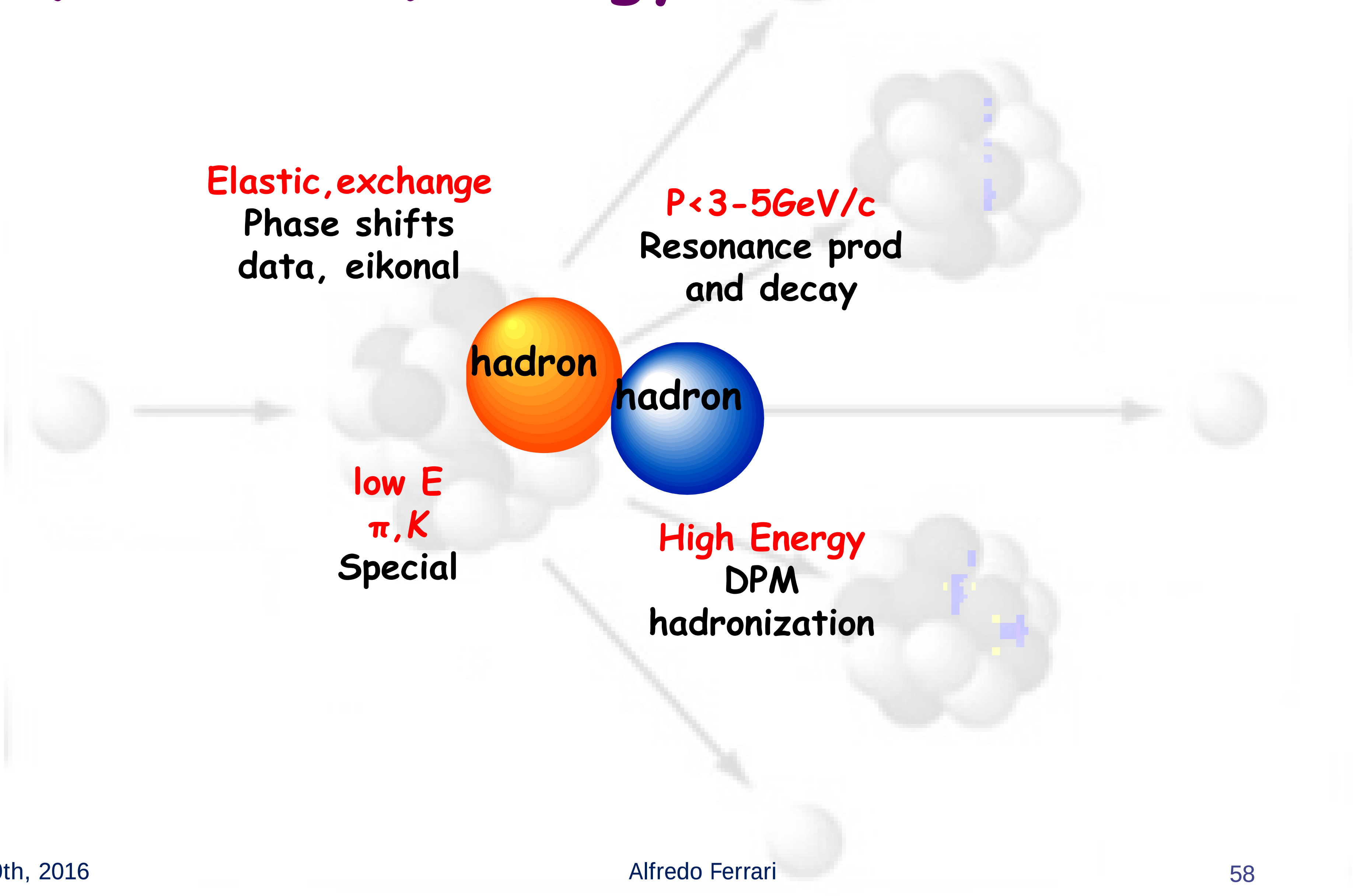

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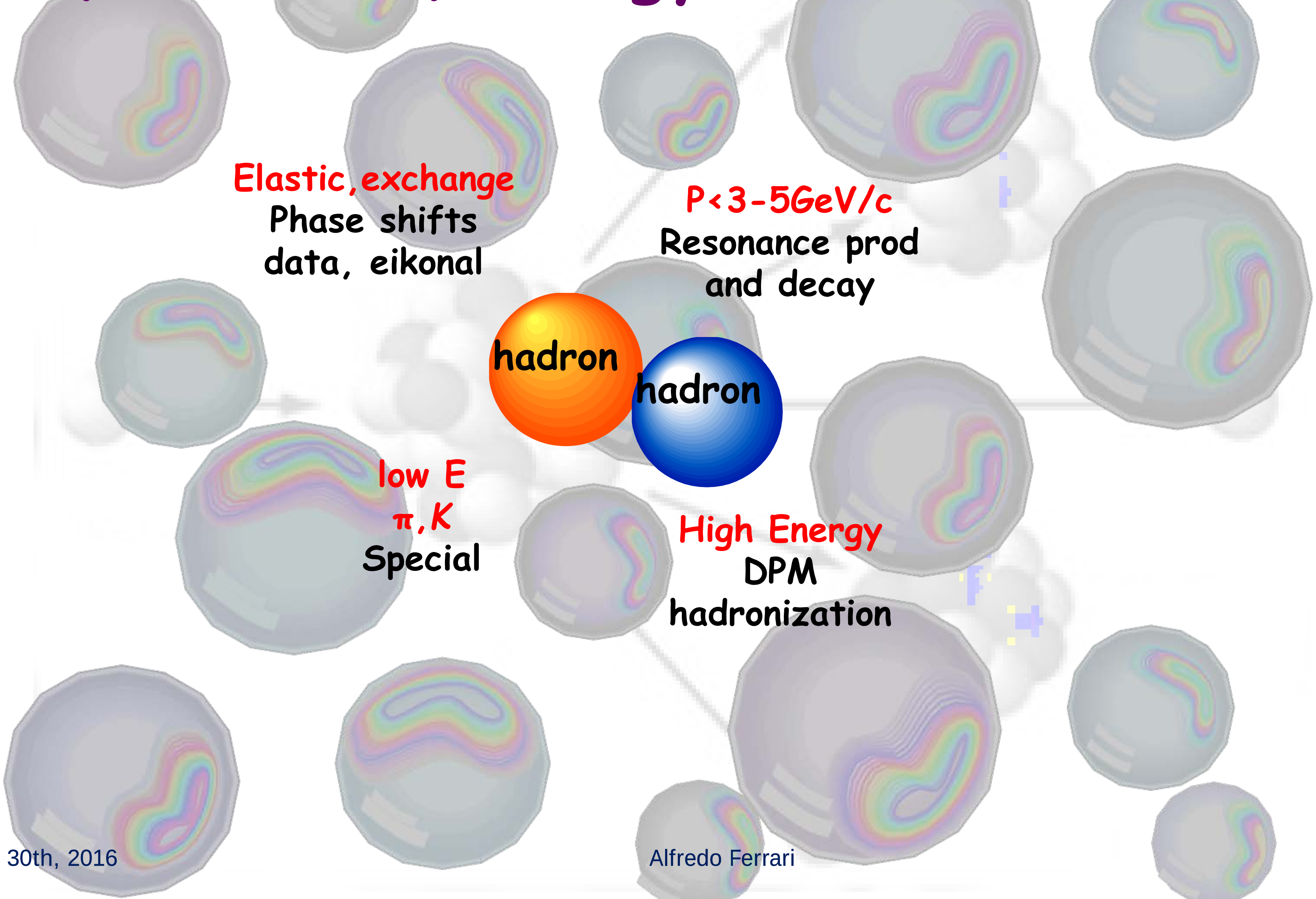


"High" (> 20 MeV) energy hA MC nuclear models:

Hadron-nucleus:

Elastic,exchange
Phase shifts
data, eikonal

P<3-5GeV/c
Resonance prod
and decay

low E
π,K
Special

High Energy
DPM
hadronization

Sophisticated
G-Intranuclear Cascade
(formation zone,
coherence length etc)

Gradual onset of
Glauber-Gribov multiple
interactions

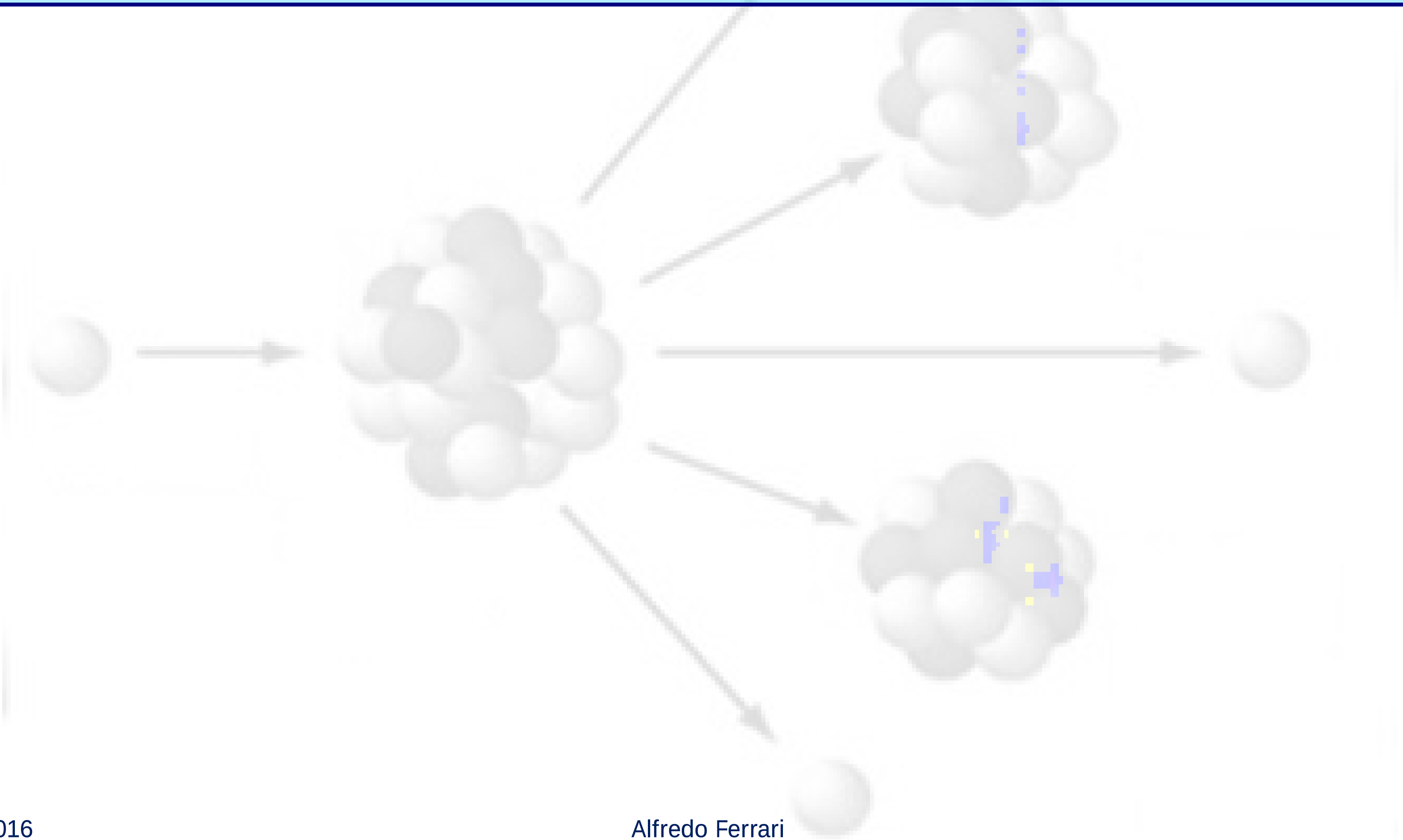
Preequilibrium

Coalescence

Evaporation/Fission/Fermi break-up
γ deexcitation

An example: nuclear interactions in PEANUT

Target nucleus description (density, Fermi motion, etc)



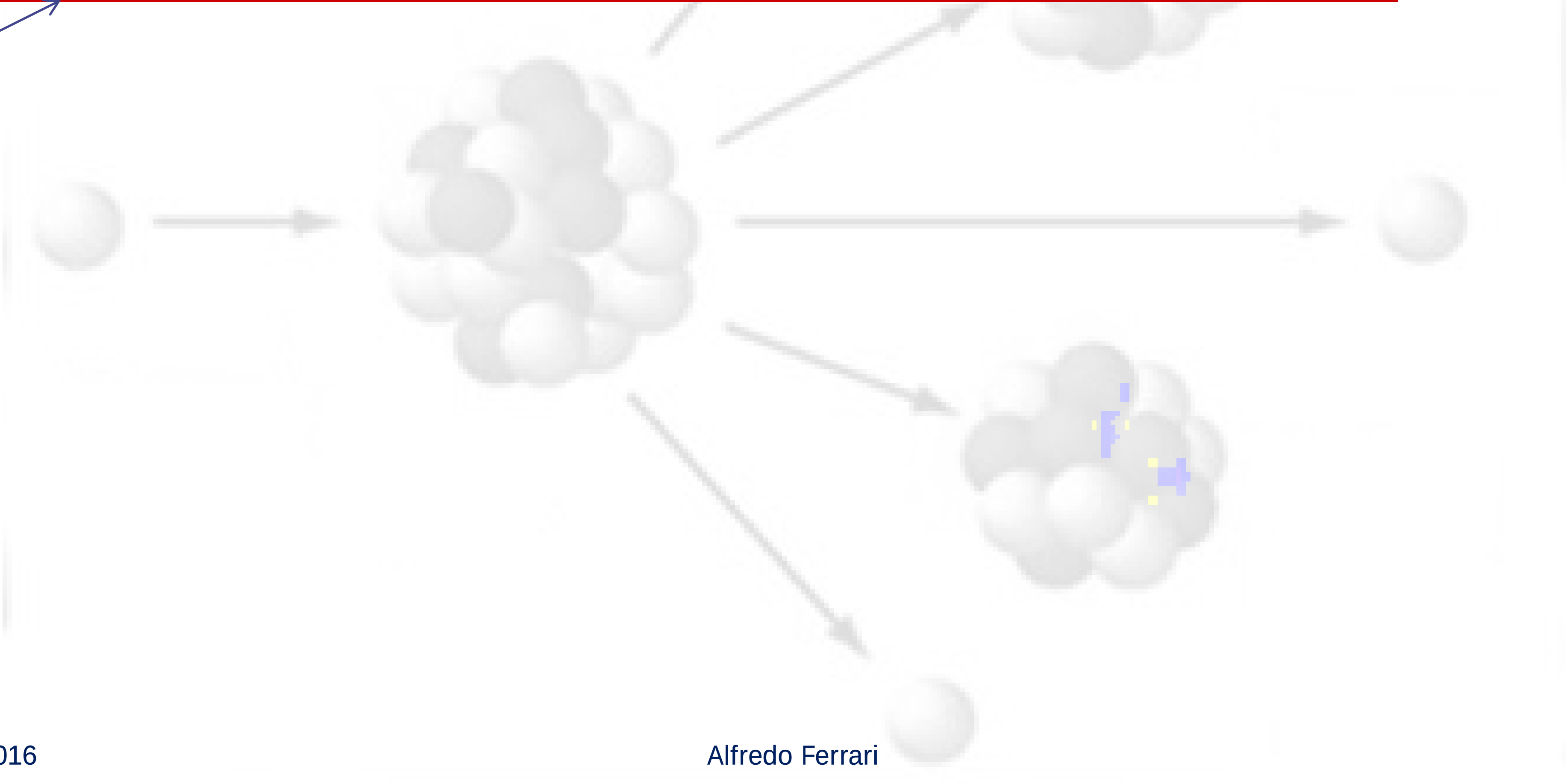
An example: nuclear interactions in PEANUT

Target nucleus description (density, Fermi motion, etc)

⇩

Glauber-Gribov cascade with formation zone

High energies (above few GeV)



An example: nuclear interactions in PEANUT

Target nucleus description (density, Fermi motion, etc)

↓

Glauber-Gribov cascade with formation zone

↓

Generalized IntraNuclear cascade

High energies (above few GeV) → Glauber-Gribov cascade with formation zone

An example: nuclear interactions in PEANUT

Target nucleus description (**density, Fermi motion**, etc)

⇩

Glauber-Gribov cascade with formation zone

High energies (above few GeV)

⇩

Generalized IntraNuclear cascade

⇩

Preequilibrium stage with current exciton configuration and excitation energy
(all non-nucleons emitted/decayed + all nucleons below 30-100 MeV)

An example: nuclear interactions in PEANUT

Target nucleus description (density, Fermi motion, etc)

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Glauber-Gribov cascade with formation zone

High energies (above few GeV)

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Generalized IntraNuclear cascade

⇩

Preequilibrium stage with current exciton configuration and excitation energy
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Evaporation/Fragmentation/Fission model

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Target nucleus description (density, Fermi motion, etc)

⇓

Glauber-Gribov cascade with formation zone

High energies (above few GeV)

⇓

Generalized IntraNuclear cascade

⇓

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⇓

Evaporation/Fragmentation/Fission model

⇓

γ deexcitation

An example: nuclear interactions in PEANUT

Target nucleus description (density, Fermi motion, etc)

⇩

Glauber-Gribov cascade with formation zone

High energies (above few GeV)

⇩

Generalized IntraNuclear cascade

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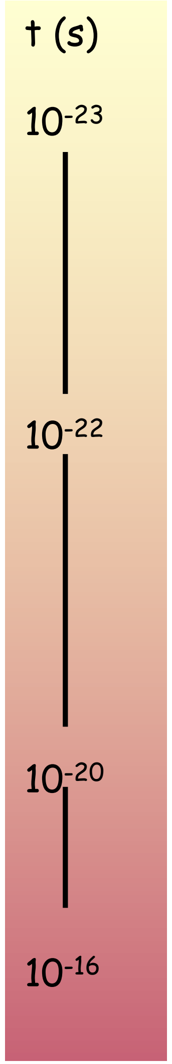
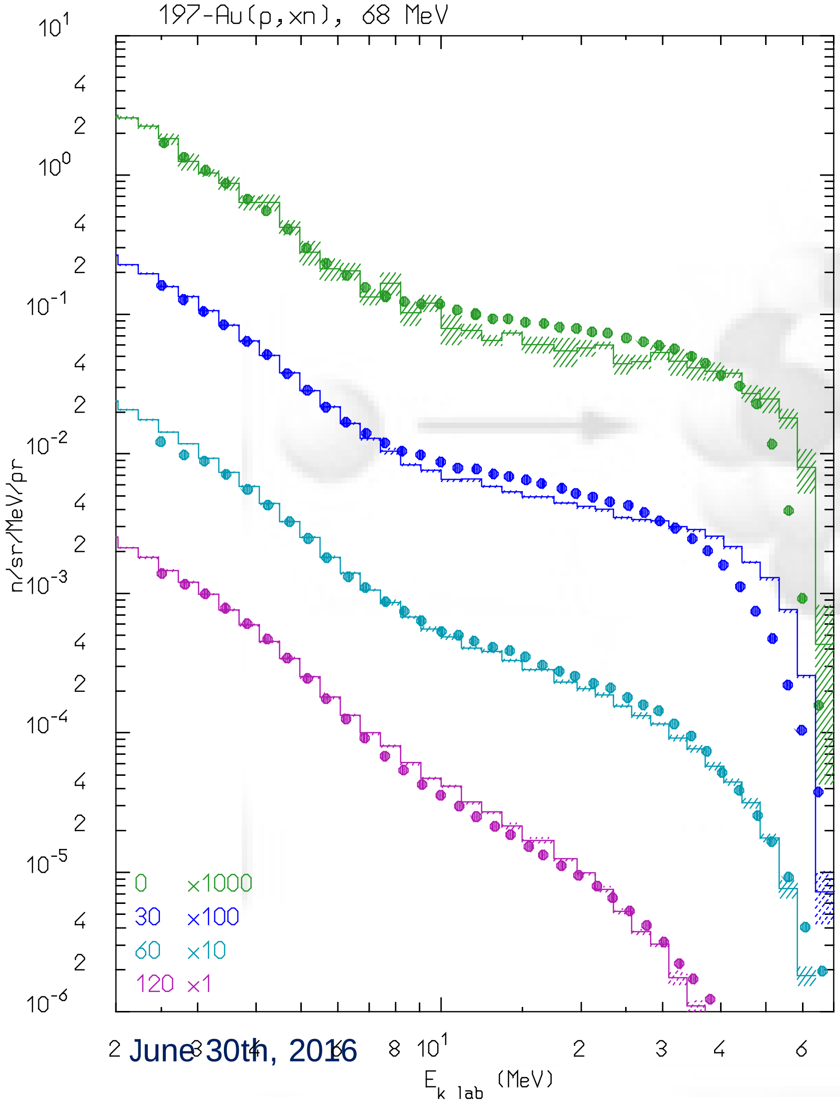
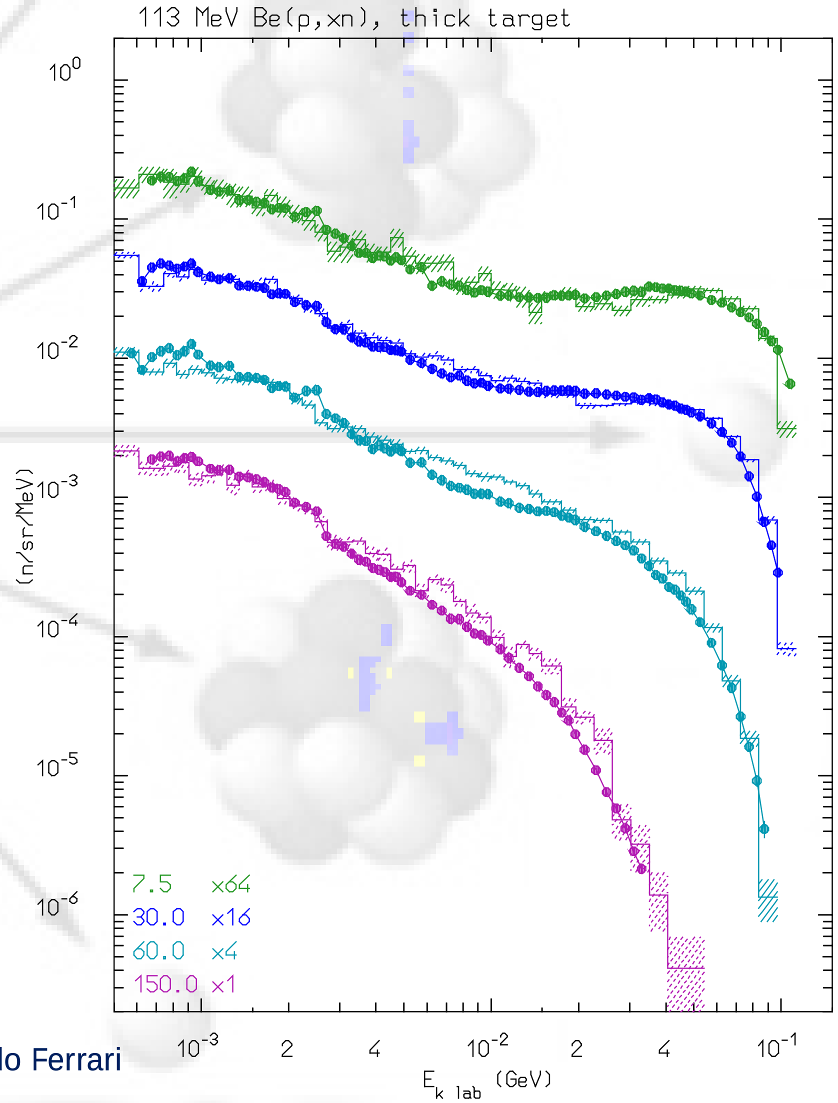


Thick target examples: neutrons

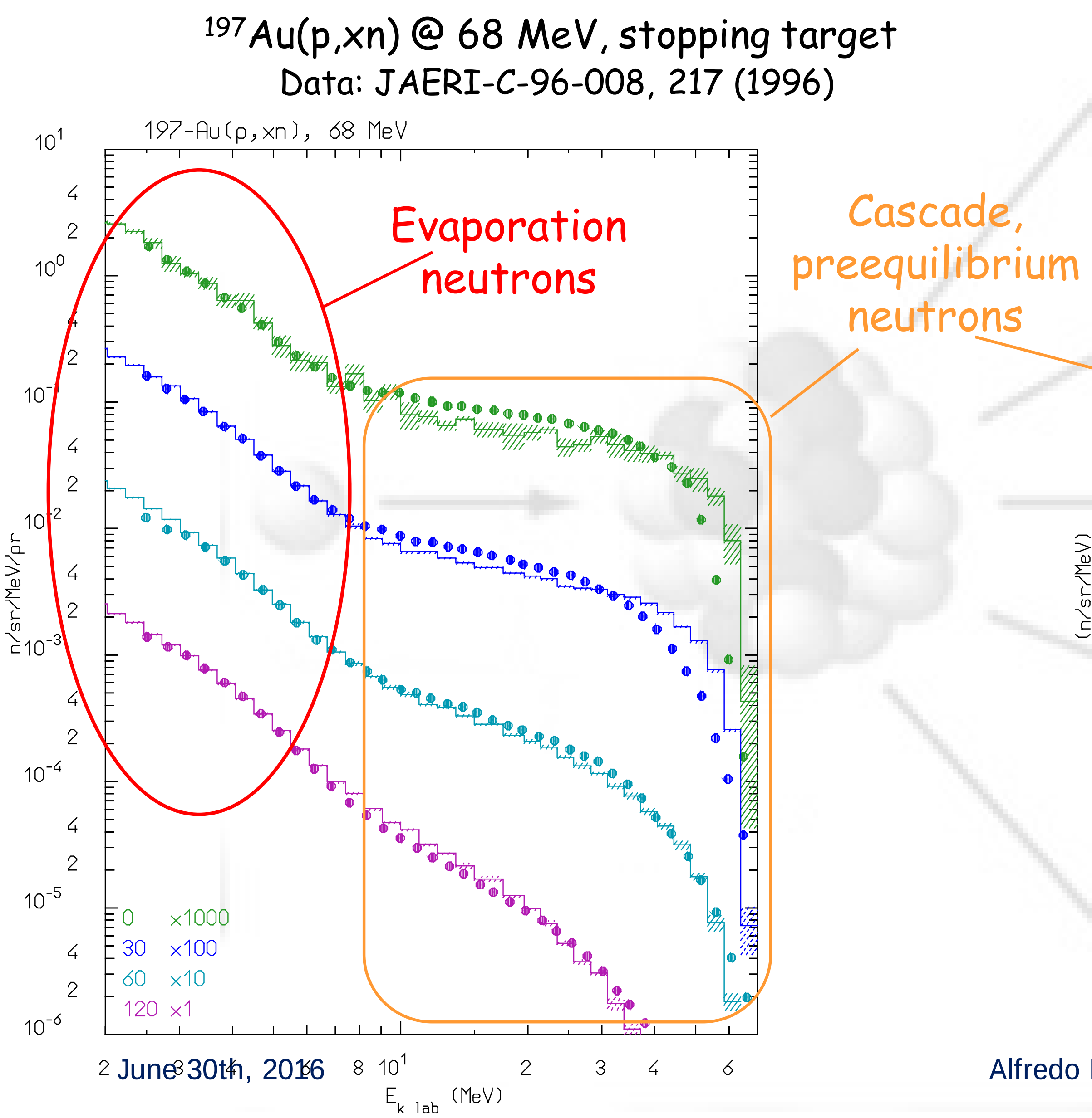
^{197}Au(p,xn) @ 68 MeV, stopping target
Data: JAERI-C-96-008, 217 (1996)

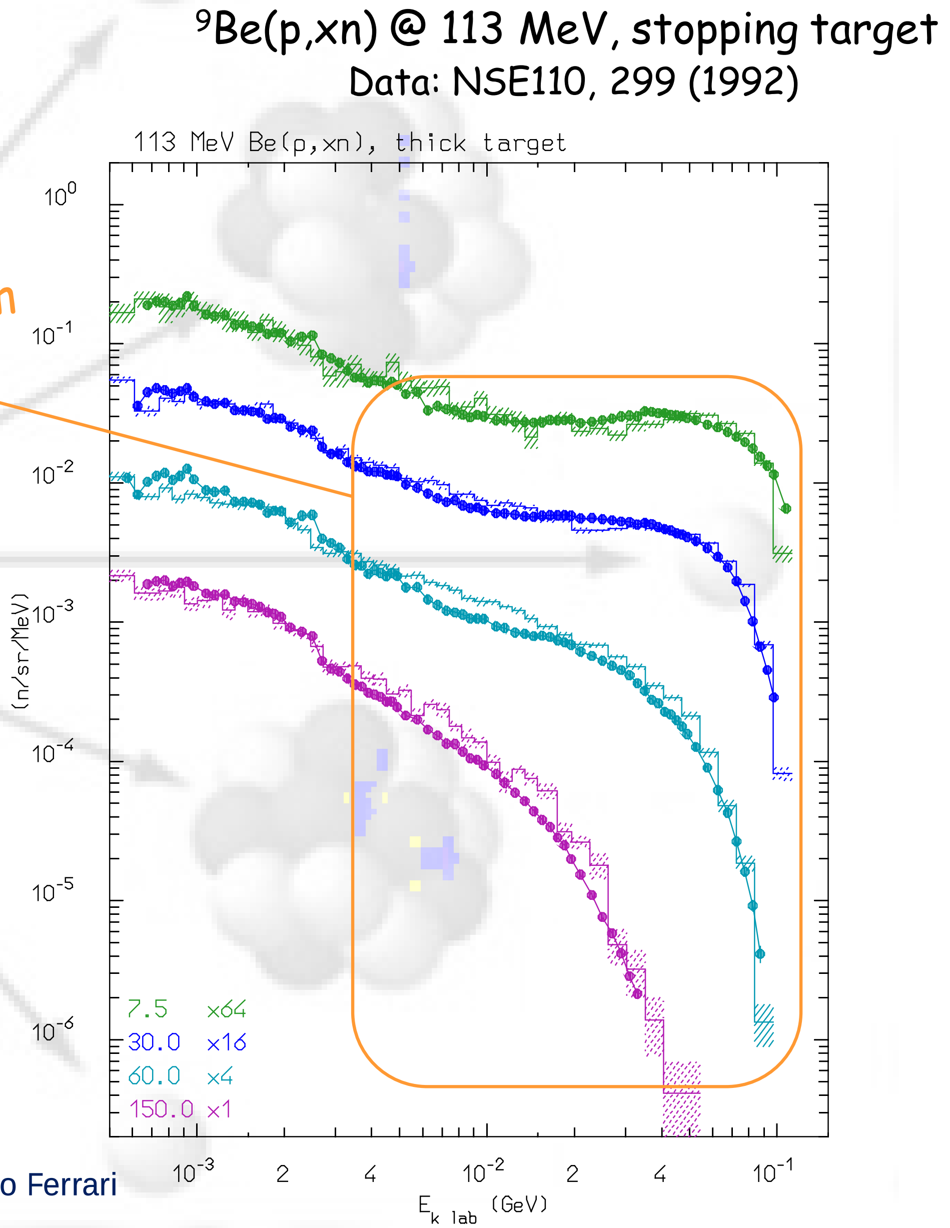


^{9}Be(p,xn) @ 113 MeV, stopping target
Data: NSE110, 299 (1992)



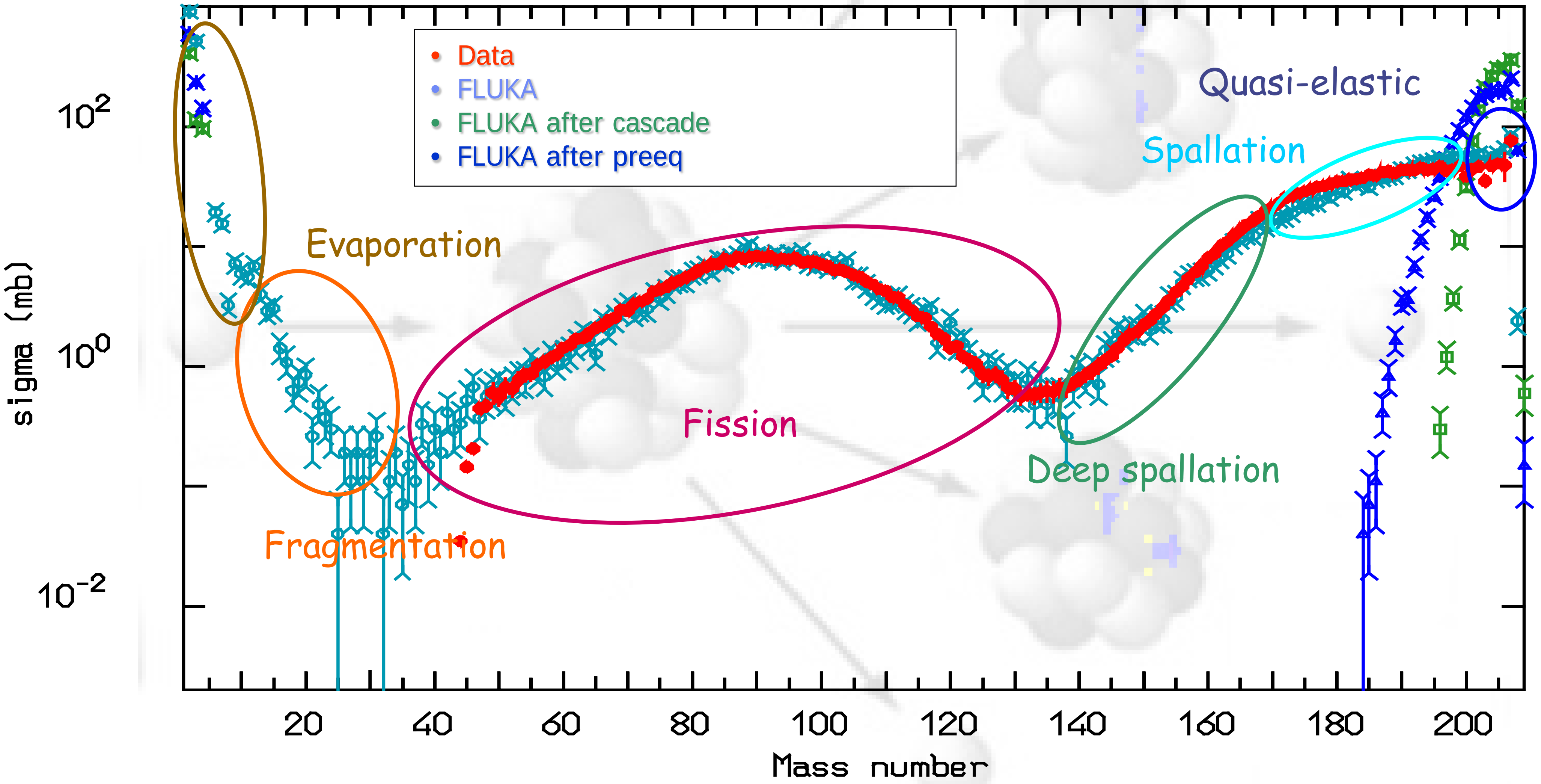
Thick target examples: neutrons





Example of fission/evaporation

1 A GeV ^{208}Pb + p reactions Nucl. Phys. A 686 (2001) 481-524

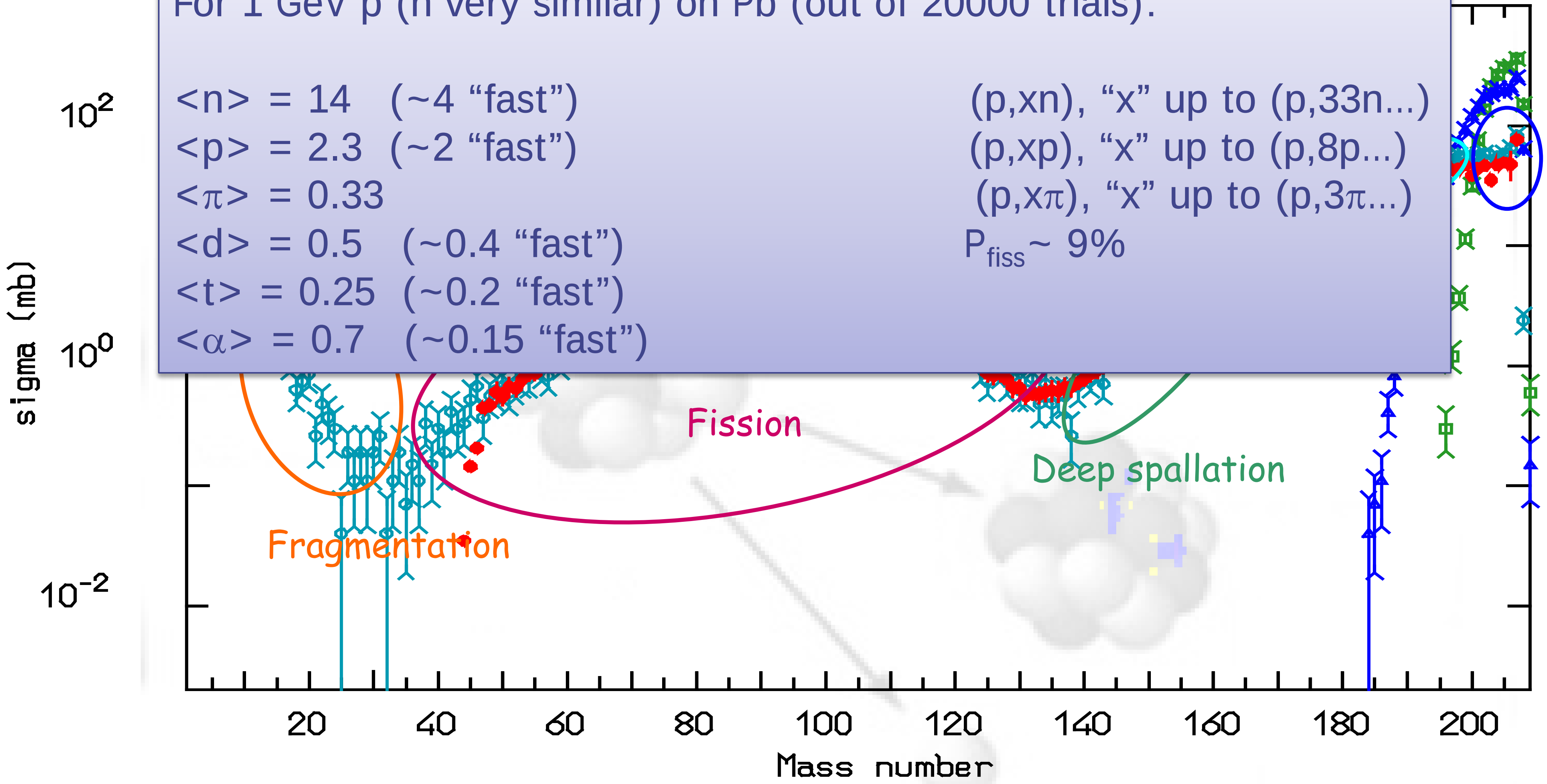


Example of fission/evaporation

1 A GeV ^{208}Pb + p reactions Nucl. Phys. A 686 (2001) 481-524

For 1 GeV p (n very similar) on Pb (out of 20000 trials):

<n> = 14	(~4 "fast")	(p,xn), "x" up to (p,33n...)
<p> = 2.3	(~2 "fast")	(p,xp), "x" up to (p,8p...)
<π> = 0.33		(p,xπ), "x" up to (p,3π...)
<d> = 0.5	(~0.4 "fast")	P_{fiss}~ 9%
<t> = 0.25	(~0.2 "fast")	
<α> = 0.7	(~0.15 "fast")	



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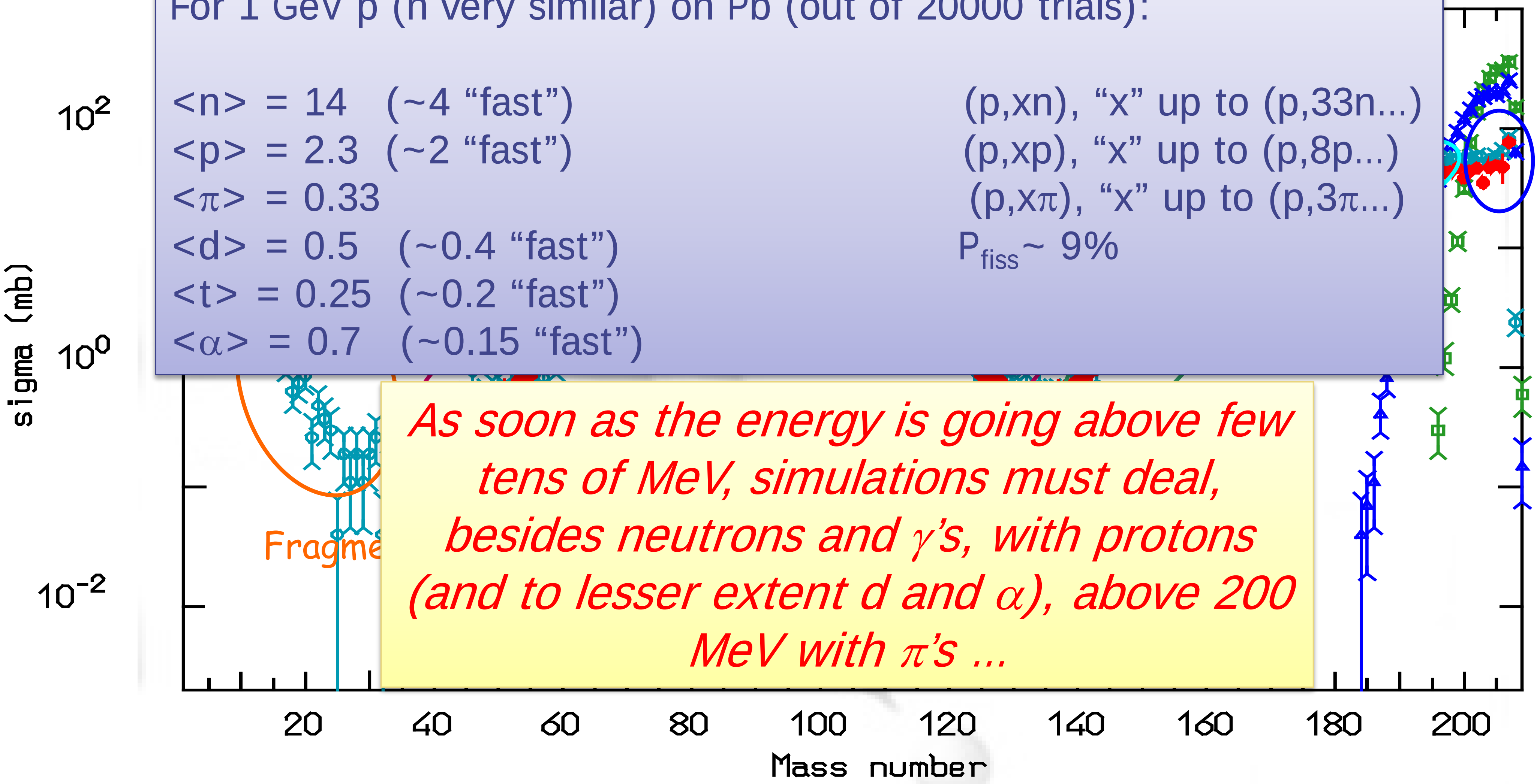
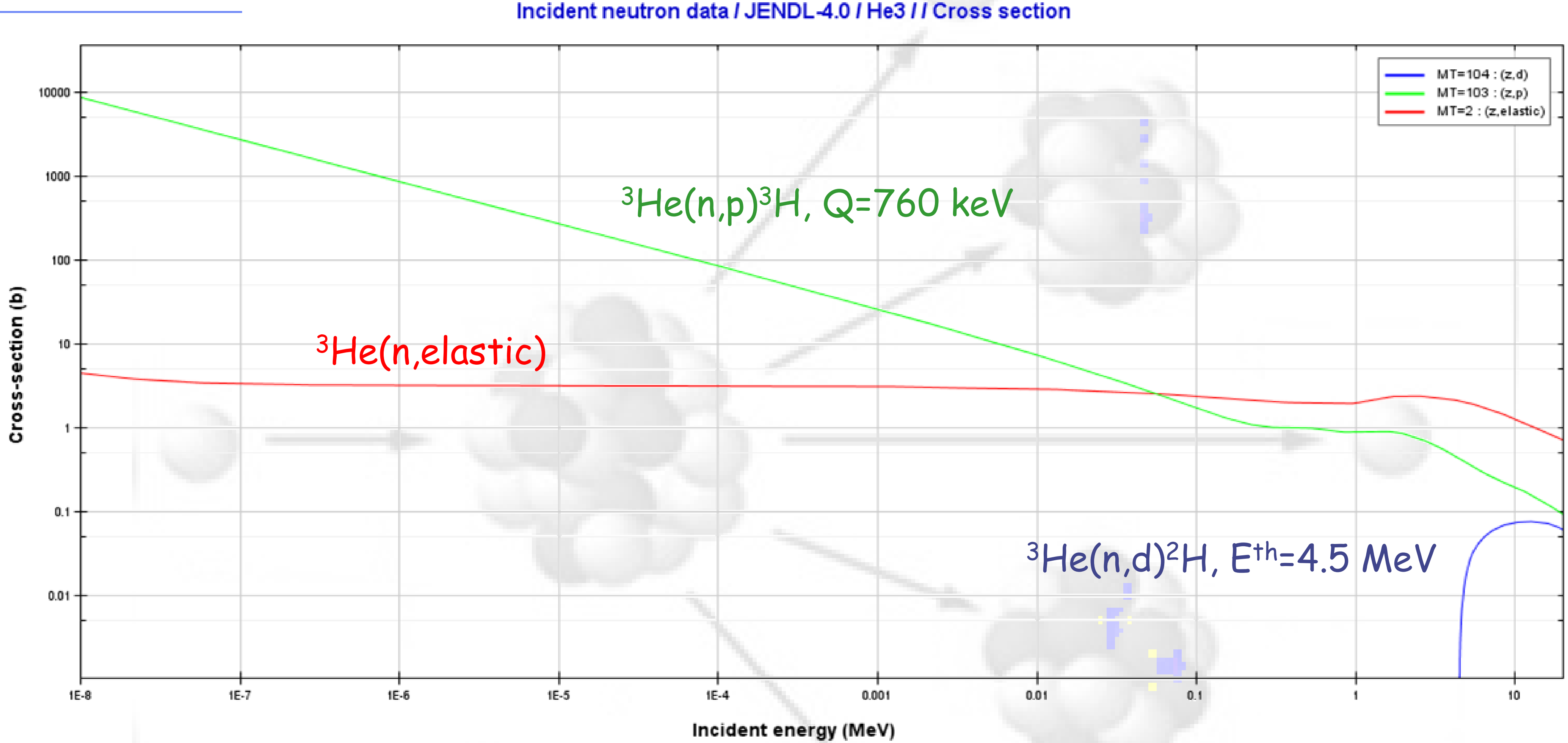


As soon as the energy is going above few tens of MeV, simulations must deal, besides neutrons and γ’s, with protons (and to lesser extent d and α), above 200 MeV with π’s ...

Examples: Bonner sphere(s) with ^{3}He detector

- Bonner sphere with ^{3}He detector at the centre
- Assumptions:
  - Most of the counts will be due to low energy (~thermal) neutrons moderated by the polyethylene
  - The vast majority of the counts will be due to the (n,p) reaction
- Compute response functions by:
  a) Folding with the cross section for ^{3}He(n,p)^{3}H only (and only for E < 20 MeV)
  b) As above but also adding the contribution of (n,el) and (n,d) when the resulting charged recoils are over a threshold set at 100, 200 and 500 keV
  c) Scoring the pulse height of energy deposition events in the detector gas (it requires a special MC able to generate correlated recoils for all reactions involving ^{3}He)
- … assuming for irradiation geometries:
  - A parallel neutron beam impinging on the sphere side
  - An uniform and isotropic neutron fluence surrounding the spheres

^{3}He cross sections:



a) Naïve approach: folding with **^{3}He(n,p)^{3}H** cross section
b) More sophisticated: … also with **(n,el)** and **(n,d)** when charged products above detection threshold
c) Full analogue one (requires a suitable ad hoc MC): compute the en.dep. in the gas event-by-event

Geometry:

The algorithms to build a geometry and to track particles inside it differ from code to code; In general:

- The geometry is built from basic solids and/or surfaces
- It must have an external boundary, to limit the tracking
- Defined by input cards, or by user-written routines
- Can allow for repetition of structures
- Can allow for “voxel” representation (CT import, medical applications)

The tasks of the geometry package:

- Find where (regions and material) is the particle
- Move particles along straight (or curved, eg magn. field) trajectories
- Find intersections with the surfaces that limit regions
- Find the next region ($\Rightarrow$ material) after a boundary crossing
- Compute the normal at interfaces

Source term:

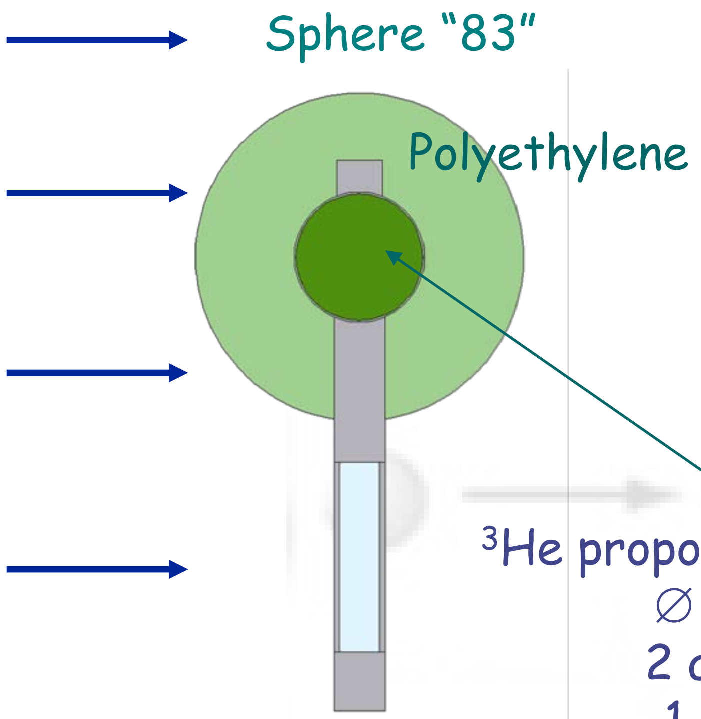
All codes allow for an arbitrarily complex description of the source term, which is a critical starting condition. In general it is possible to describe:

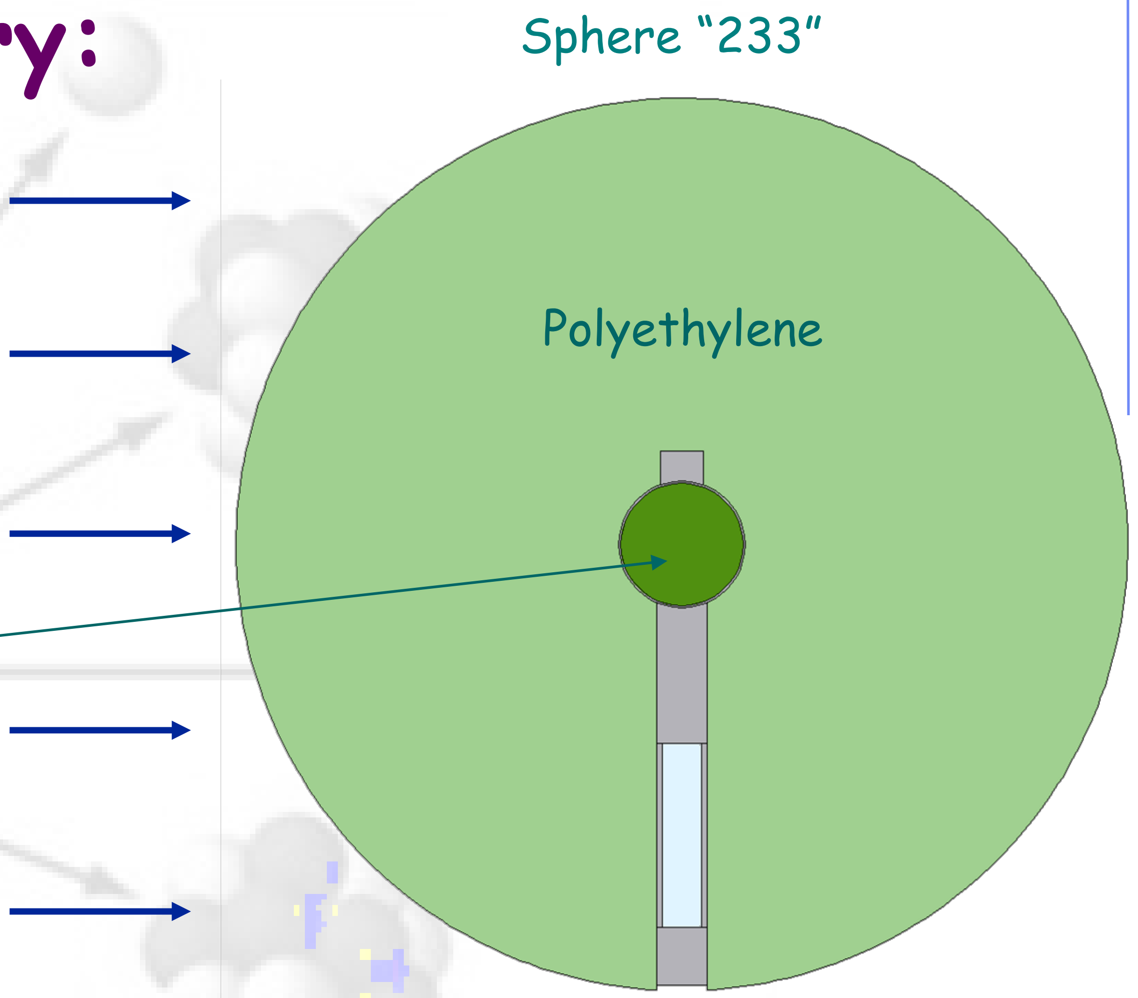
- The energy spectrum of the source "beam" (monoenergetic, several lines, line with a spread, continuous spectrum, …)
- The angular distribution (parallel, with a divergence, isotropic, …)
- The spatial distribution (point-like, linear, planar, volume, …)
- The time distribution (instantaneous, with a given irradiation profile, …)

Many codes have built-in options for simple energy, angle, spatial, distributions. Arbitrary ones can always be built by means of ad-hoc user routines

Some codes have built-in databases for radioactive isotope γ, α, and electron conversion lines, together with automatic sampling of $\beta^{+/-}$ spectra

Lateral irradiation geometry:

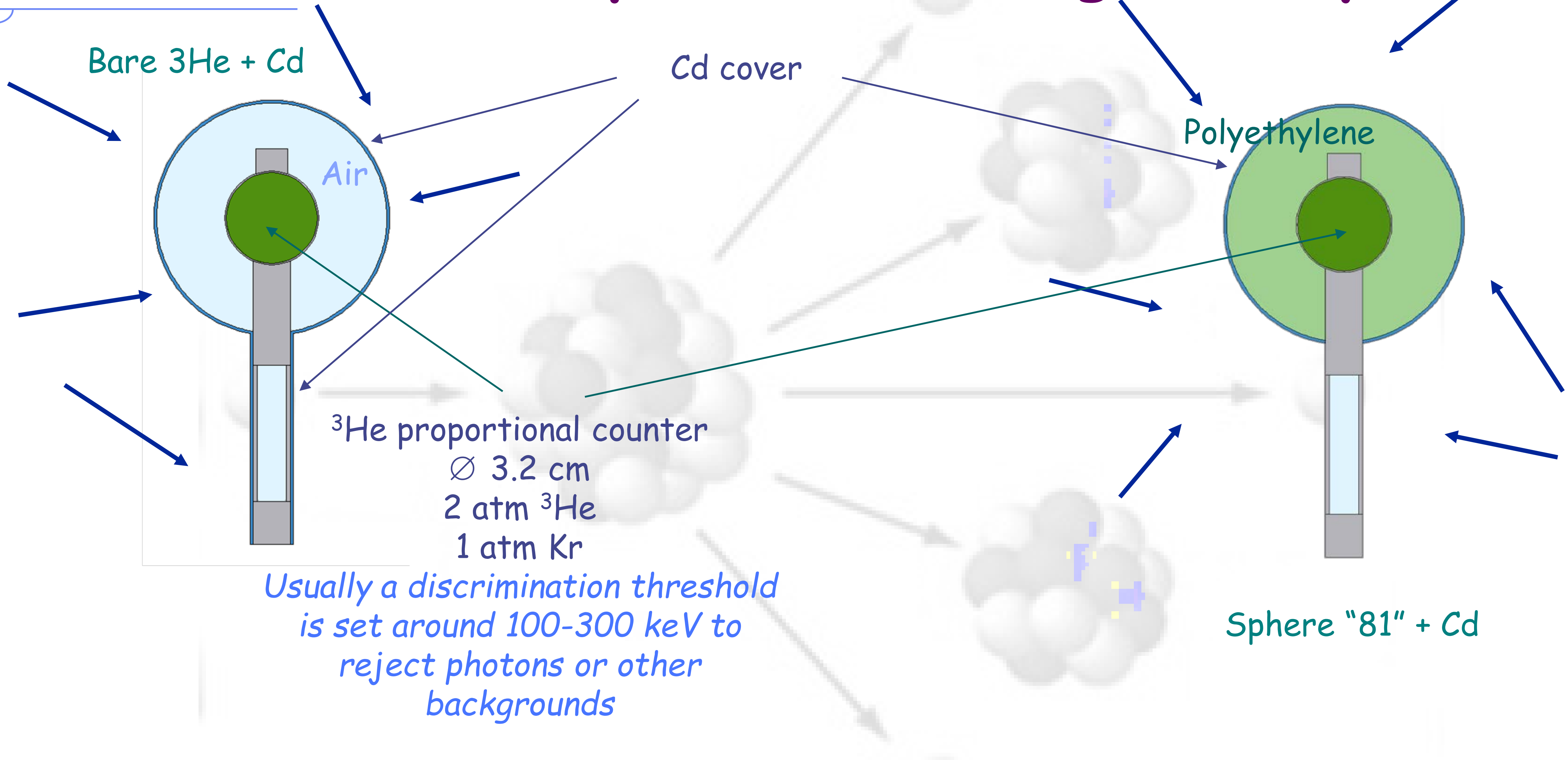




^{3}He proportional counter
∅ 3.2 cm
2 atm ^{3}He
1 atm Kr

Usually a discrimination threshold is set around 100-300 keV to reject photons or other backgrounds

Uniform and isotropic irradiation geometry:



^{3}He proportional counter
∅ 3.2 cm
2 atm ^{3}He
1 atm Kr

Usually a discrimination threshold is set around 100-300 keV to reject photons or other backgrounds

Results from a MC calculation:

Estimators (or "tallies"):

- It is often said that Monte Carlo is a "mathematical experiment". The MC equivalent of the result of a real experiment (*i.e.* of a measurement) is called an estimator
- Just as a real measurement, an estimator is obtained by sampling from a statistical distribution and has a statistical uncertainty (and in general also a systematic error)
- There are often several different techniques to measure the same physical quantity: in the same way the same quantity can be calculated with different kinds of estimators

Estimators:

Most MC codes have built-in estimators, to be activated and tailored by the user. The results are usually averaged over one run and normalized to one primary particle. Additional flexibility can be achieved by

- Convolution off-line or on-line. For instance: convolution of fluence with conversion factors to obtain reaction rates or equivalent dose.
- Event-by-event estimators for correlated data analysis
- Full or partial dumping of events: steps, interactions, etc, for off-line analysis. To be used only if absolutely necessary.

Two main categories of calculations discussed in the following:

- "average"
- event-by-event

Estimator (or "Tallies") Types:

Various types, depending on the quantity to be estimated and on the topology

- Boundary Crossing: estimates the fluence or the current of particles on a physical boundary between two regions. Results are mono or multi-dimensional fluence spectra, function of energy, angle, id, …
- Track length: estimates the fluence of particles inside one volume, based on their path length within the volume. Results are fluence spectra as a function of particle energy
- Collision: estimates the fluence of particles inside one volume, based on the number of collisions occurring within the volume. Results are fluence spectra as a function of particle energy.
- Pulse height: deposited energy spectrum within a volume *(event-by-event!)*
- Mono-dimensional deposited energy, inelastic interactions (star), activity.. estimates the density of a given quantity within a volume.
- Meshes: regular subdivision of a part of the geometry in sub-volumes. Can estimate fluence, energy deposition, stars… Can be independent from the tracking geometry, and result in a 2D or 3D spatial distribution of the estimated quantity

Folding fluence with response functions:

- Whenever the sensitive medium ***cross section/response function*** is ***known*** and there is no need for an event-by-event analysis, the most accurate and CPU "cheap" way is to evaluate the detector response by ***folding*** the known ***cross section/response function with the*** (differential in energy) ***neutron fluence*** inside the sensitive volume
- In practice, recalling the fluence definition in terms of track-length (x is the "sensitive" isotope, ρ_x, P_{Ax} its density and atomic weight, σ_x the microscopic cross section for the reaction of interest):

$$R = \int \frac{dl(E)}{dE} \sigma_x(E) \frac{\rho_x N_{Av}}{P_{Ax}} dE$$

This method works nicely if σ is known, which is often the case in the energy range of the evaluated data files

At higher energies where models are used and where several reactions are possible its validity depends on the detector configuration (eg it can still be used for a thermal neutron detector embedded in a moderator)

Examples: Bonner sphere(s) with ^{3}He detector

- Bonner sphere with ^{3}He detector at the centre
- Assumptions:
  - Most of the counts will be due to low energy (~thermal) neutrons moderated by the polyethylene
  - The vast majority of the counts will be due to the (n,p) reaction
- Compute response functions by:
  a) Folding with the cross section for ^{3}He(n,p)^{3}H only (and only for $E < 20$ MeV)
  b) As above but also adding the contribution of (n,el) and (n,d) when the resulting charged recoils are over a threshold set at 100, 200 and 500 keV
  c) Scoring the pulse height of energy deposition events in the detector gas (it requires a special MC able to generate correlated recoils for all reactions involving ^{3}He)
- … assuming for irradiation geometries:
  - A parallel neutron beam impinging on the sphere side
  - An uniform and isotropic neutron fluence surrounding the spheres

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→ Source term

Examples: Bonner sphere(s) with ^{3}He detector

- Bonner sphere with ^{3}He detector at the centre

Geometry description

- Assumptions:
  - Most of the counts will be due to low energy (~thermal) neutrons [in the] polyethylene
  - The vast majority of the counts will be due to the (n,p) reaction

Track-length estimator in the gas volume, folding with ^{3}He σ's

- Compute response functions by:
  a) Folding with the cross section for ^{3}He(n,p)^{3}H only (and only for E < 20 MeV)
  b) As above but also adding the contribution of (n,el) and (n,d) when the resulting charged recoils are over a threshold set at 100, 200 and 500 keV
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  - A parallel neutron beam impinging on the sphere side
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Source term

Examples: Bonner sphere(s) with ^{3}He detector

- Bonner sphere with ^{3}He detector at the centre
- Assumptions:
  - Most of the counts will be due to low energy (~thermal) neutrons polyethylene
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- … assuming for irradiation geometries:
  - A parallel neutron beam impinging on the sphere side
  - An uniform and isotropic neutron fluence surrounding the spheres

Geometry description

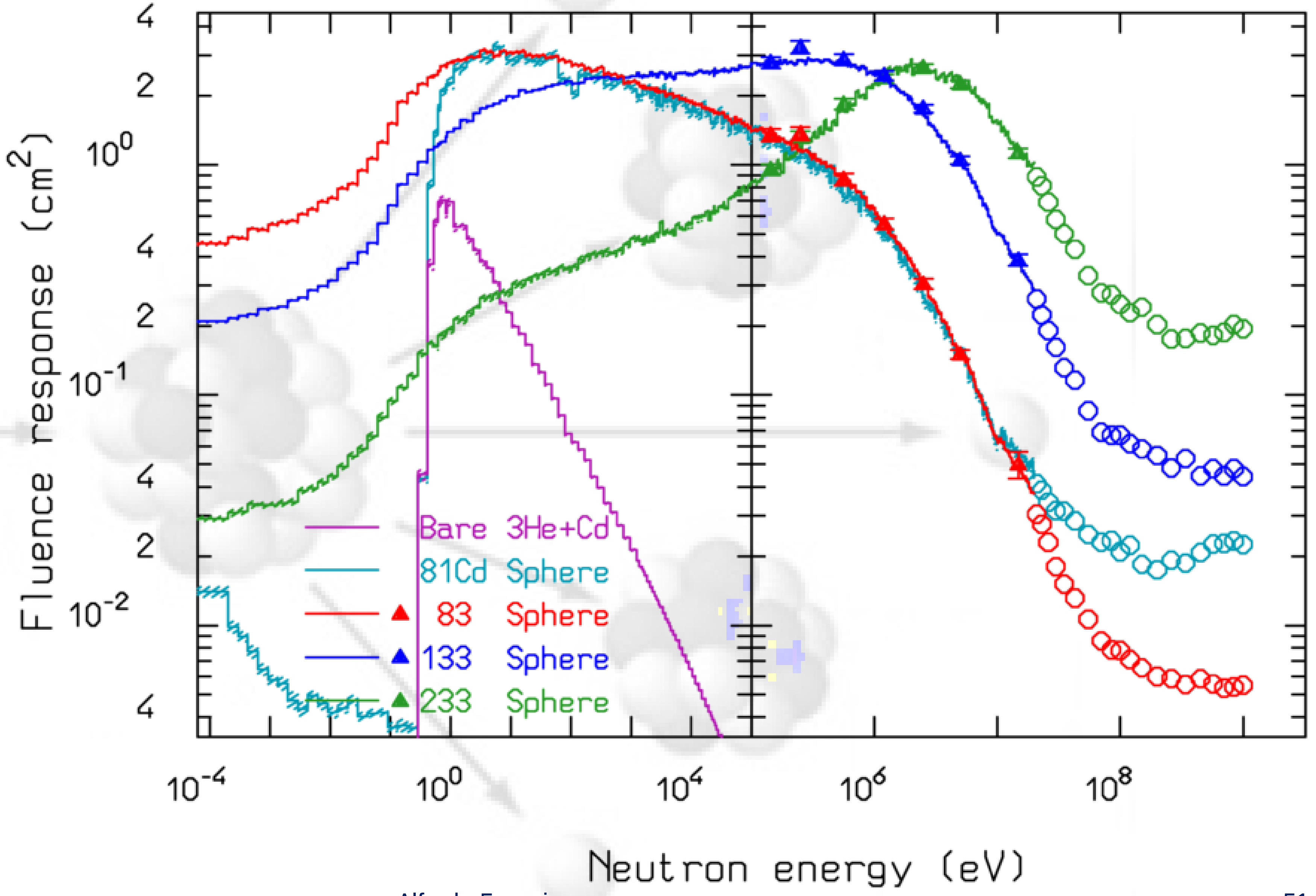
Track-length estimator in the gas volume, folding with ^{3}He σ's

Source term

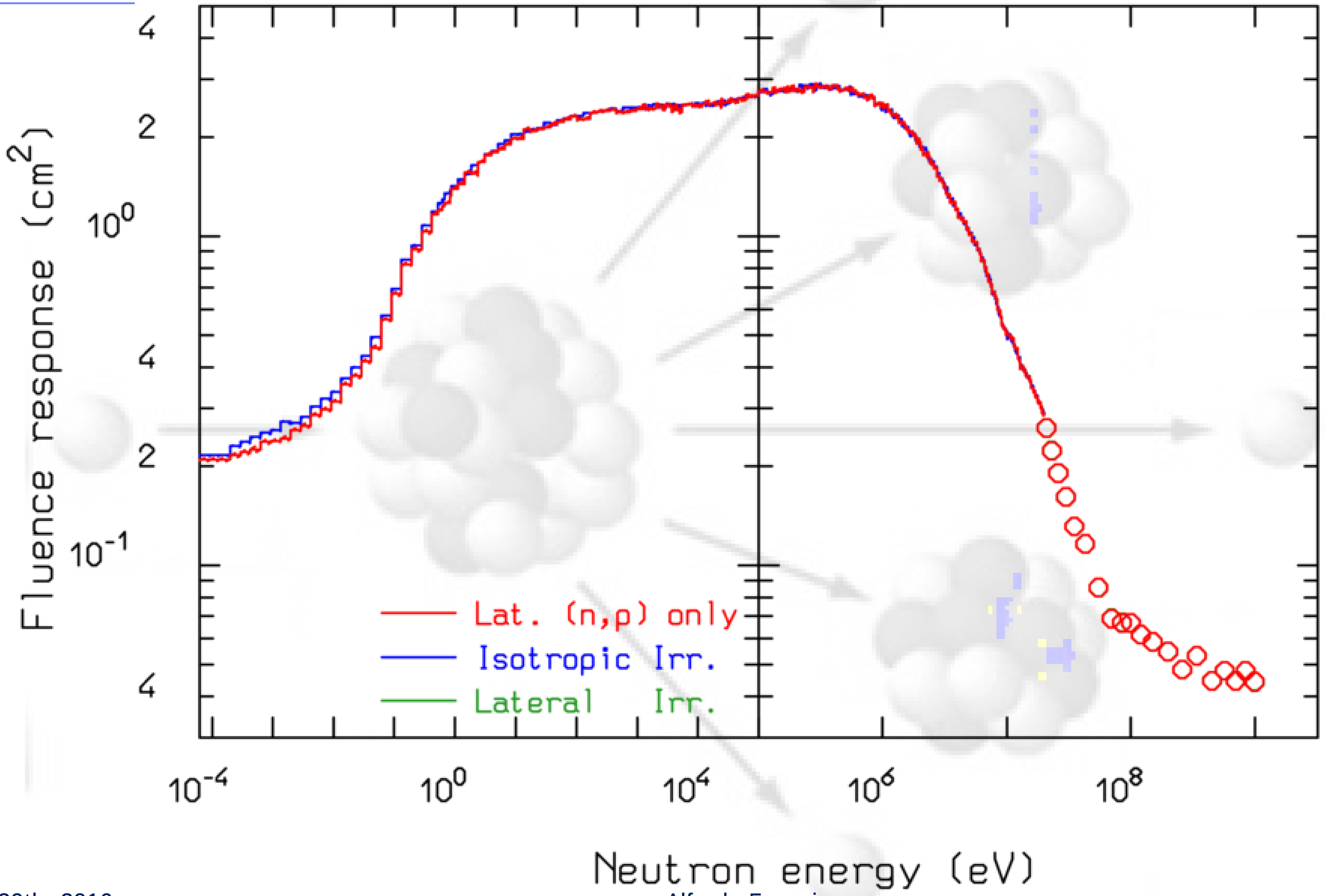
Pulse-height of energy deposition in the gas, no quenching, 5%/√E(MeV) resolution

Response functions:

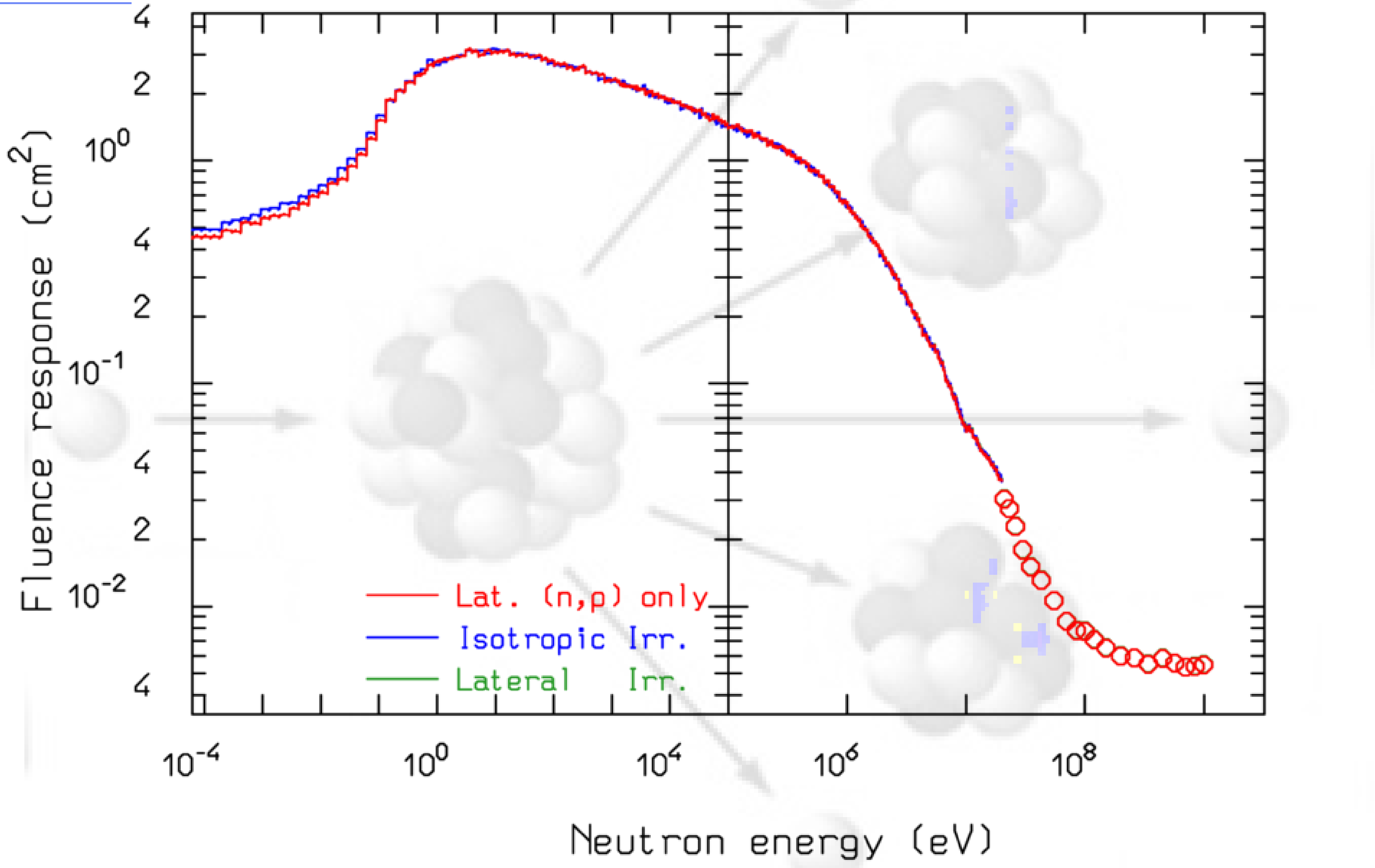
Computed response functions by folding (option b)), using 200 keV as threshold for (n,el), (n,d). The symbols are exp. data obtained with mono-energetic neutron beams at PTB



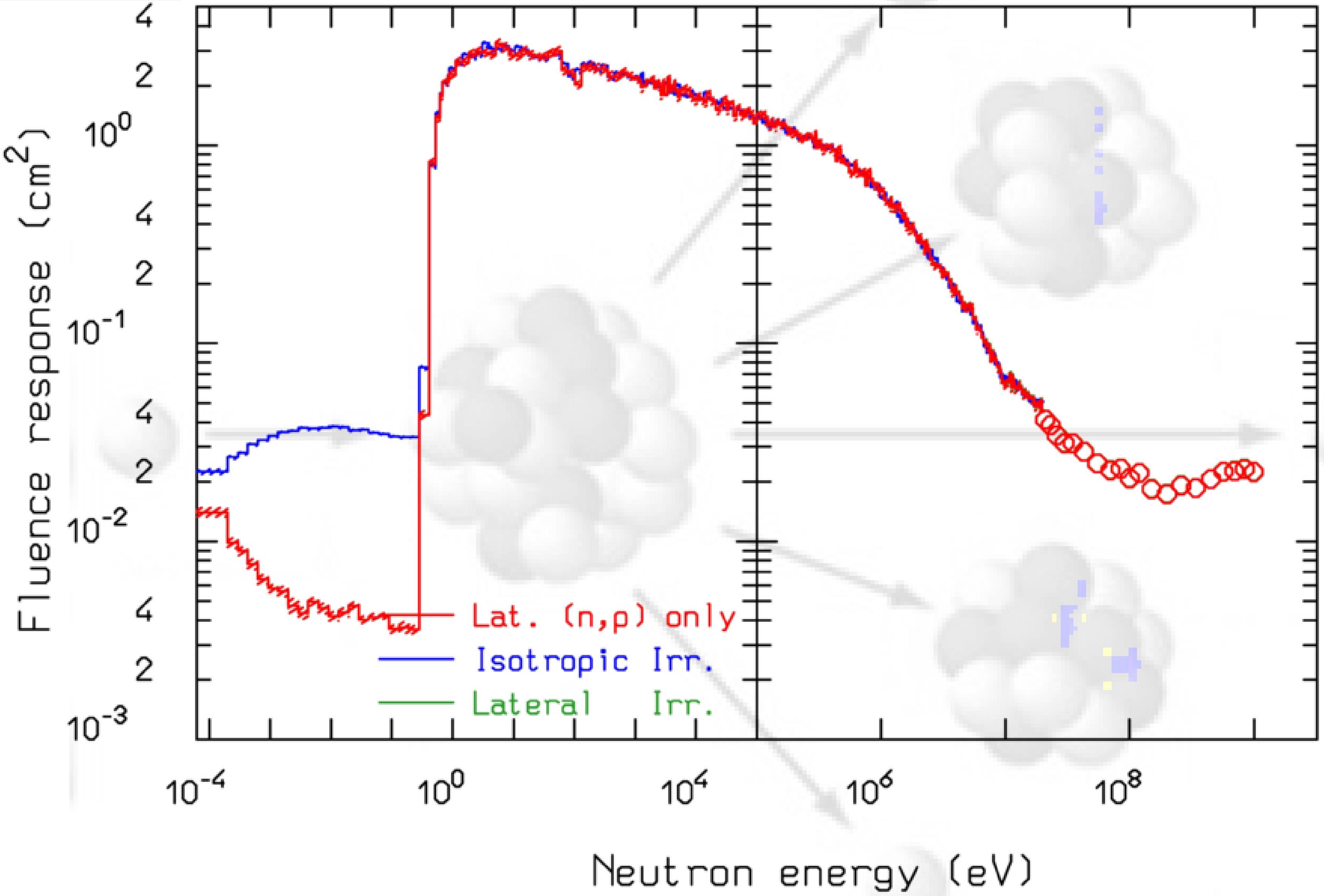
Lateral vs isotropic, a) vs b): Sphere 133

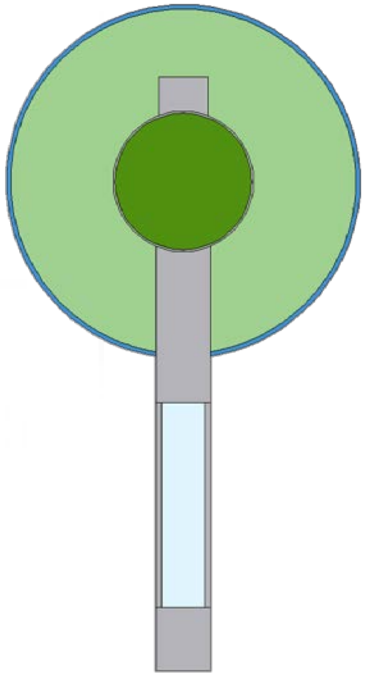


Lateral vs isotropic, a) vs b): Sphere 83

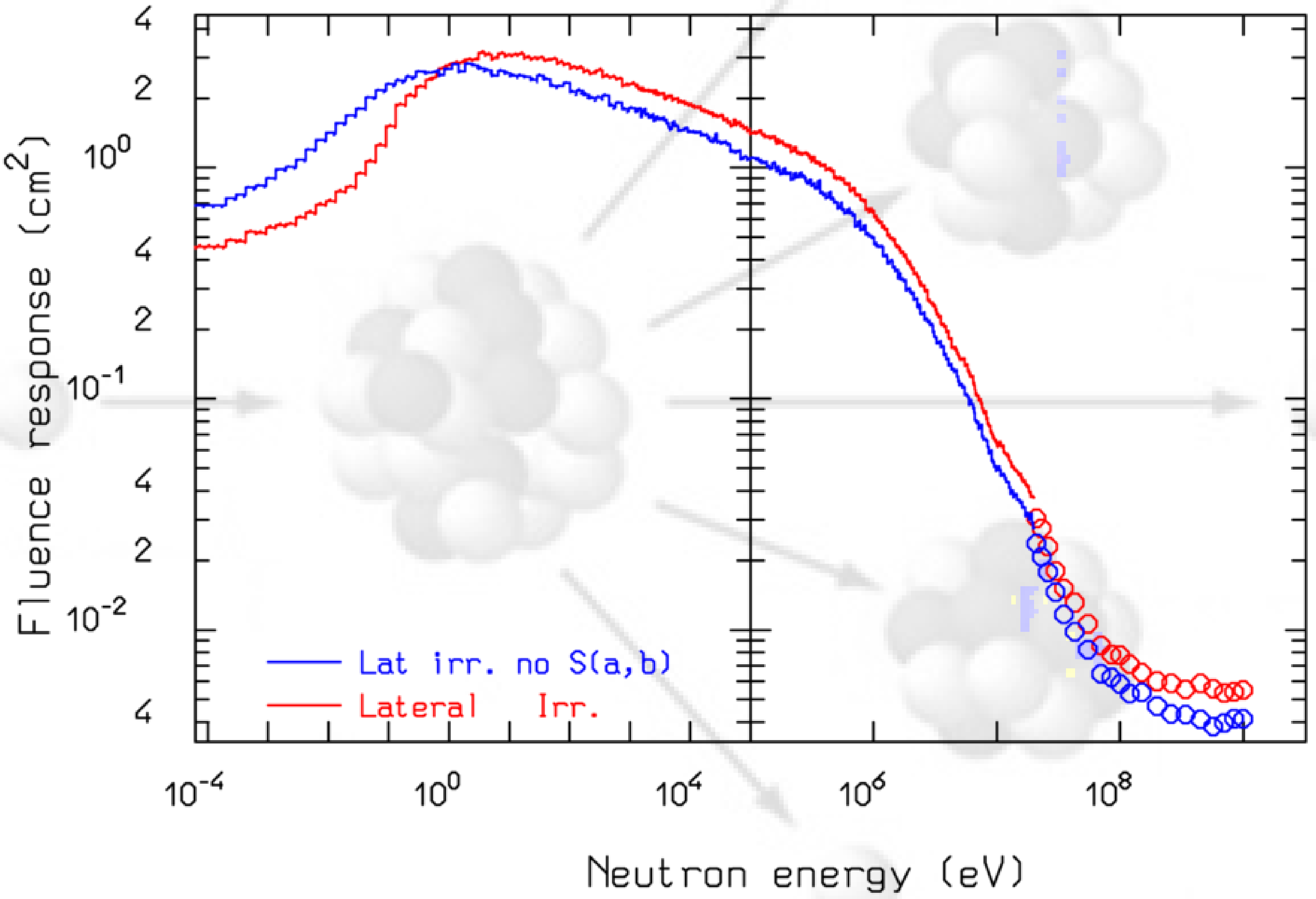


Lateral vs isotropic, a) vs b): Sphere 81+Cd

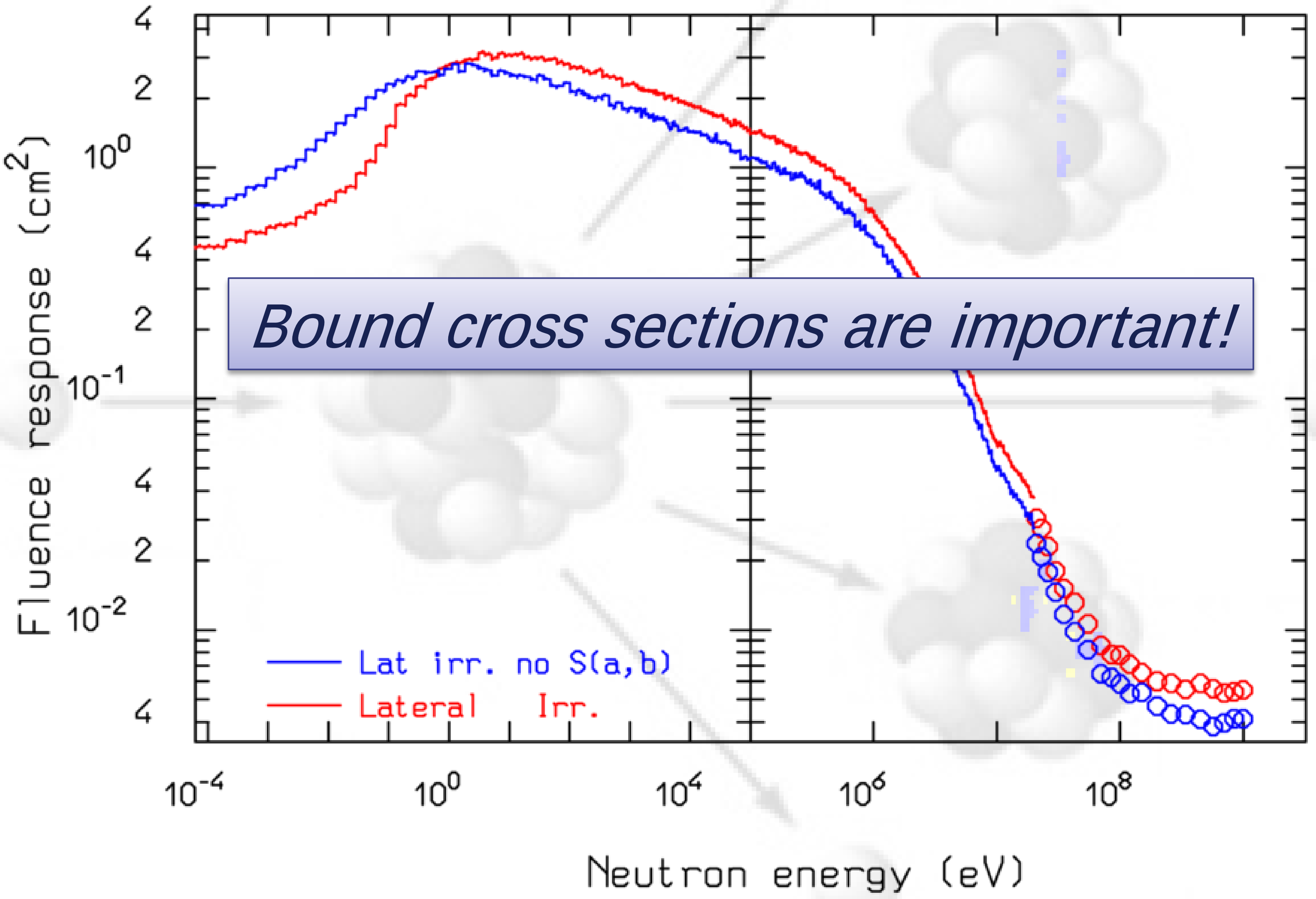




S(α,β) vs free gas for H: Sphere 83



S(α,β) vs free gas for H: Sphere 83

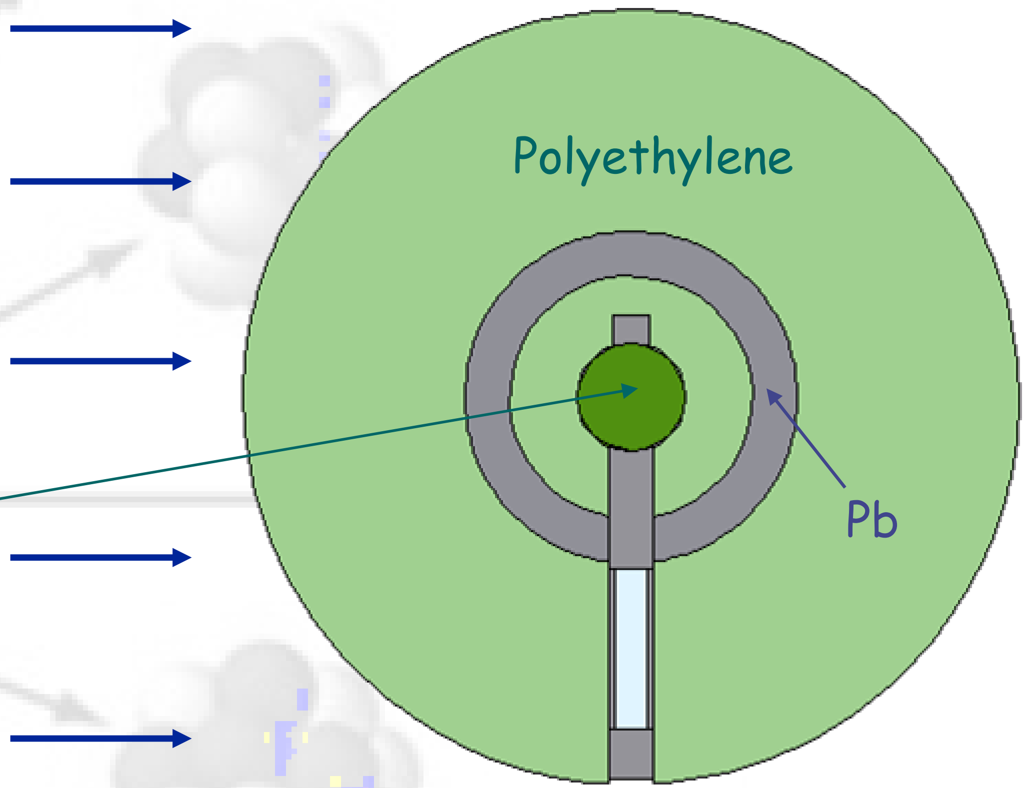


Sphere 233 with 1.5 cm $CH_2 \rightarrow$ Pb:

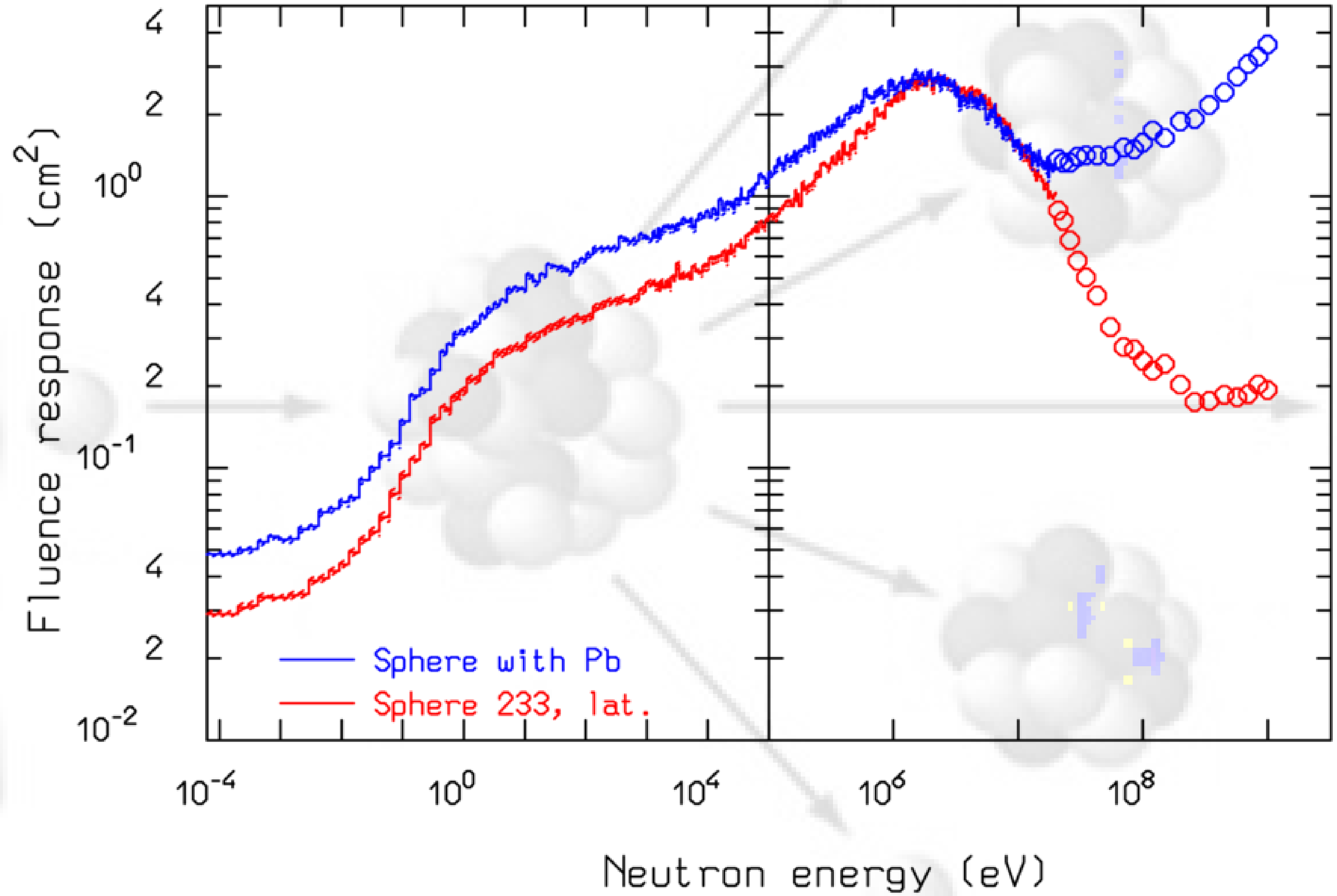
What is the effect of Pb? "High" energy neutrons interacting with Pb produce several evaporation neutrons (~1-2 MeV) among the others, which in turn are effectively moderated by CH_2 exactly like "primary" neutrons of the same energy

^{3}He proportional counter
∅ 3.2 cm
2 atm ^{3}He
1 atm Kr

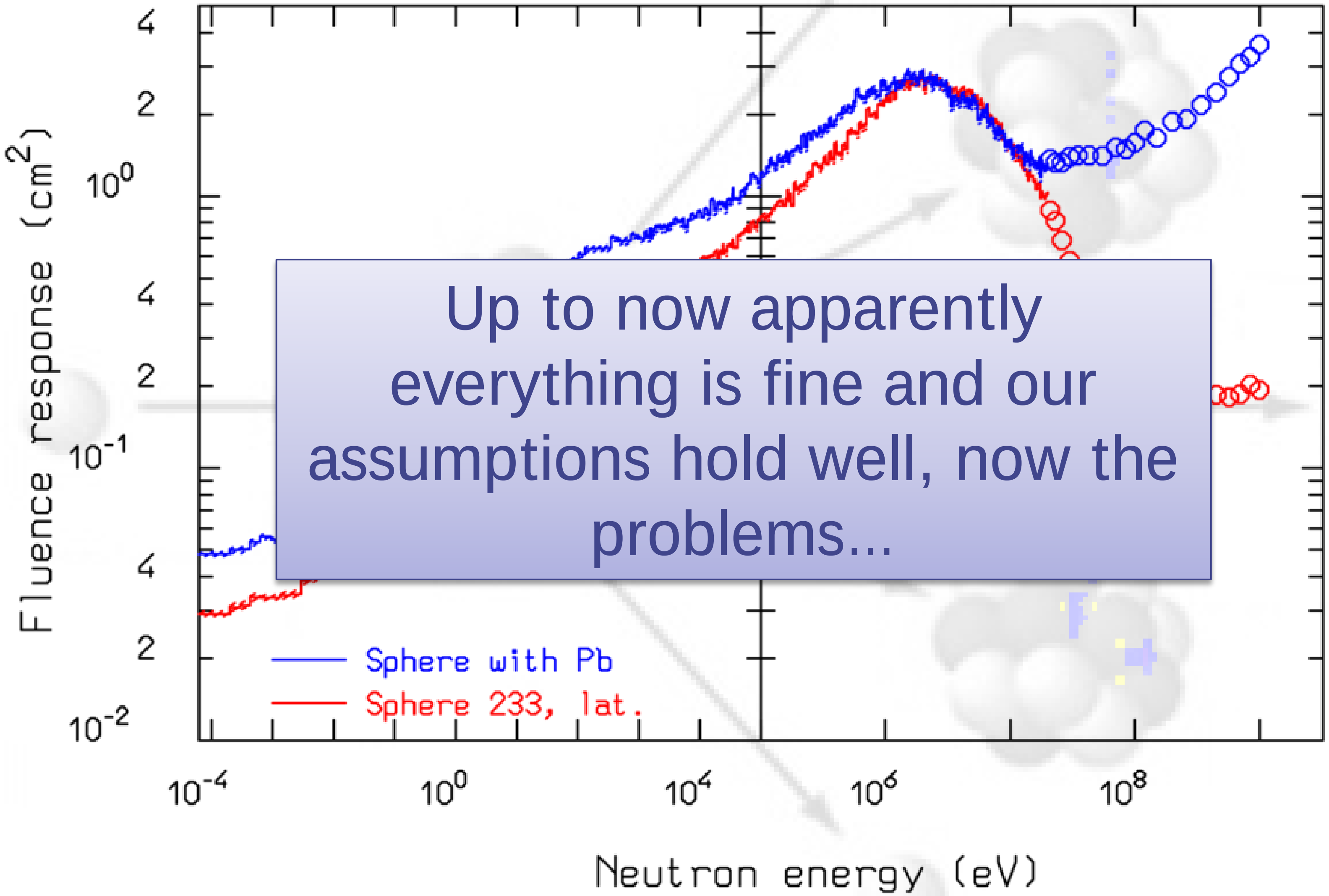
Sphere "233 with Pb"



Sphere 233 vs Sphere 233 + Pb

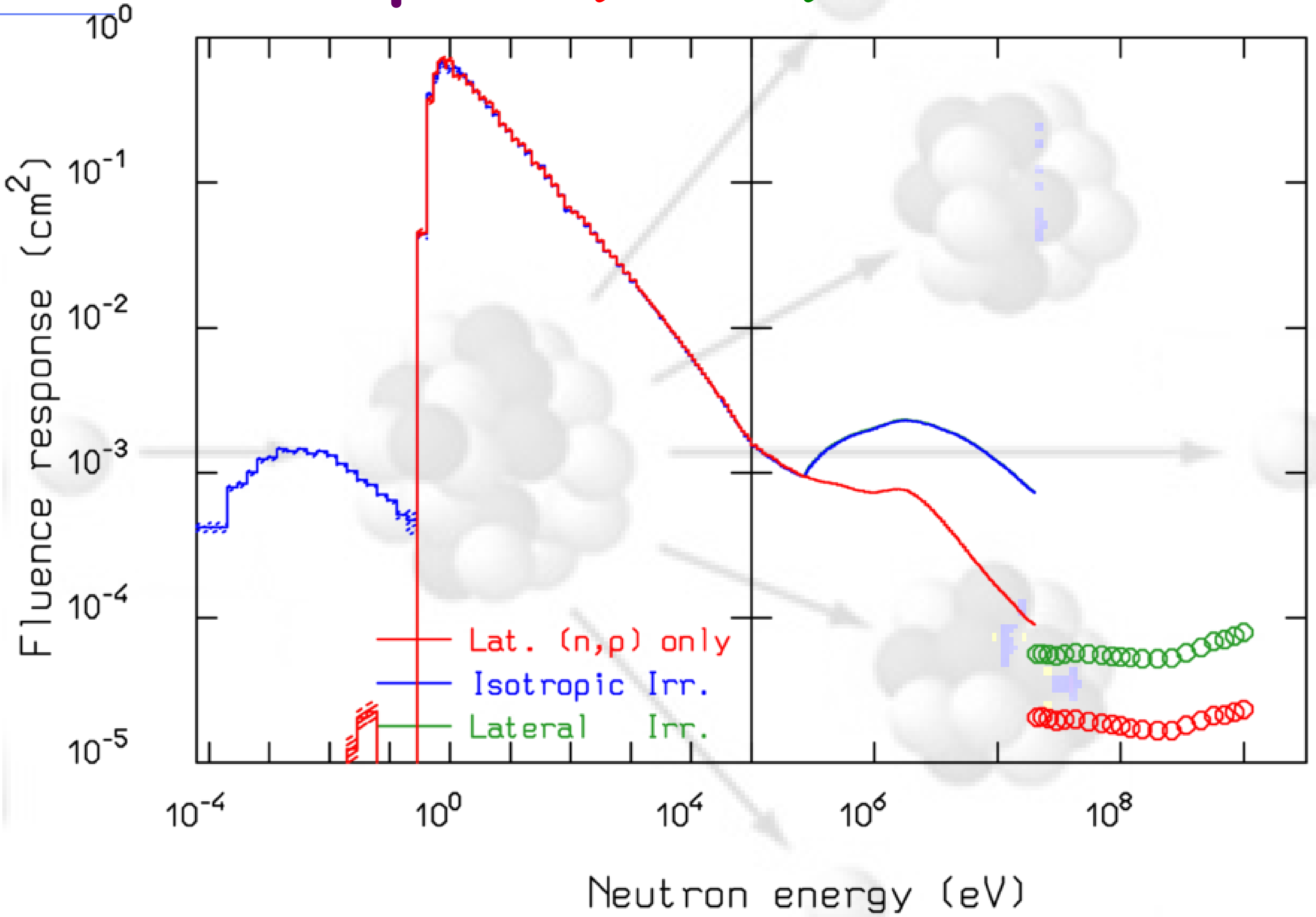


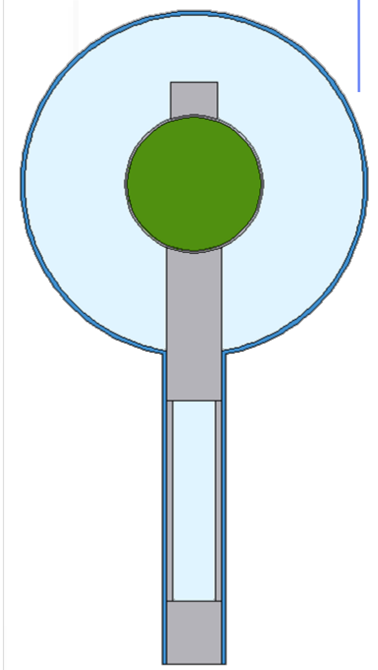
Sphere 233 vs Sphere 233 + Pb



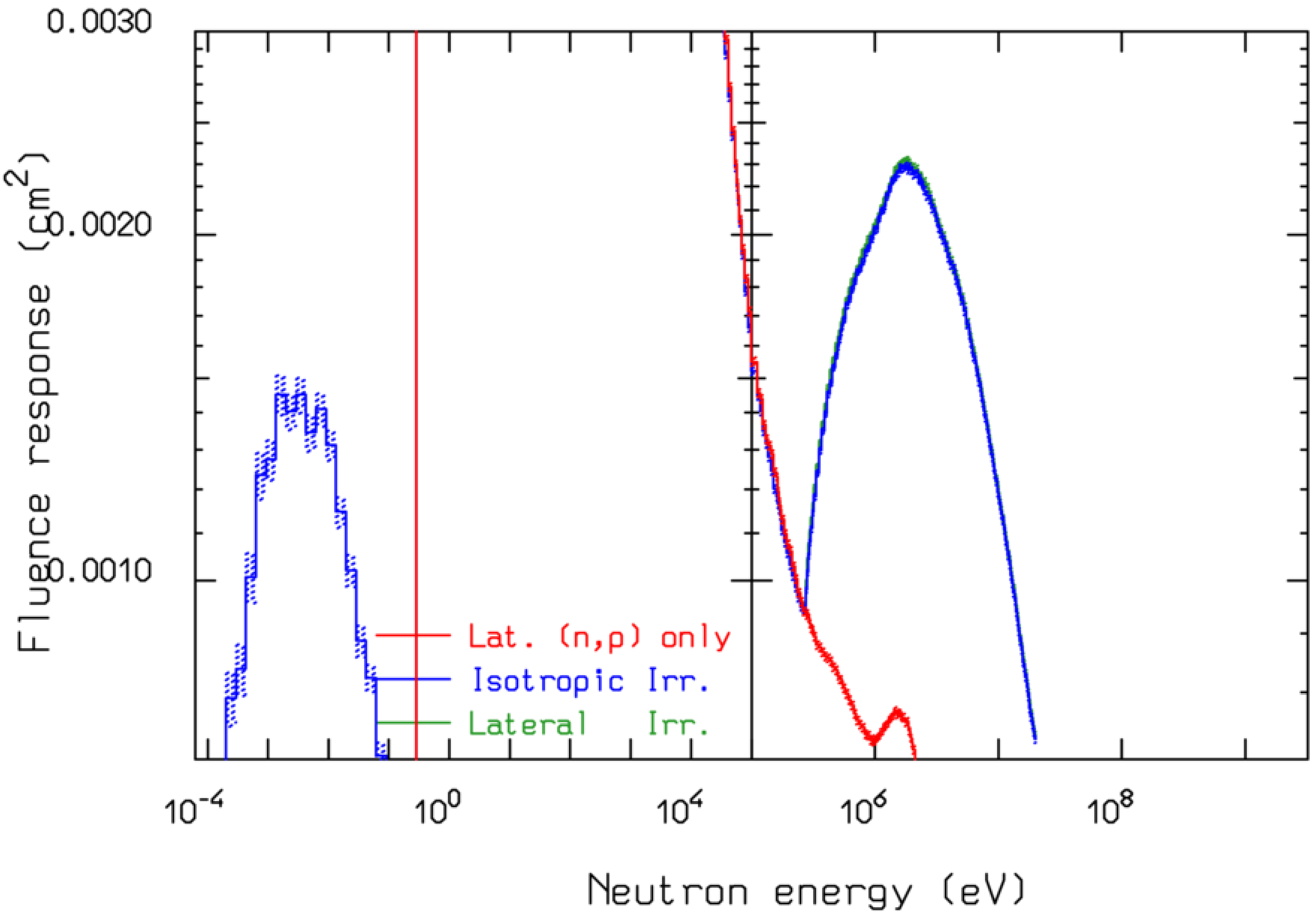
Up to now apparently everything is fine and our assumptions hold well, now the problems...

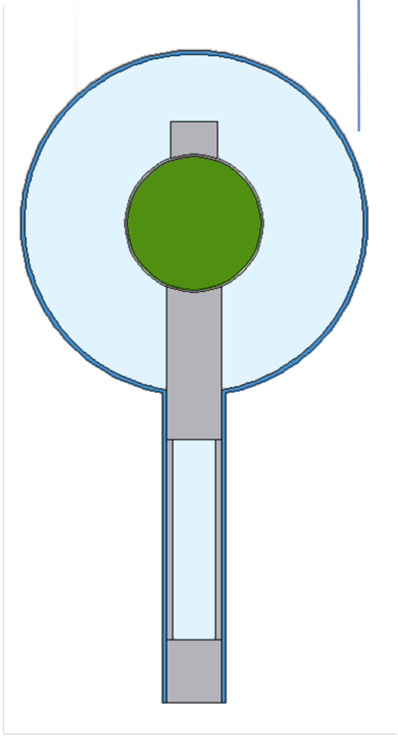
Lateral vs isotropic, a) vs b): Bare ^{3}He+Cd



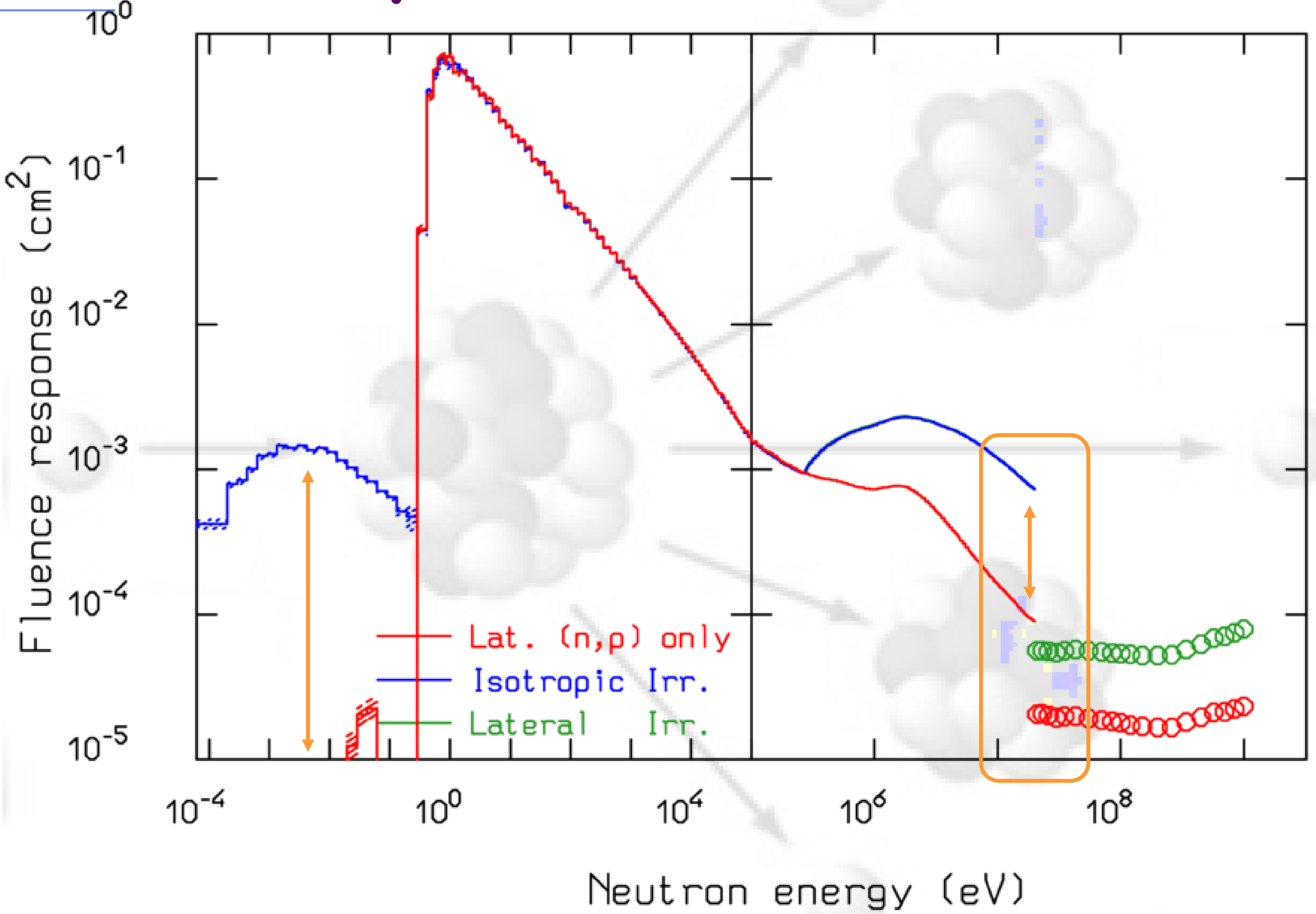


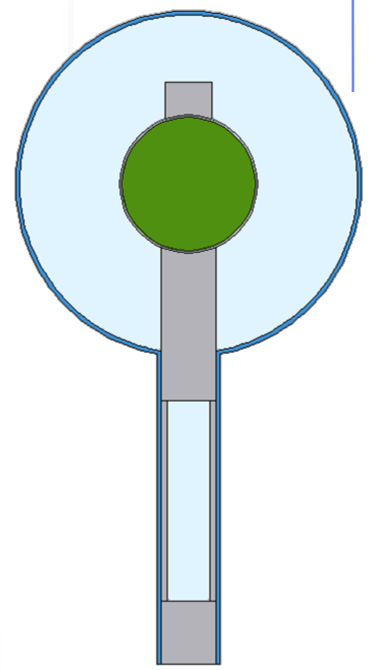
Lateral vs isotropic, a) vs b): Bonn ^3He:Cd



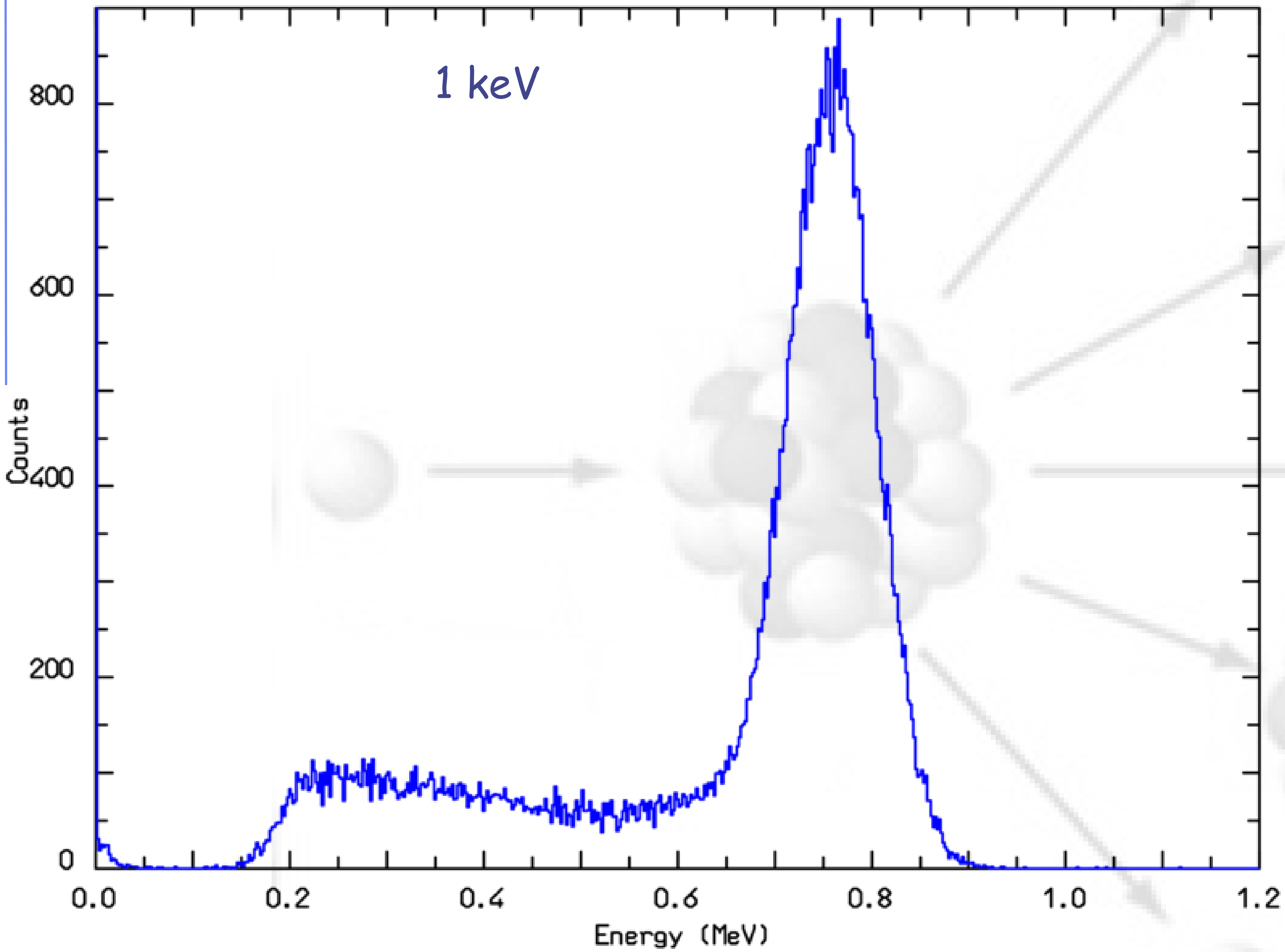


Lateral vs isotropic, a) vs b): Bare ^{3}He+Cd



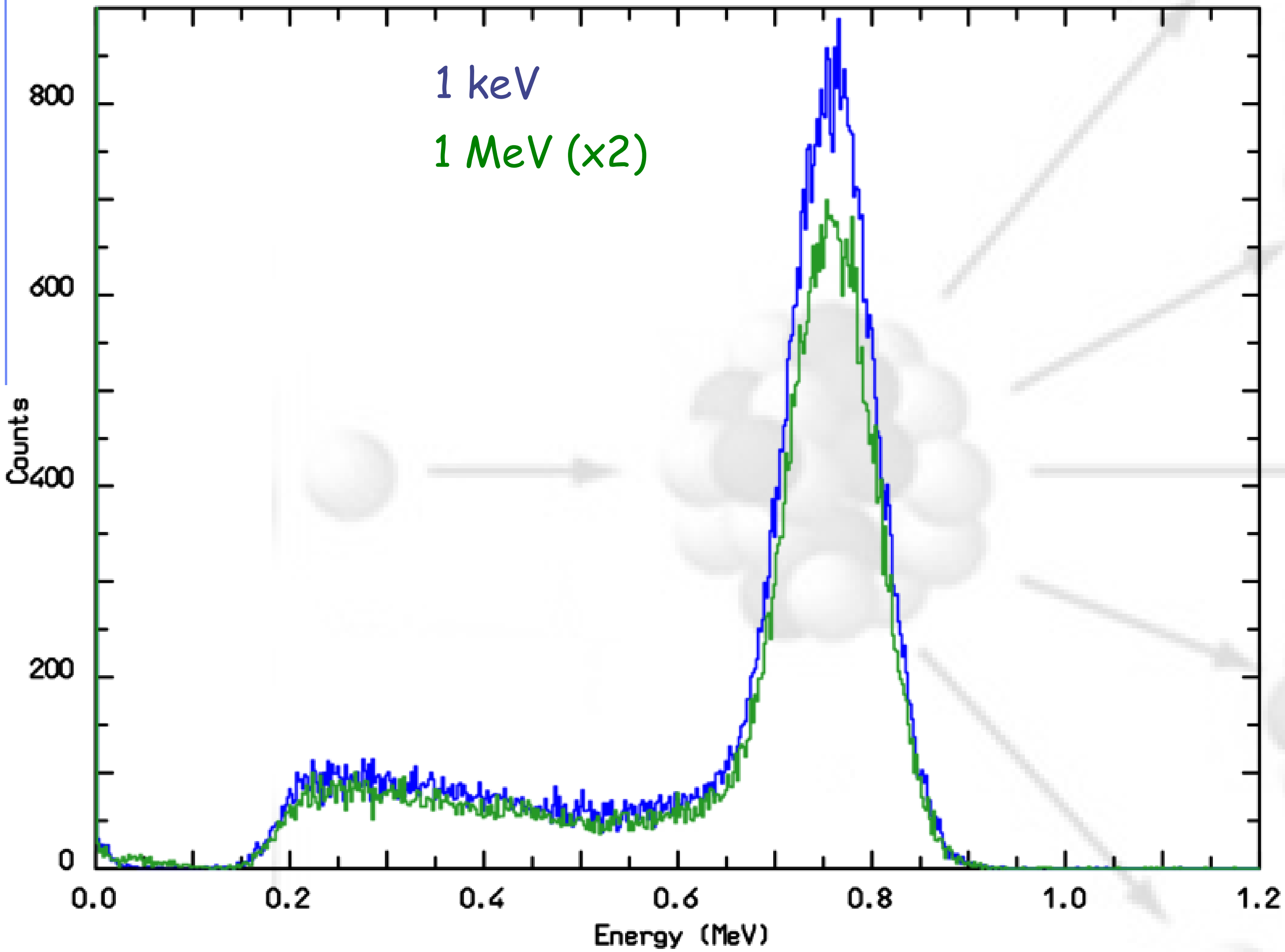


Sphere "83", option c): pulse height distributions



Response (cm^{-2})				
Thr. (keV):	100	200	500	*Fold*
Energy				
1 keV	2.30	2.28	1.85	*2.22*

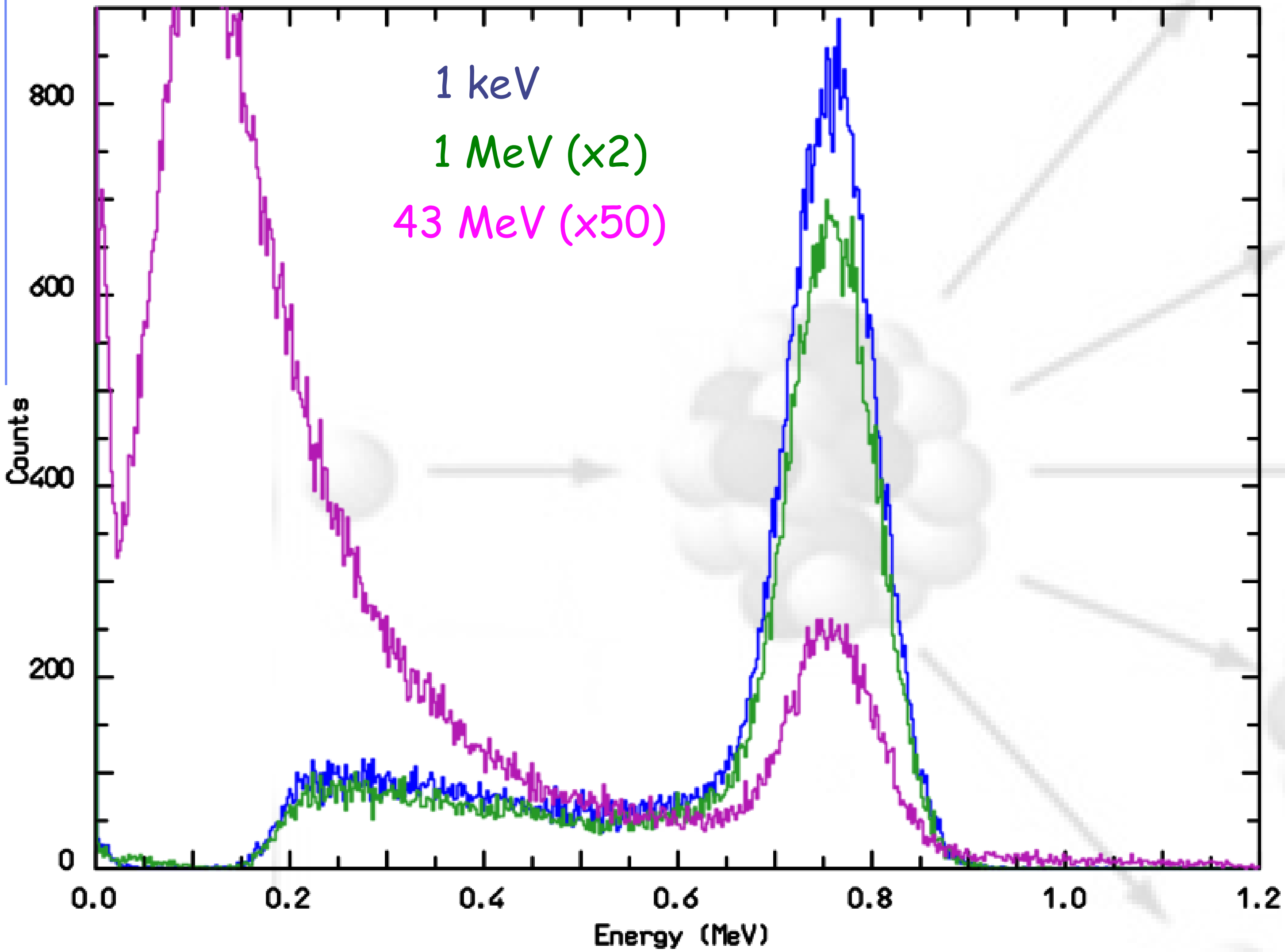
Sphere "83", option c): pulse height distributions



Response (cm^{-2})

Thr. (keV):	100	200	500	*Fold*
Energy				
1 keV	2.30	2.28	1.85	*2.22*
1 MeV	0.636	0.629	0.508	*0.651*

Sphere "83", option c): pulse height distributions



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43 MeV	0.067	0.038	0.015	*0.013*

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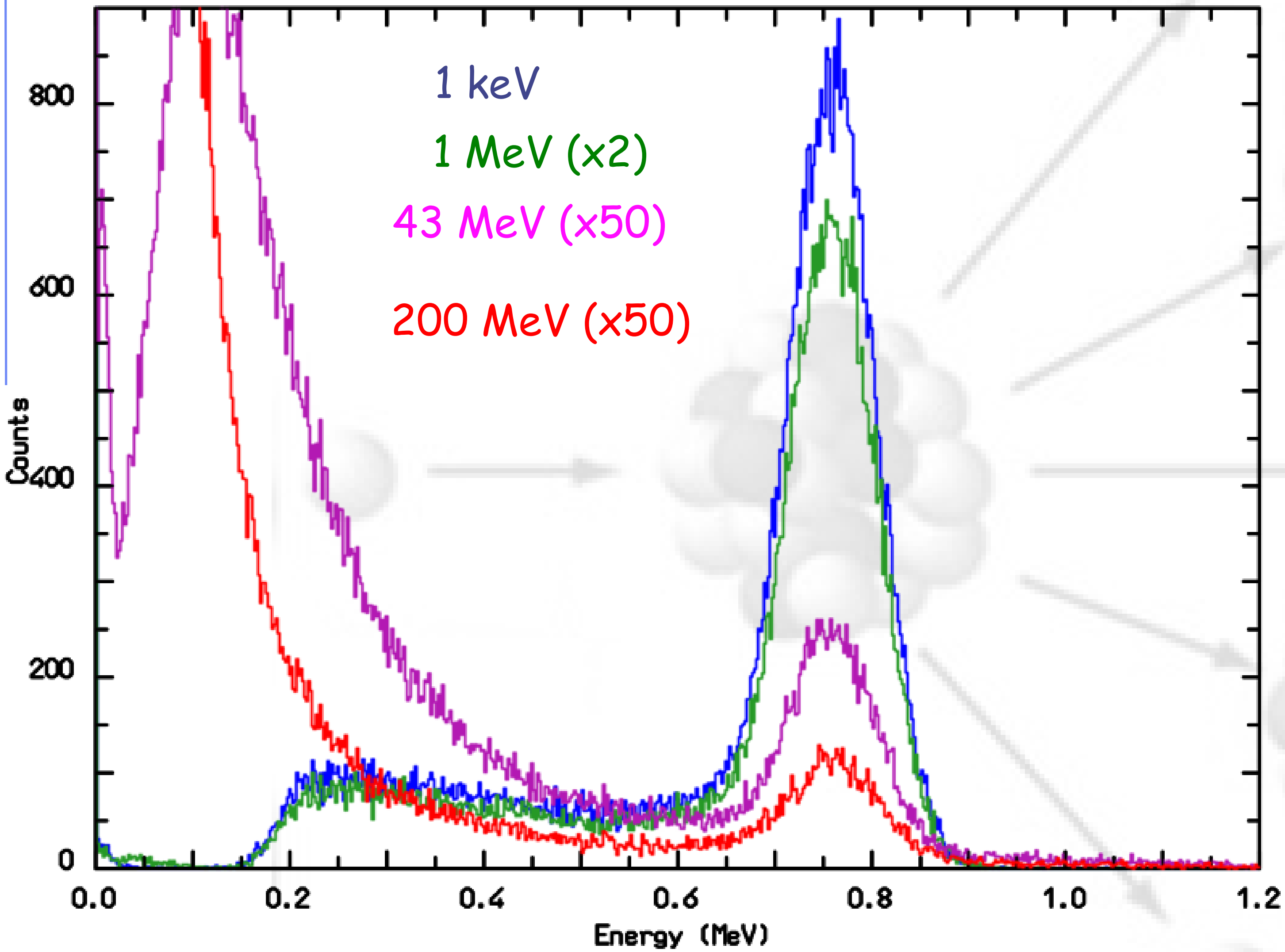

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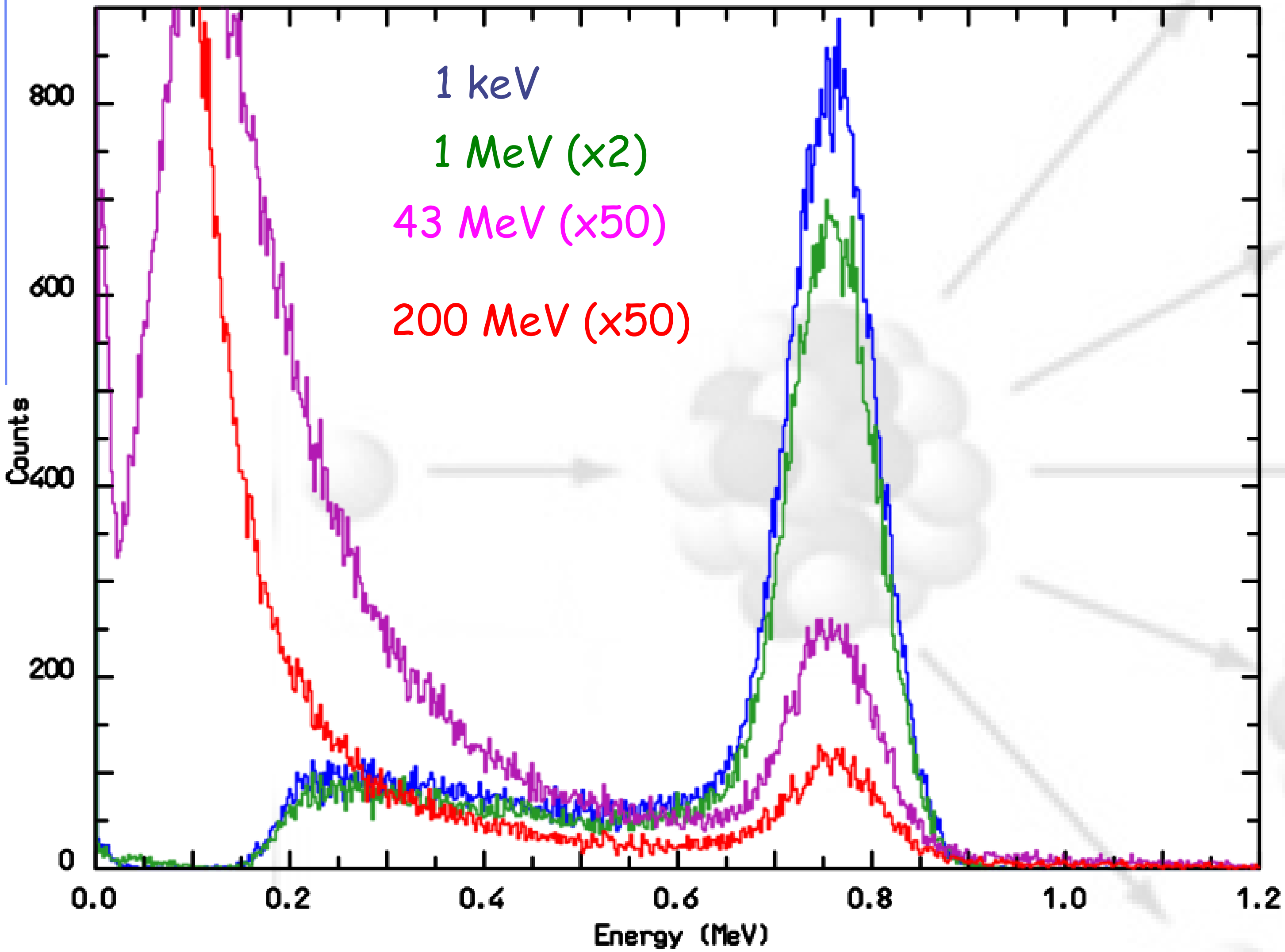
43 MeV	0.067	0.038	0.015	*0.013*
200 MeV	0.033	0.016	.0073	*.0070*

Sphere "83", option c): pulse height distributions



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1 MeV	0.636	0.629	0.508	*0.651*
43 MeV	0.067	0.038	0.015	*0.013*
200 MeV	0.033	0.016	.0073	*.0070*

A calculation with no knowledge of actual experimental procedures and/or an experiment with no check (multichannel...) at "high" energies of the discrimination set at low energies would be meaningless

Simulations of/with scintillation detectors:

Folding with known scintillator efficiencies:

Pros:

- ✓ As reliable as the efficiencies…
- ✓ … and computed fluences
- ✓ Very efficient CPU usage

Cons:

- Efficiencies often unknown …
- … or available for a limited energy range
- … or available only for a limited number of projectiles (eg issues with competing/background reactions)

Computing directly the scintillator response:

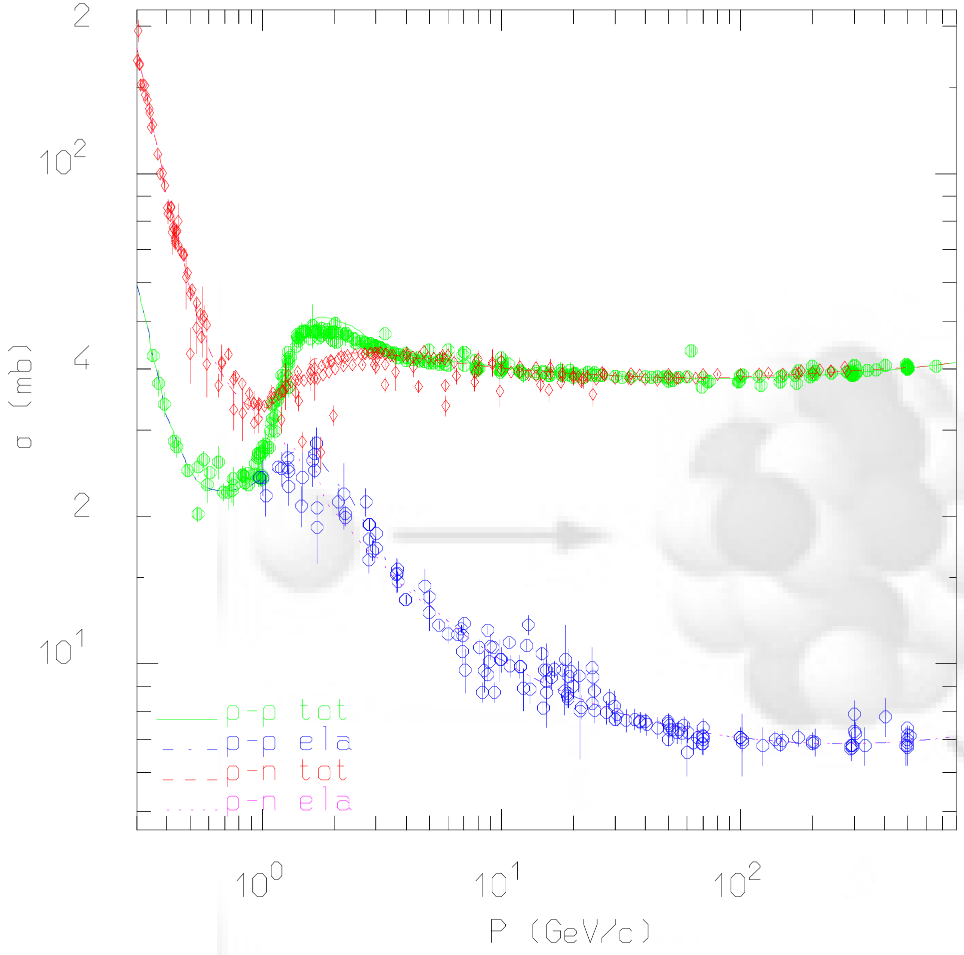
Pros:

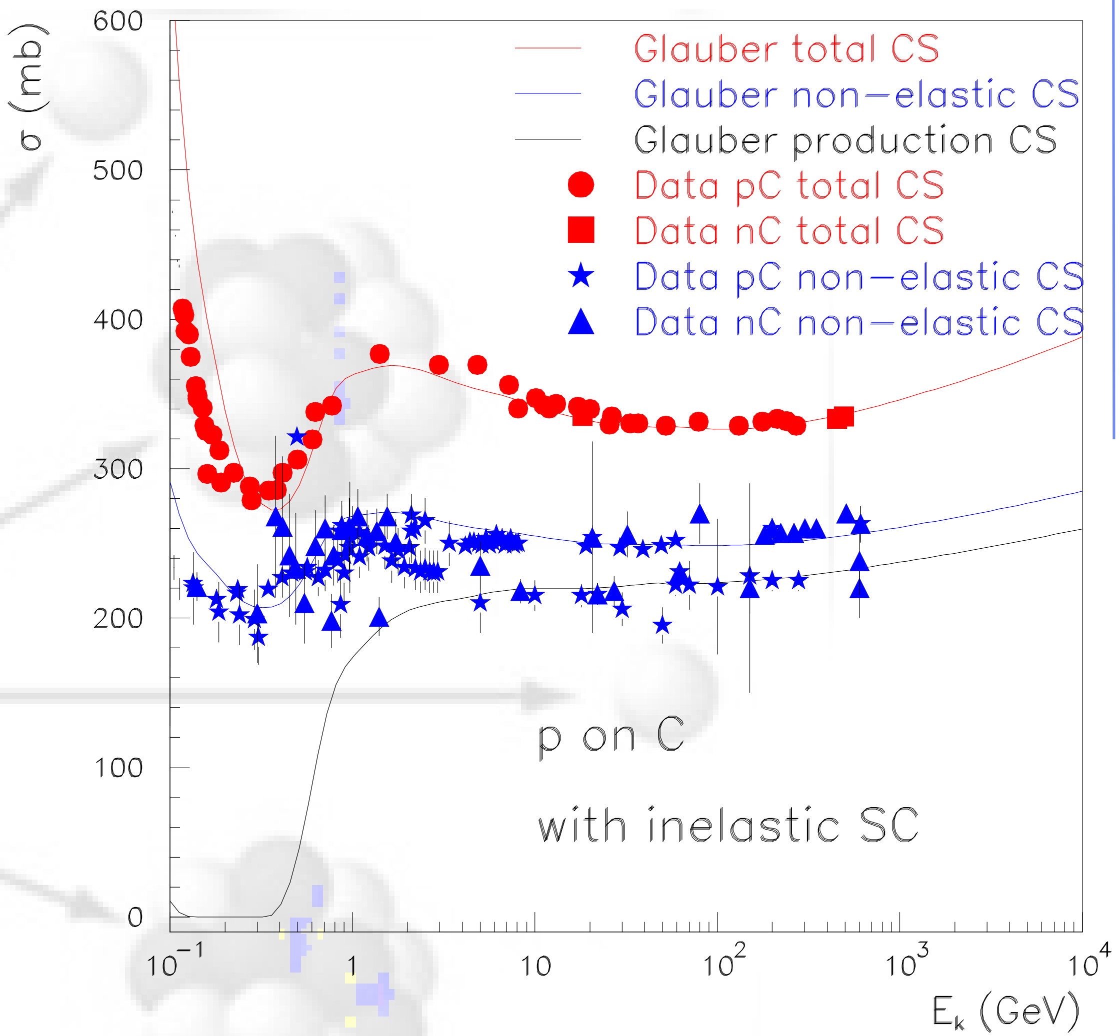
- ✓ Available for whichever projectile,
- ✓ … target …
- ✓ … and energy…
- ✓ At low energies as reliable as evaluated data/quenching parameters

Cons:

- Some sensitivity on nuclear models above 20 MeV (… unavoidable anyway)
- Quenching (light output as a function of energy/particle) must be known
- Systematics hard to evaluate

np/n^{12}C cross section:





Proton (Neutron) Carbon cross sections computed in self-consistent Glauber approach accounting for inelastic screening

Please note the ambiguity of the non-elastic exp. results, almost 2-population like

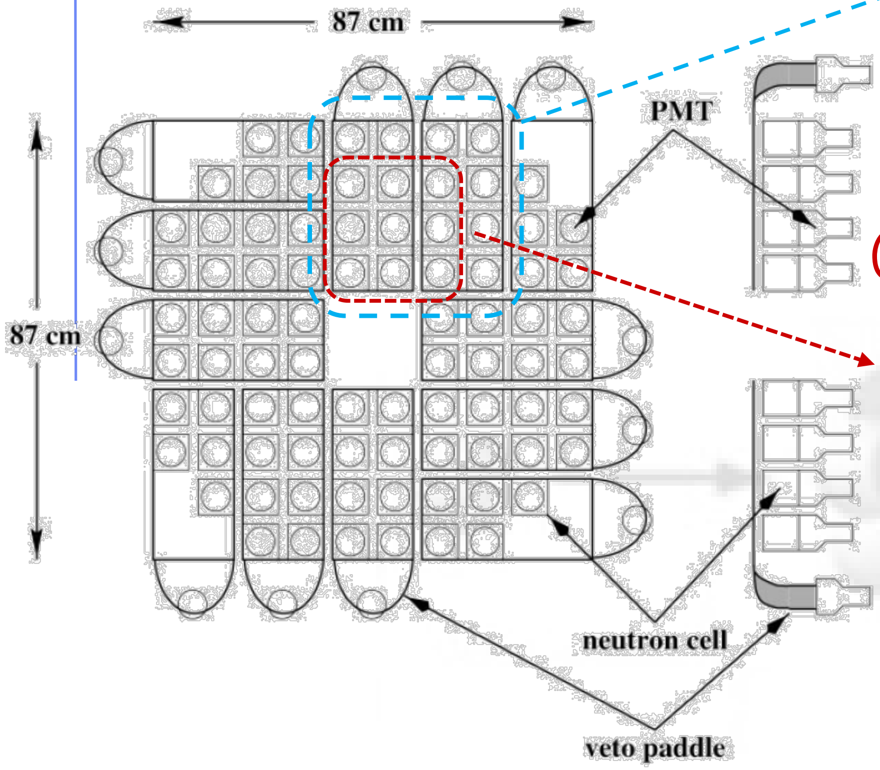
TRIUMF BC505 array expt.:

Resolution: $\sigma(E) = \sigma_0 + \frac{\sigma_1}{E[\mathrm{MeV}]^{1/2}}$

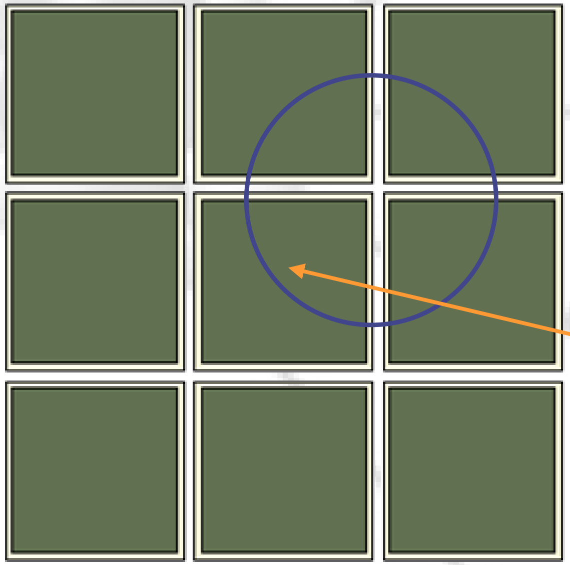
$\sigma_0 = 0.005\,\mathrm{MeV},\ \sigma_1 = 0.077\,\mathrm{MeV}^{3/2}$

$$\frac{dE_{ee}}{dx} = \frac{dE/dx}{1 + k_B \frac{dE}{dx} + c\left(\frac{dE}{dx}\right)^2}$$

Subset used for the neutron calibration



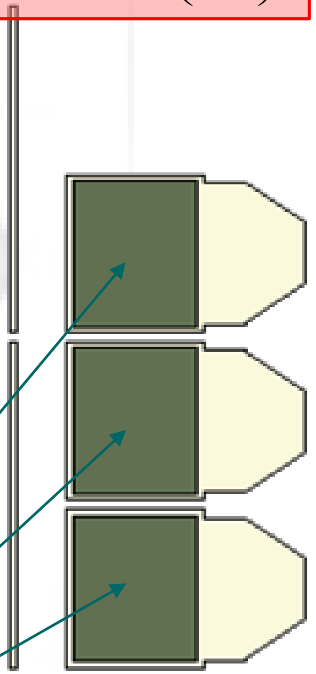
(Further) reduced subset for the MC simulation



Front view

8.9 MeV neutrons from $\pi^- p \rightarrow \gamma n$

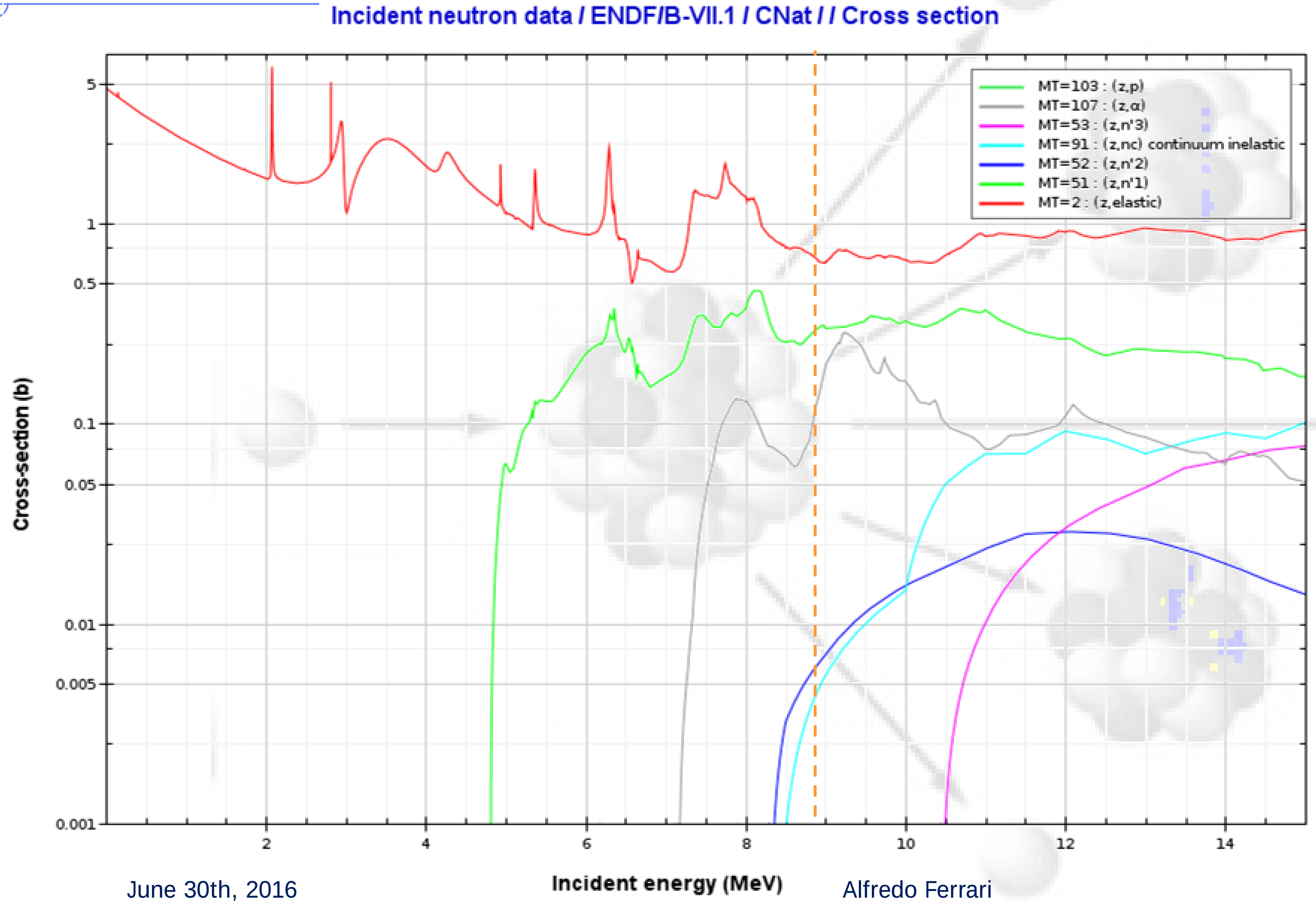
Signal cell



Bottom view

BC505 cells $7.6 \times 7.6 \times 6.4\ \mathrm{cm}^3$

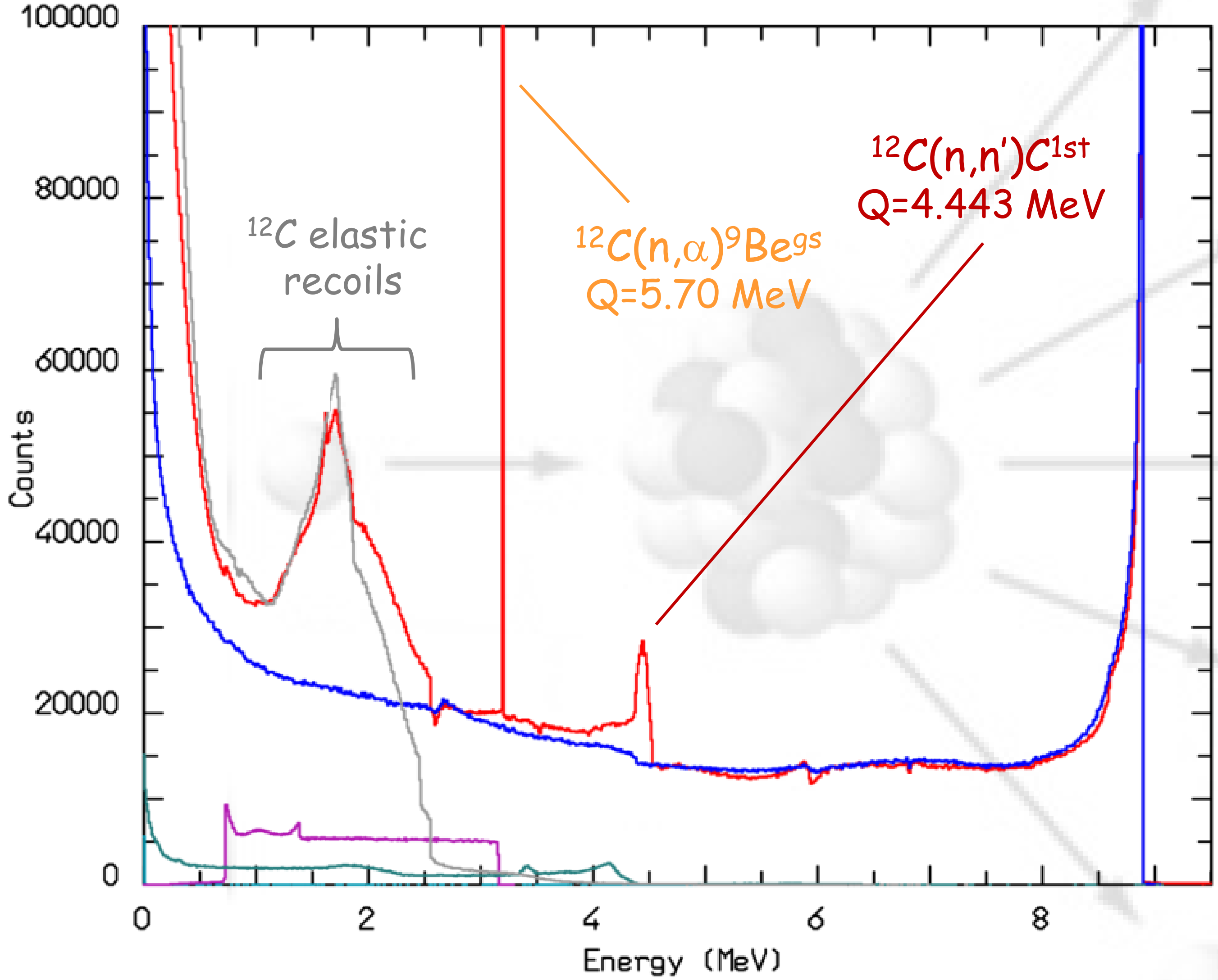
Relevant C cross section @ 8.9 MeV:



Main xsecs @ 8.9 MeV
(sigma(np) ~1.03 b)

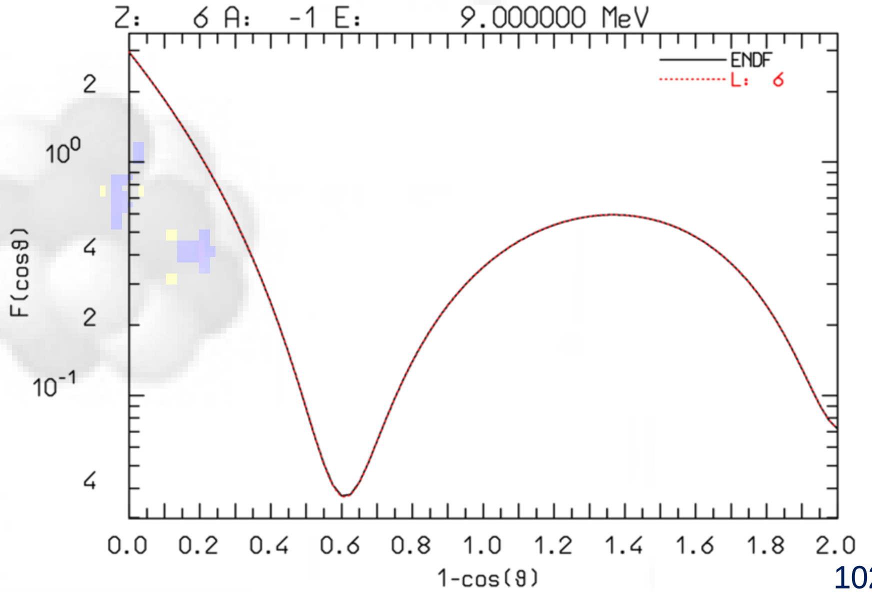
- $^{12}C(n,el)$
- $^{12}C(n,n')^{12}C^{1st}$
- $^{12}C(n,\alpha)^{9}Be^{gs}$

BC505 pulse height response to 8.9 MeV neutrons: (res:no,quen:no)

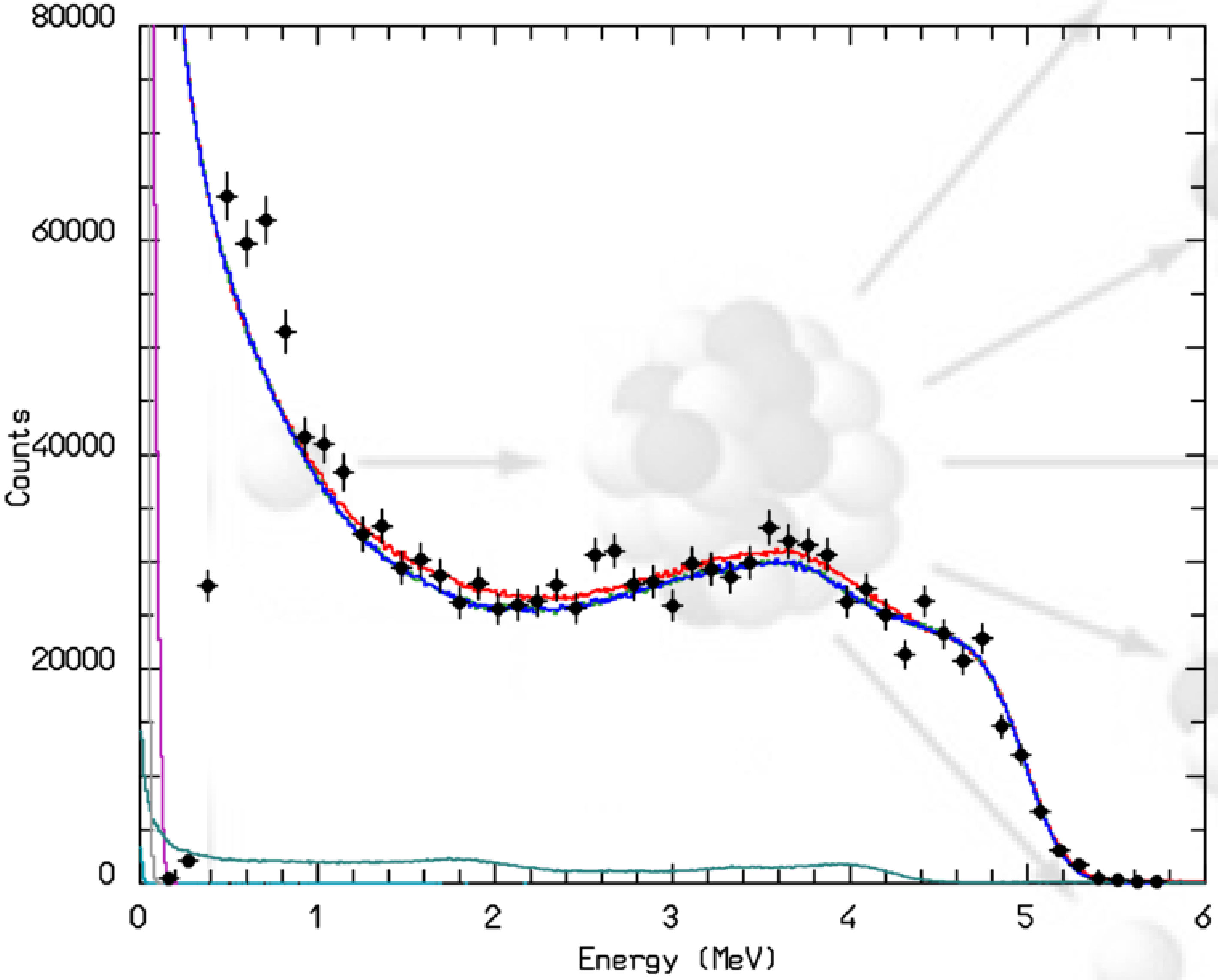


Color coding:

All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Other heavies
e+e- and photons



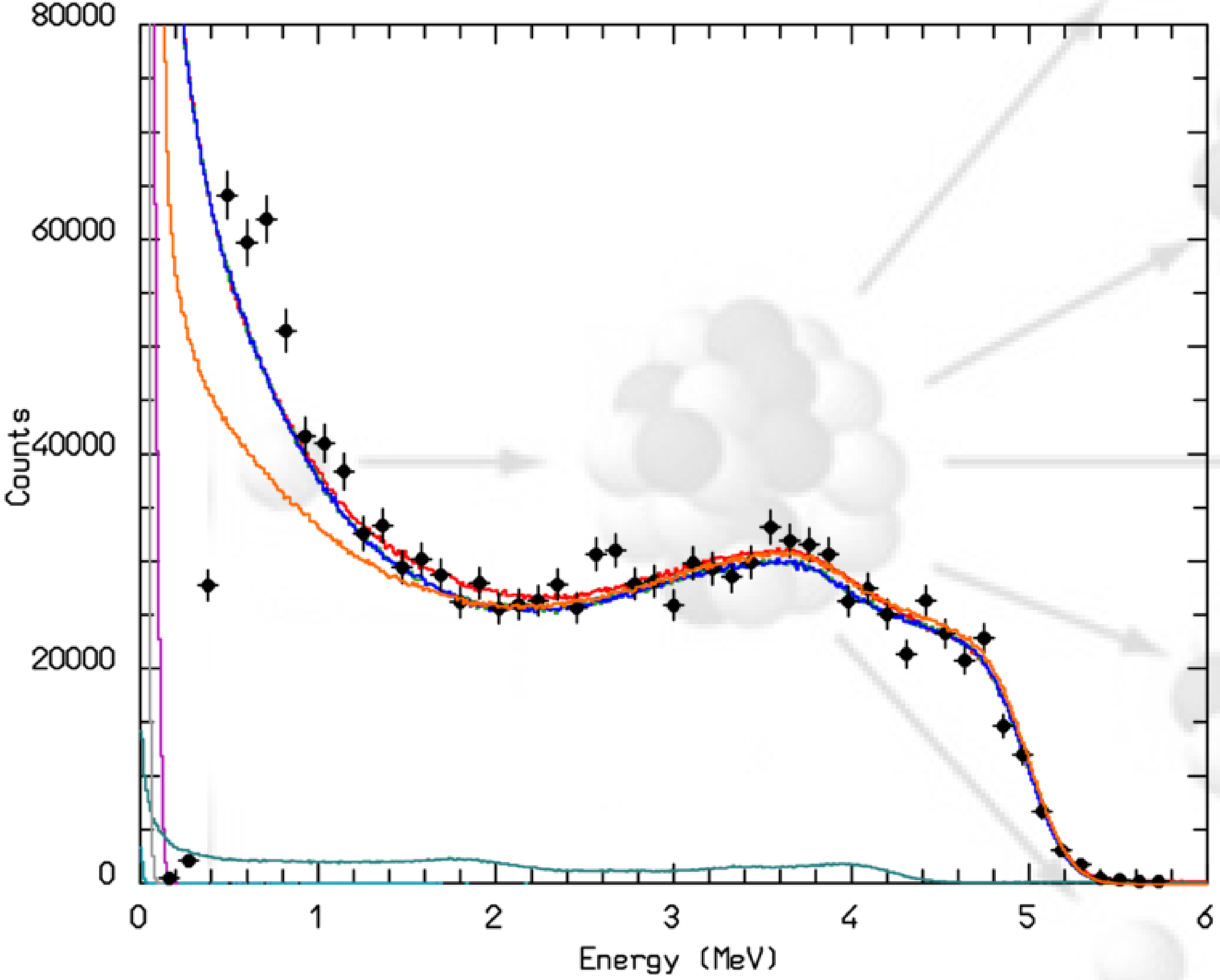
BC505 pulse height response to 8.9 MeV neutrons: (res:yes,quen:yes)



Color coding:

All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Other heavies
e+e- and photons
Exp. Data (NIMA431,446,1999)

BC505 pulse height response to 8.9 MeV neutrons: (res:yes,quen:yes)



Color coding:

All particles

Protons from elastic recoils

All protons

Deuterons

Alphas

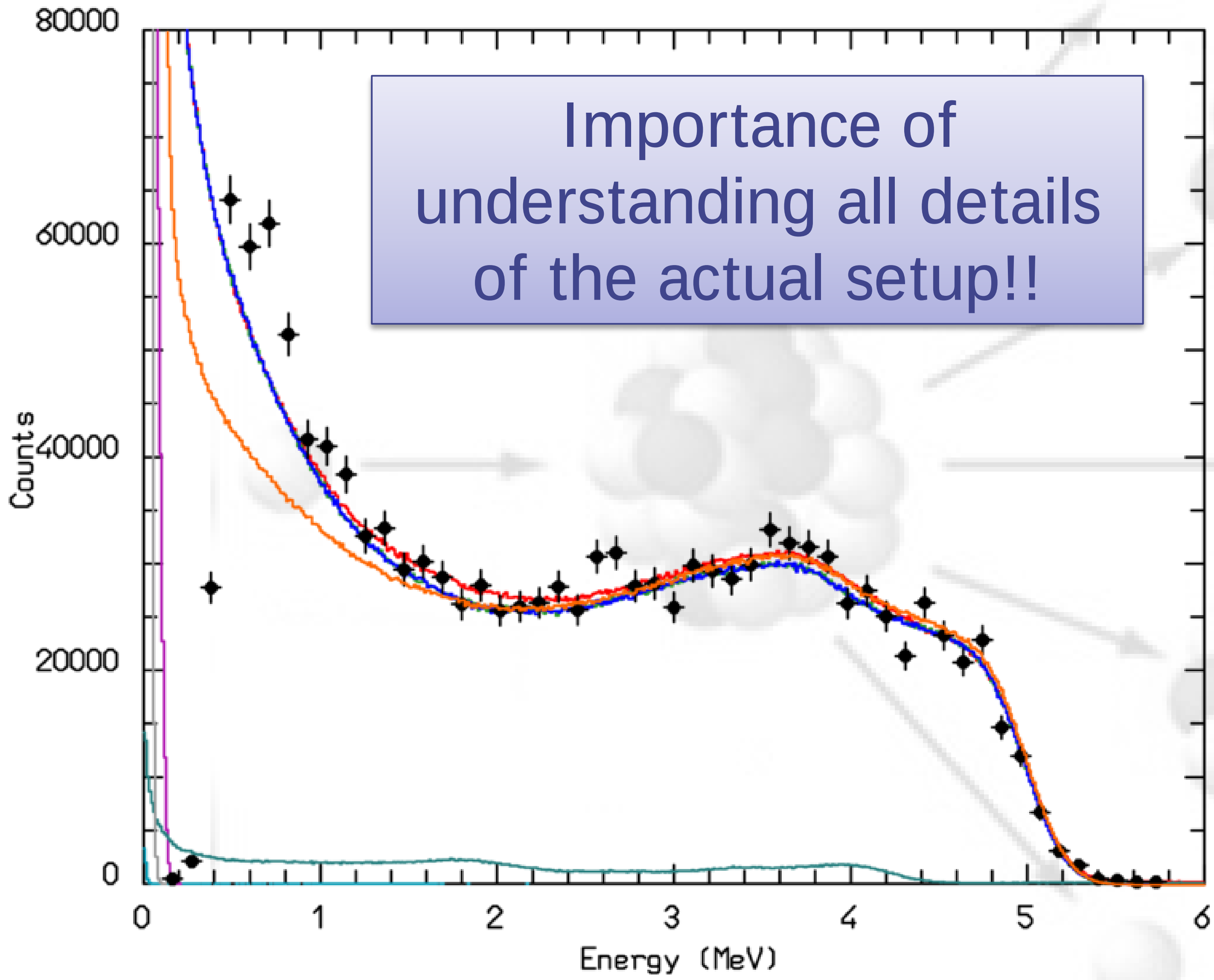
Other heavies

e+e- and photons

Exp. Data (NIMA431,446,1999)

If only the signal cell is included in the geometry the low energy part looks very different!!

BC505 pulse height response to 8.9 MeV neutrons: (res:yes,quen:yes)



Color coding:

All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Other heavies
e+e- and photons
Exp. Data (NIMA431,446,1999)

If only the signal cell is included in the geometry the low energy part looks very different!!

Example of MC induced errors:

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Nuclear Instruments and Methods in Physics Research A 583 (2007) 507–515

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH
Section A

www.elsevier.com/locate/nima

Reevaluation of secondary neutron spectra from thick targets upon heavy-ion bombardment

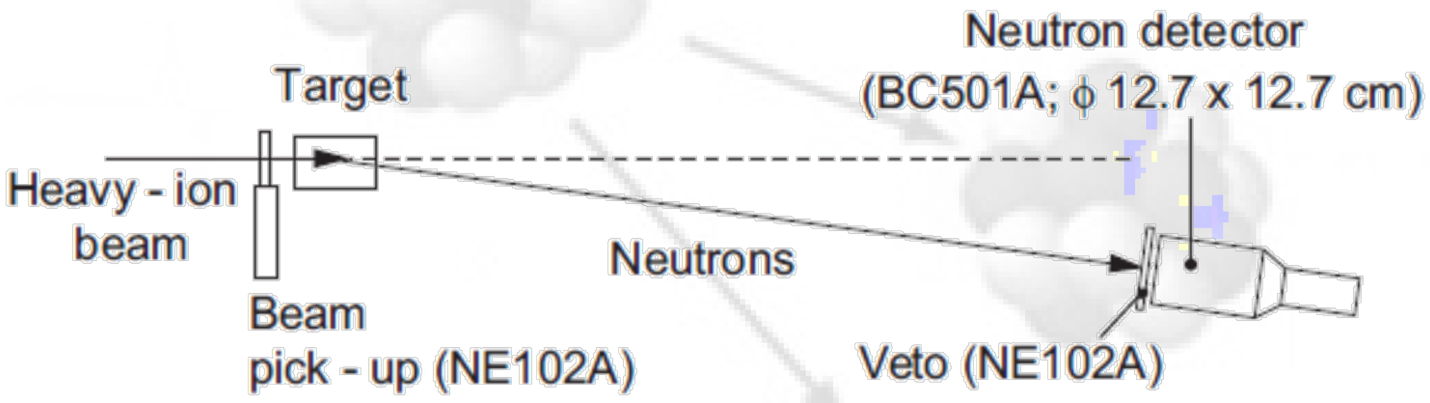


Fig. 2. Schematic of the experimental arrangement.

Effect of the "wrong" scintillator efficiency

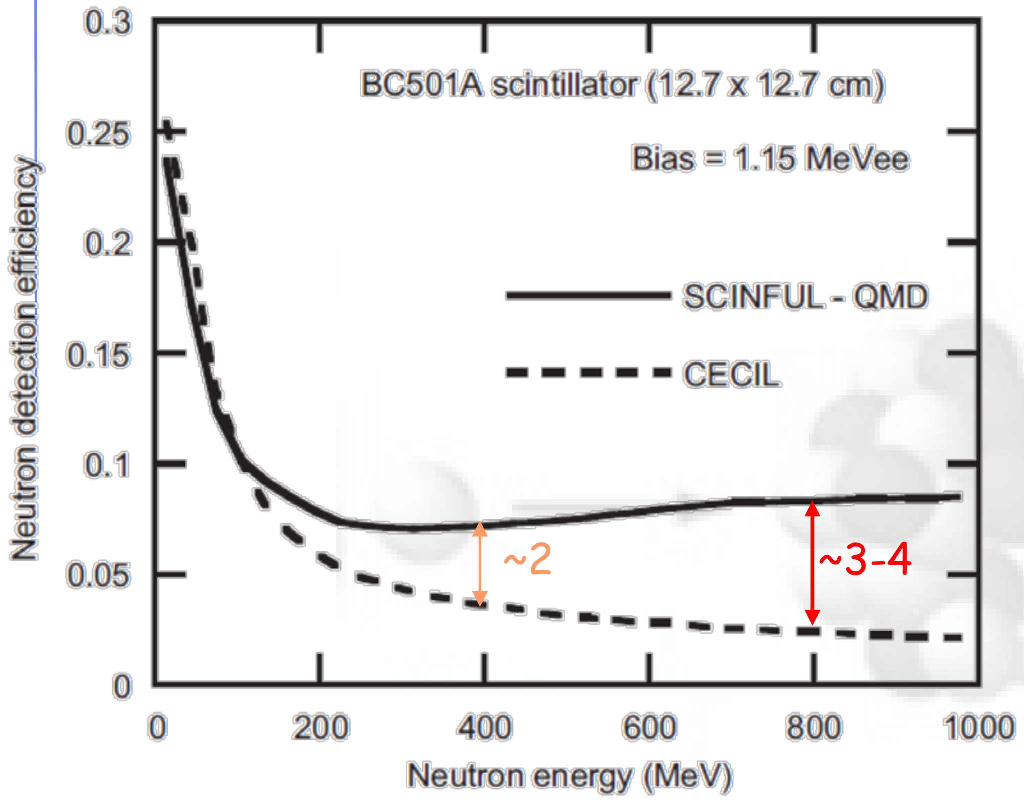


Fig. 1. Neutron-detection efficiency of a BC501A-type liquid organic scintillator with bias of 1.15 MeVee. Solid and dashed lines indicate the calculation results of SCINFUL-QMD and CECIL, respectively. The escaping proton events were eliminated in both calculations.

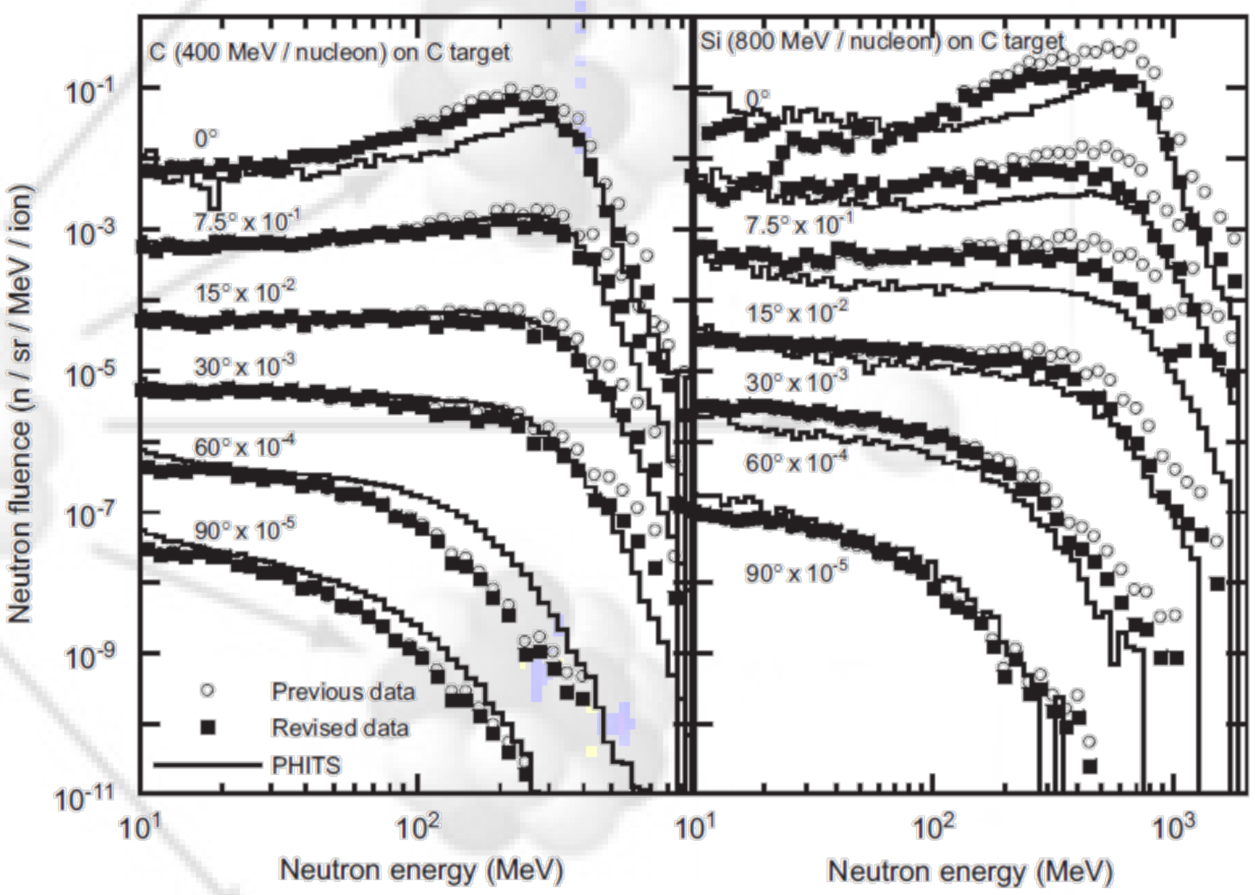


Fig. 5. Revised neutron spectra for 400-MeV/nucleon C-ion and 800-MeV/nucleon Si-ion bombardment of C targets.

Example with a ∅12.7x12.7 BC501A liq. Sci. det

- Take a ***very*** simplified BC501A liquid scintillator detector (just a cylinder with ∅12.7 cm and height 12.7 cm)
- Irradiate the front face with uniform and parallel mono-energetic neutrons (5, 50, and 500 MeV)
- Quench the energy deposition signals with parameters suitable for BC501A (eg Birks law)

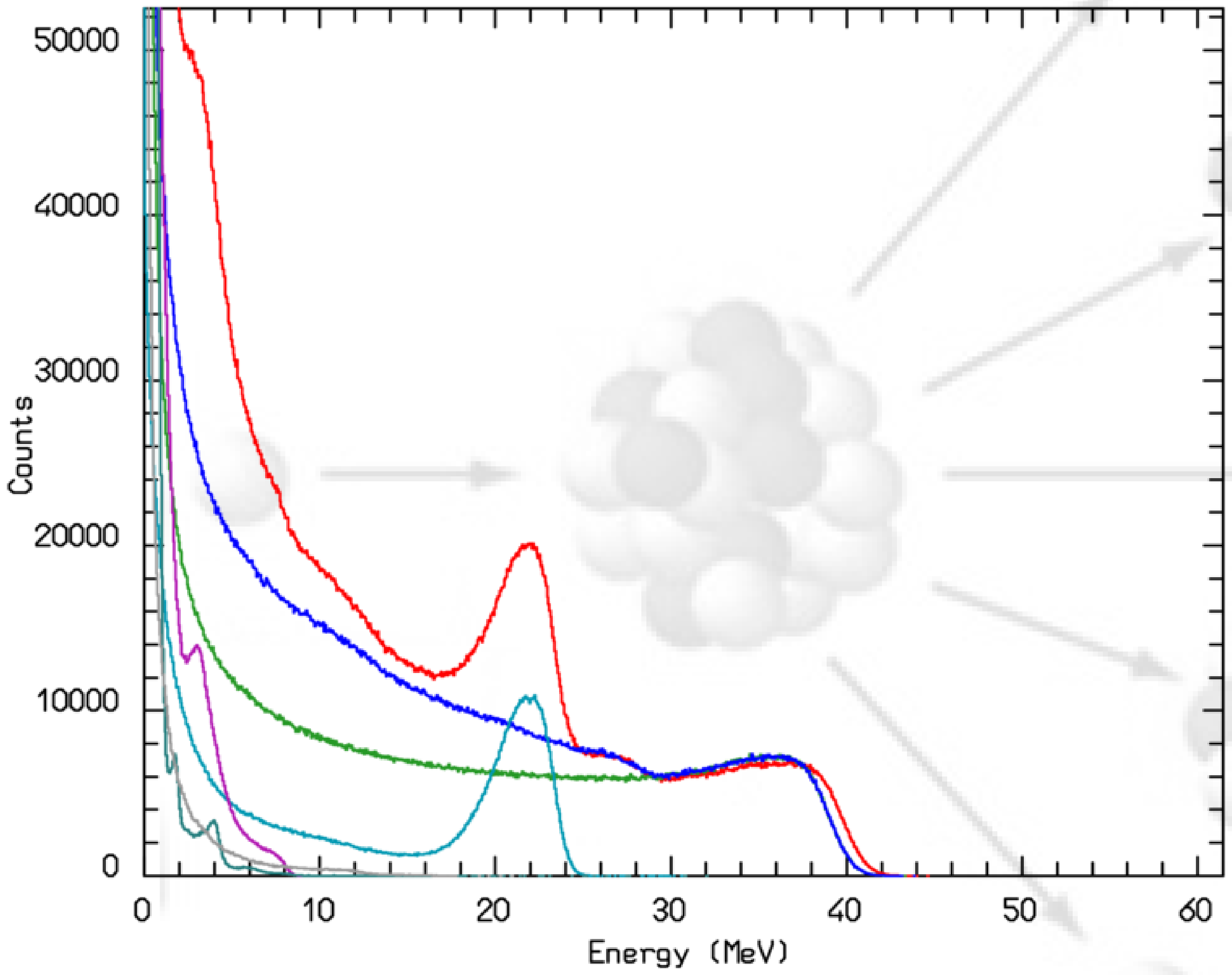
$$\frac{dL}{dx} = \frac{dE/dx}{1+kB\frac{dE}{dx}+c\left(\frac{dE}{dX}\right)^2}$$

k, c=quenching parameters

- Apply the smearing due to the scintillator resolution
- Observe the total "energy" (light) output distribution in units of MeV_{ee}, and the individual contributions of various particles*
- Compute a naïve (given the simplified setup) efficiency for E_{dep} > 1.15 MeV_{ee}

**Requires event-by-event correlations, fine above 20 MeV, mostly H important below*

Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:

All particles

Protons from elastic recoils

All protons

Deuterons

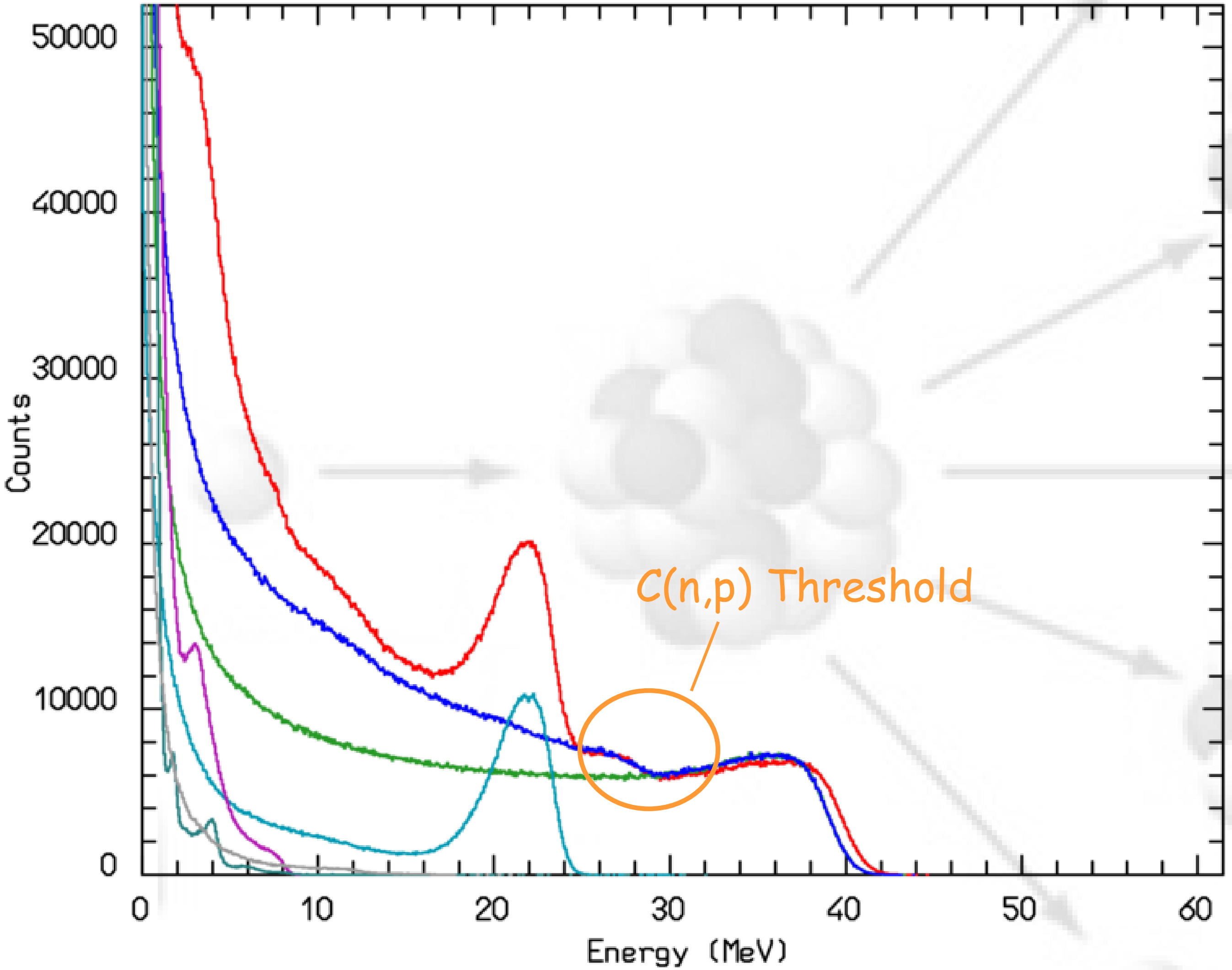
Alphas

Charged pions

Other heavies

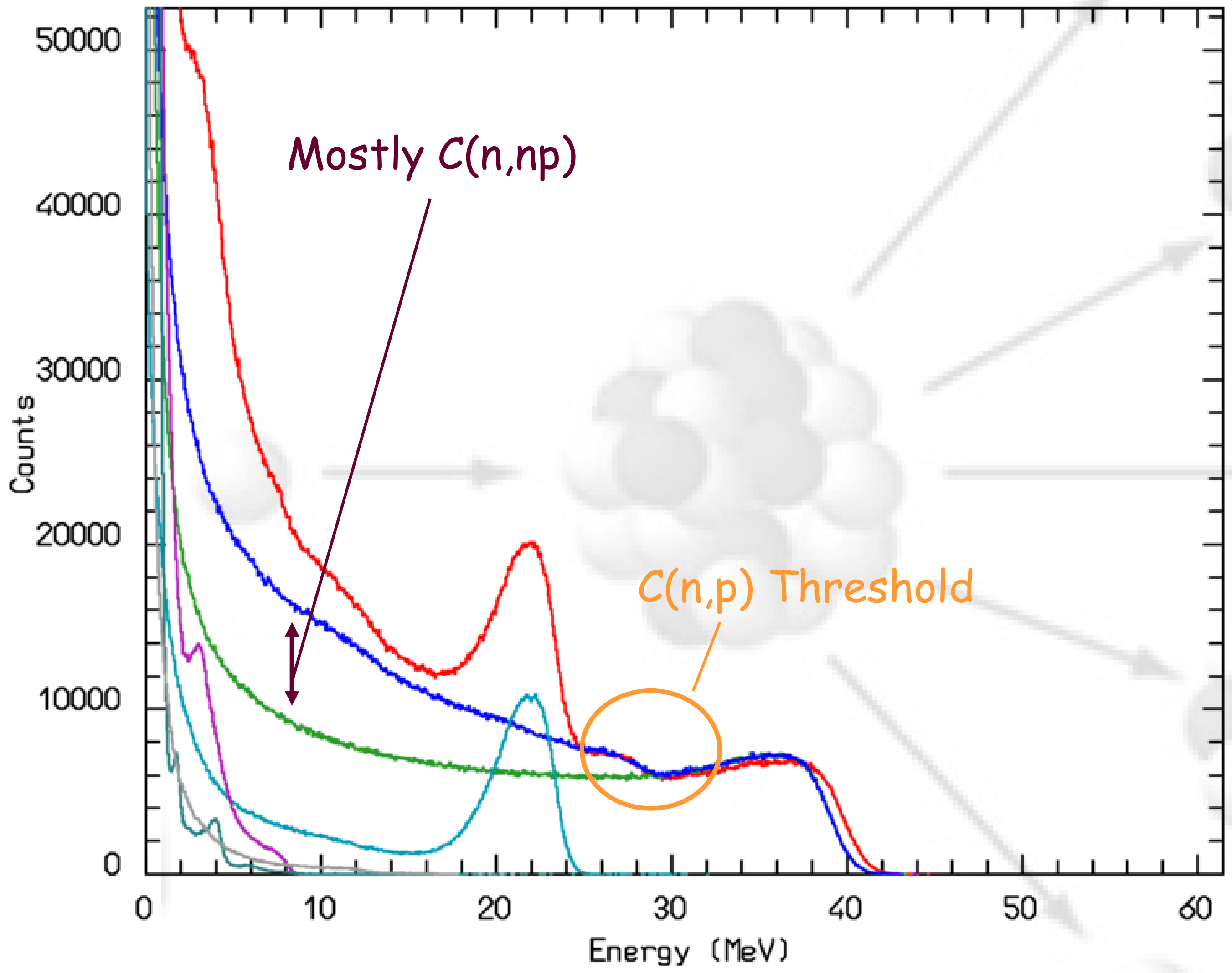
e+e- and photons

Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:
All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Charged pions
Other heavies
e+e- and photons

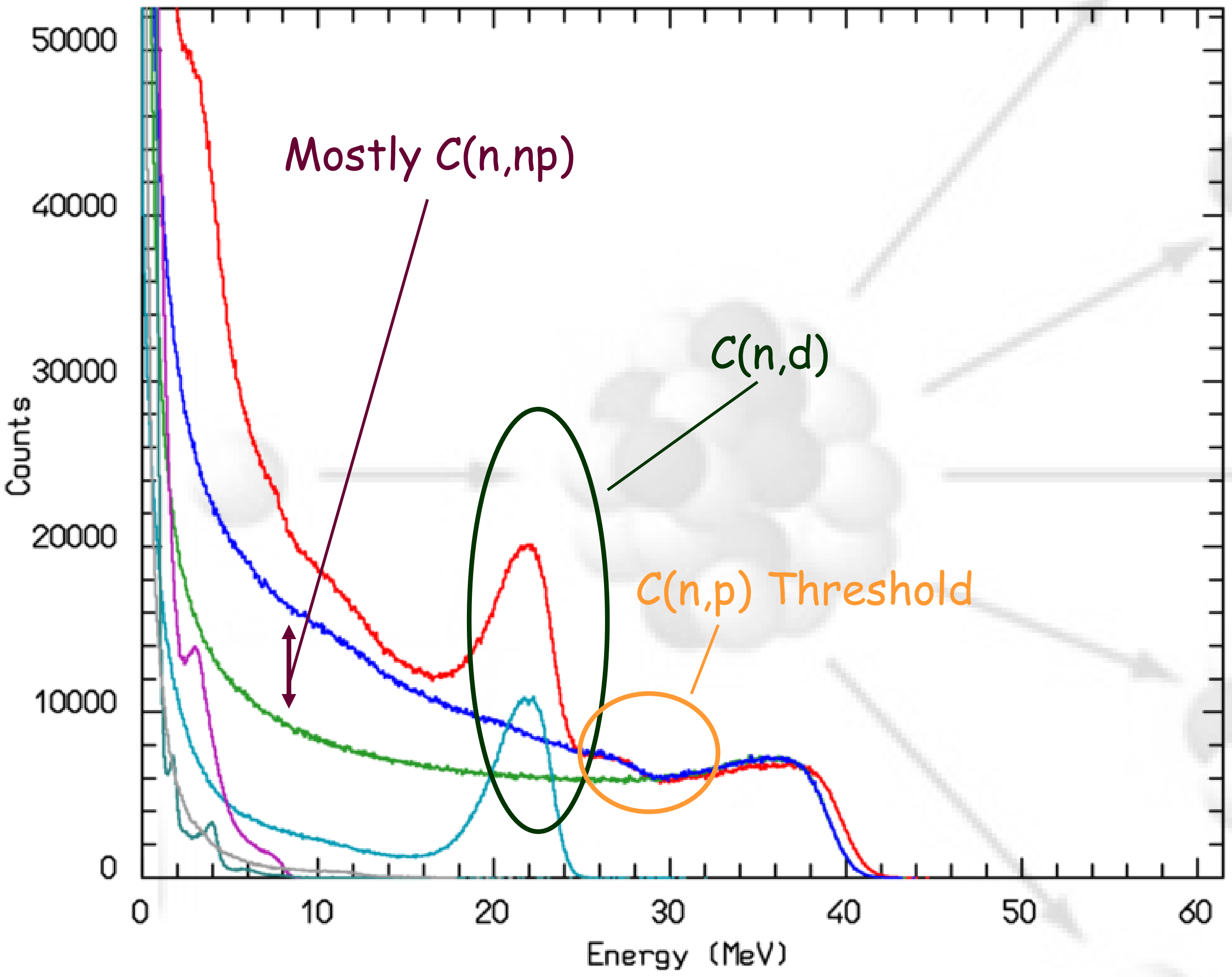
Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:

All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Charged pions
Other heavies
e+e- and photons

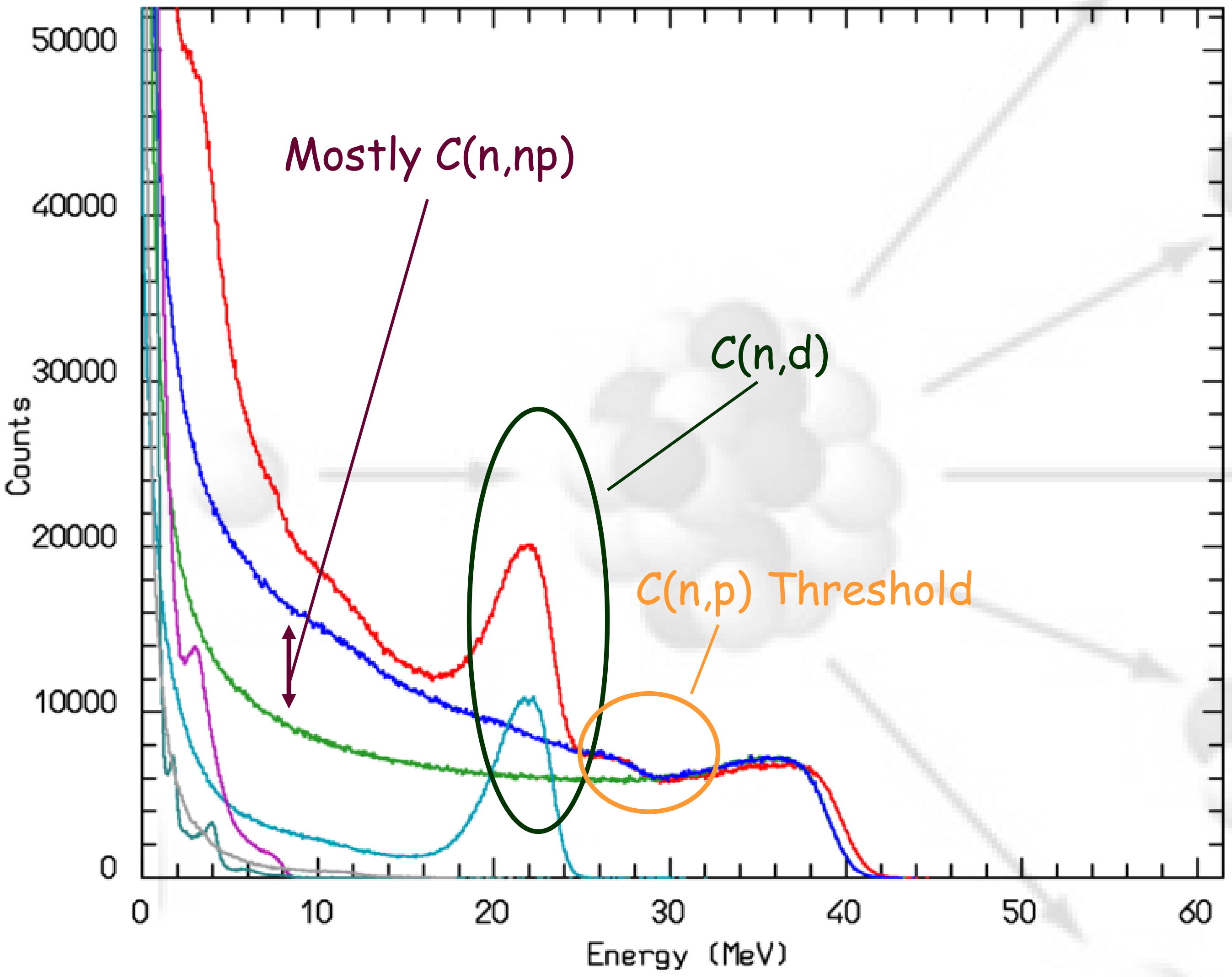
Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:

All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Charged pions
Other heavies
e+e- and photons

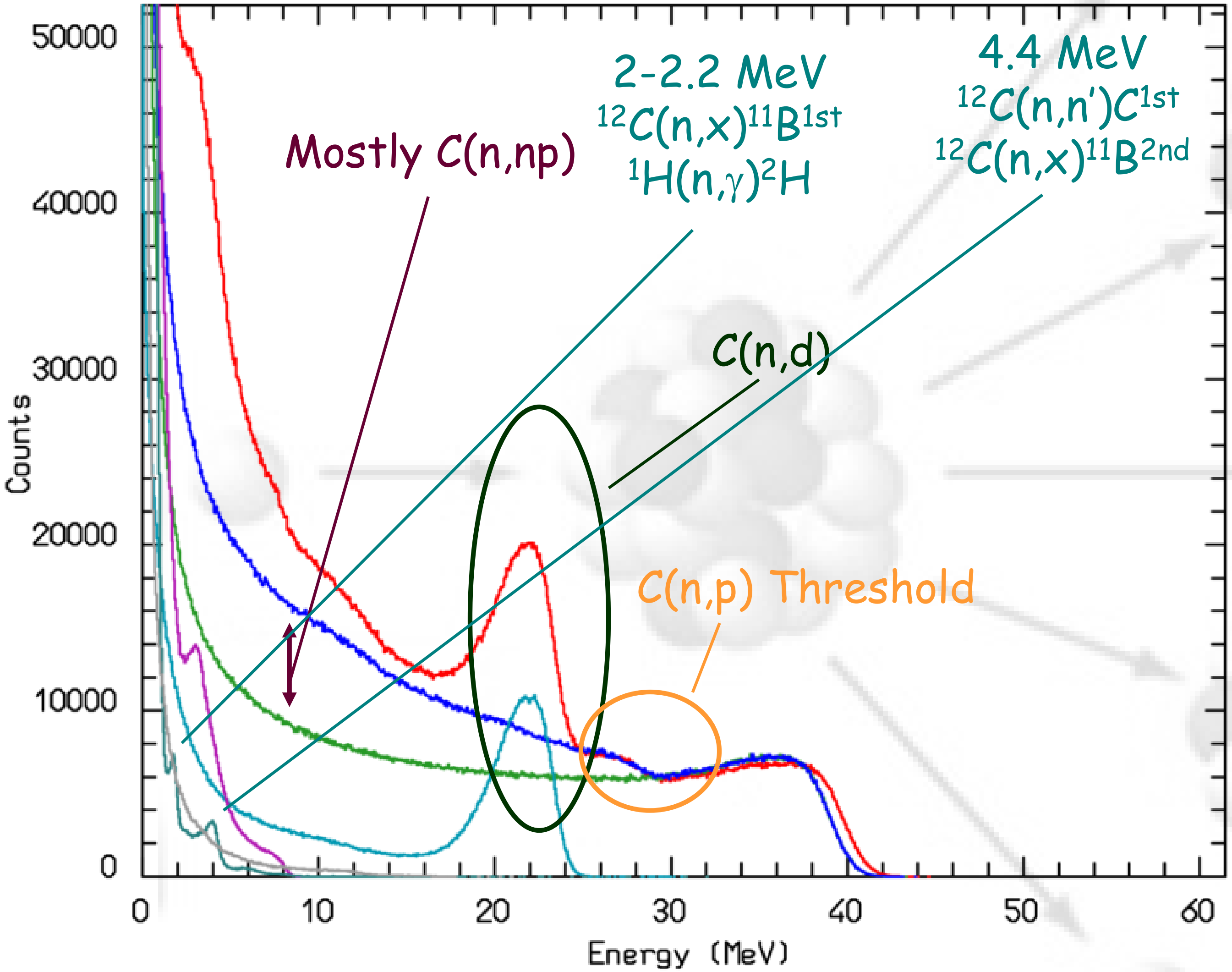
Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:

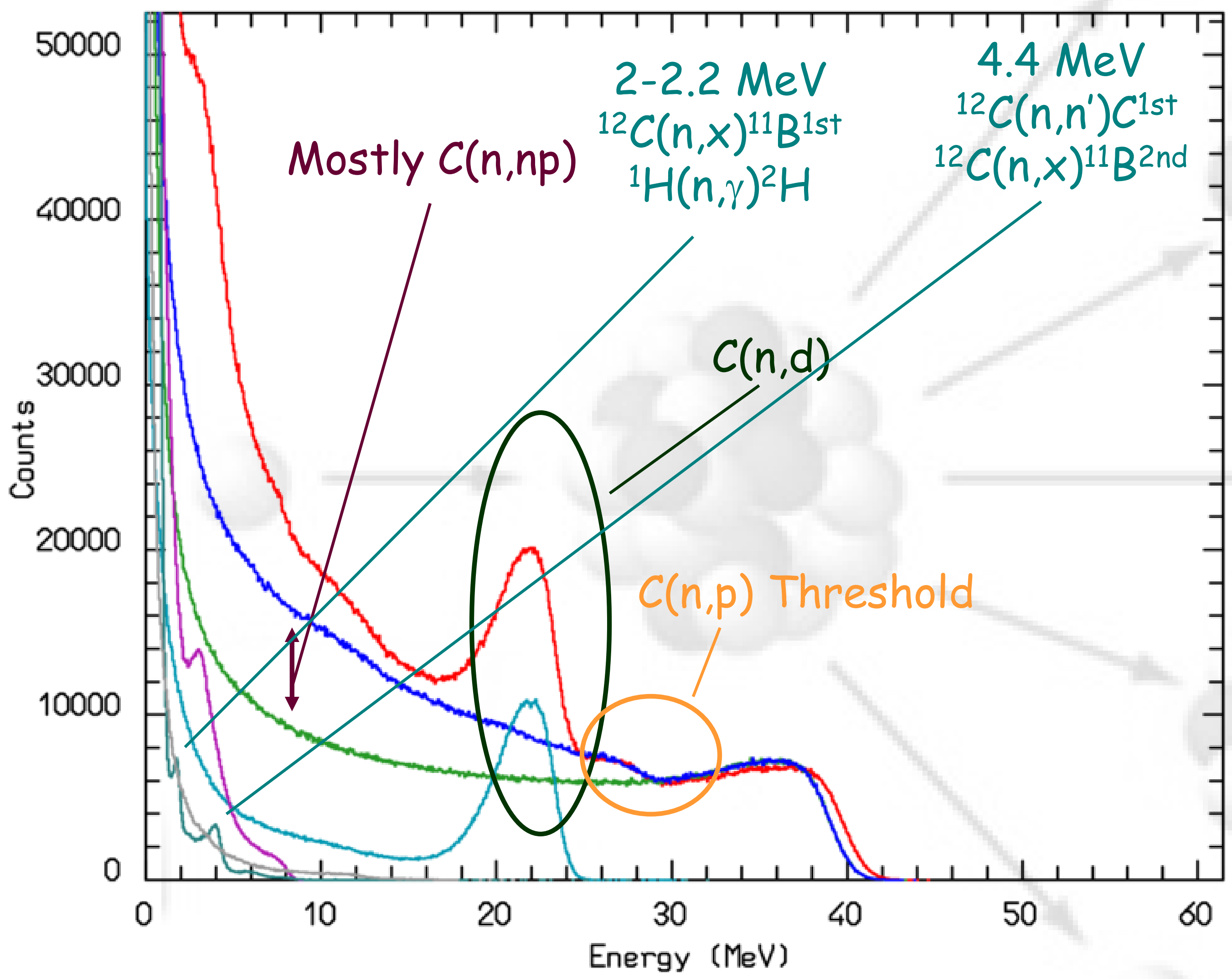
All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Charged pions
Other heavies
e+e- and photons

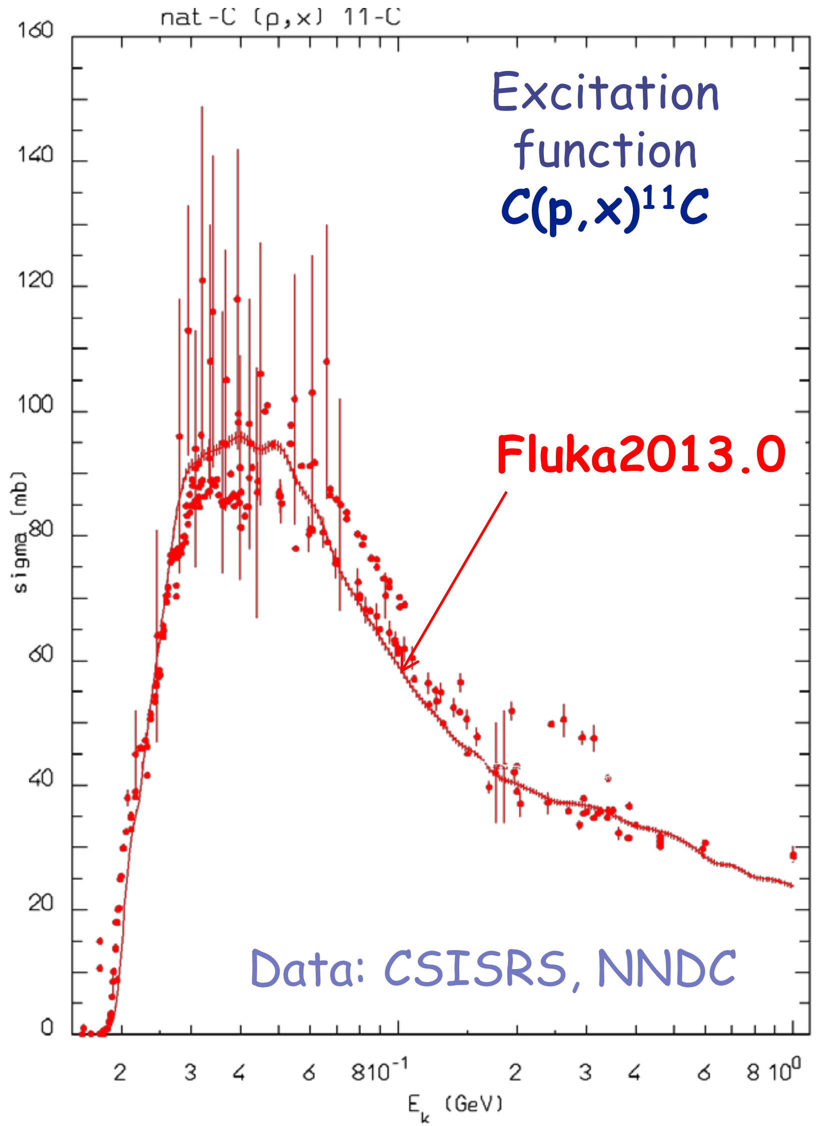
Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:
All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Charged pions
Other heavies
e+e- and photons

Pulse height response to 50 MeV neutrons (res:yes,quen:yes)





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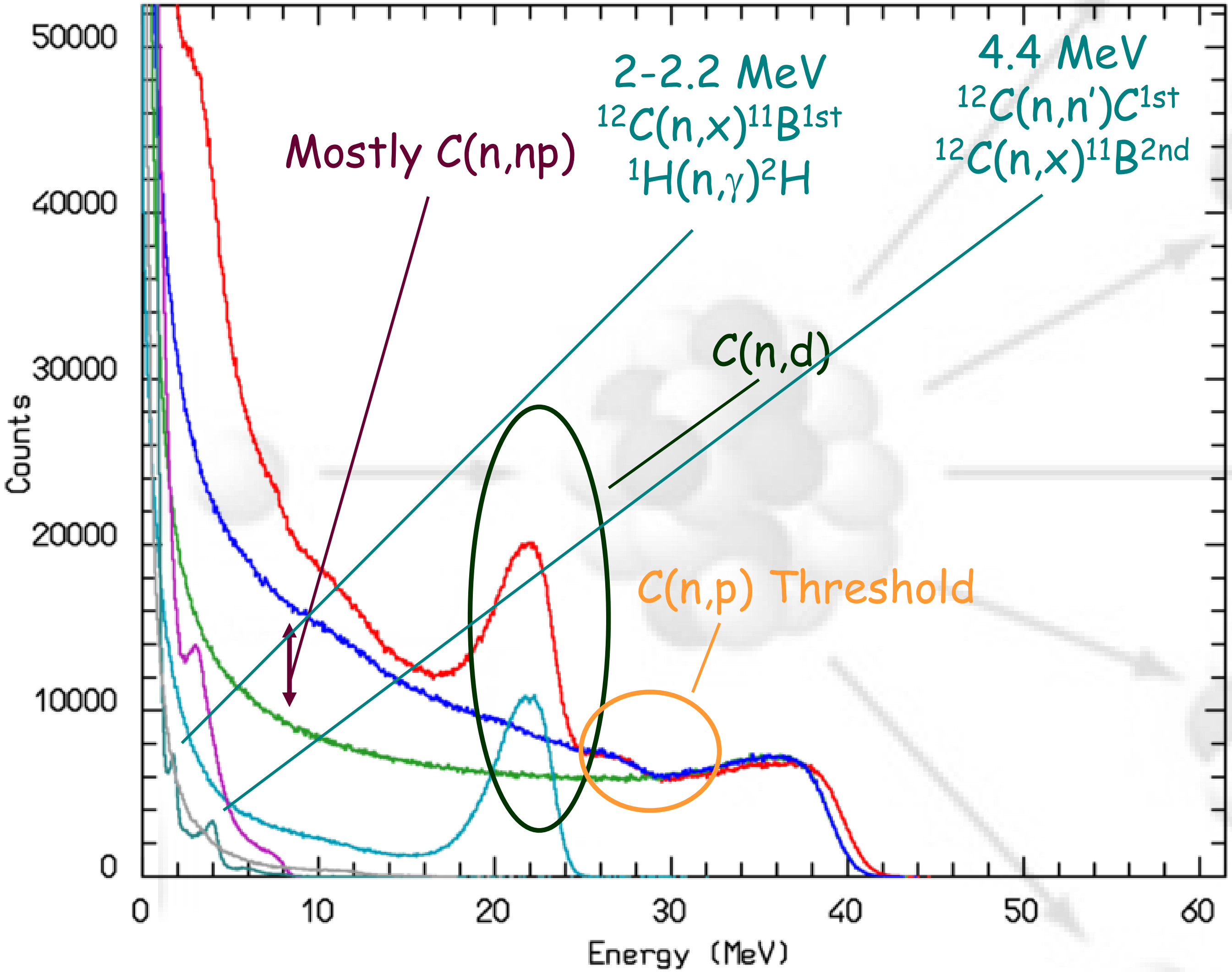
Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:

All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
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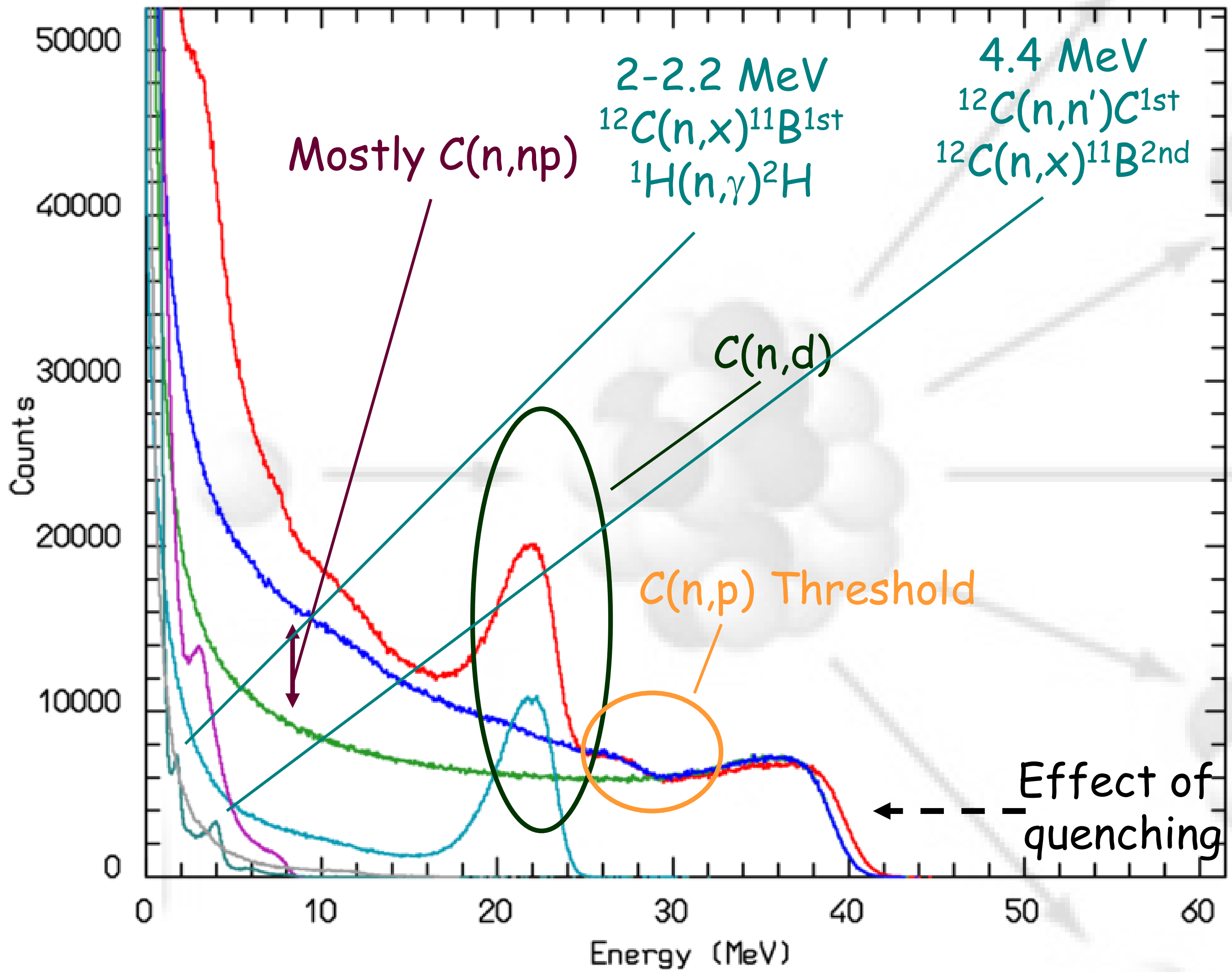
Pulse height response to 50 MeV neutrons (res:yes,quen:yes)



Color coding:

All particles

Protons from elastic recoils

All protons

Deuterons

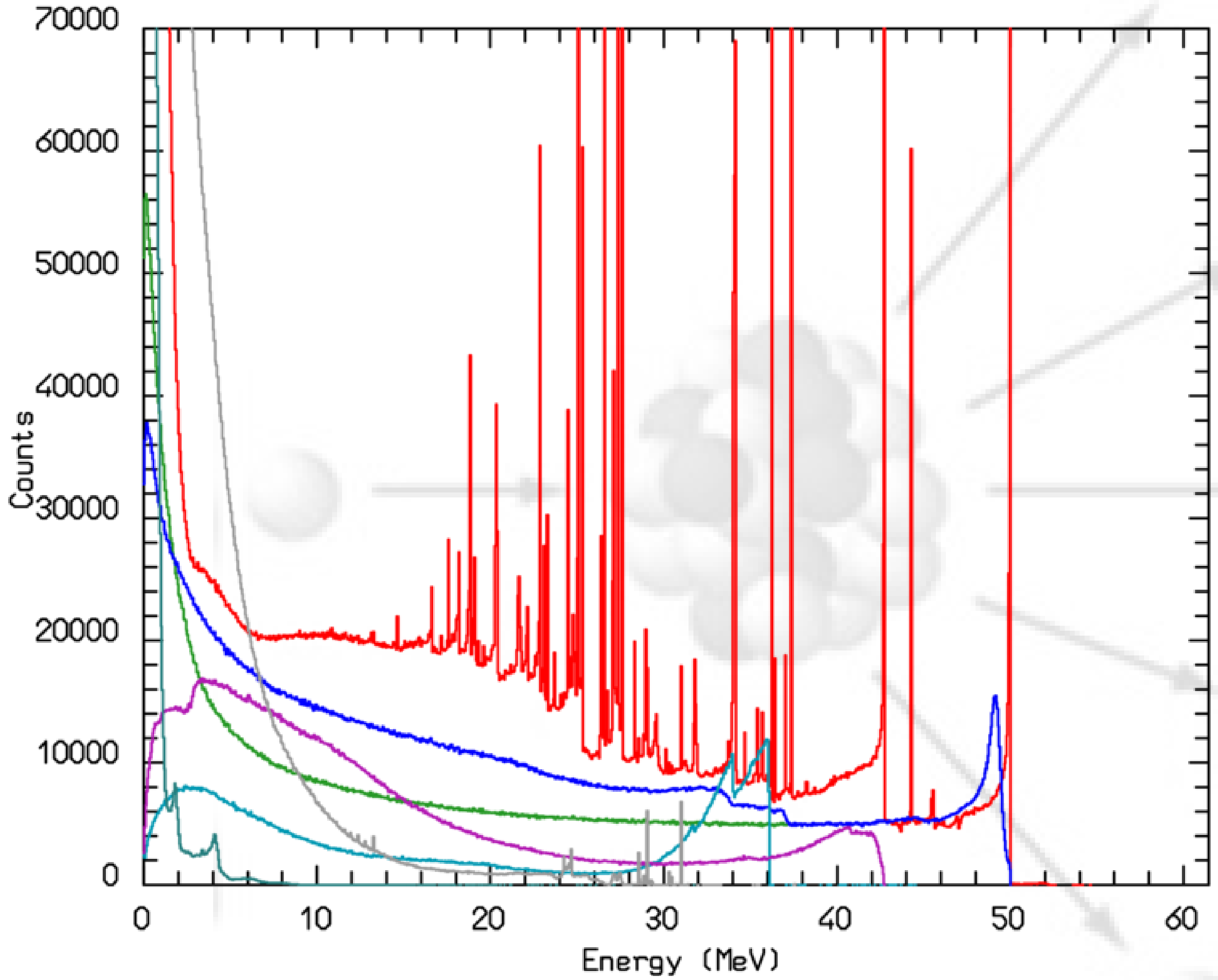
Alphas

Charged pions

Other heavies

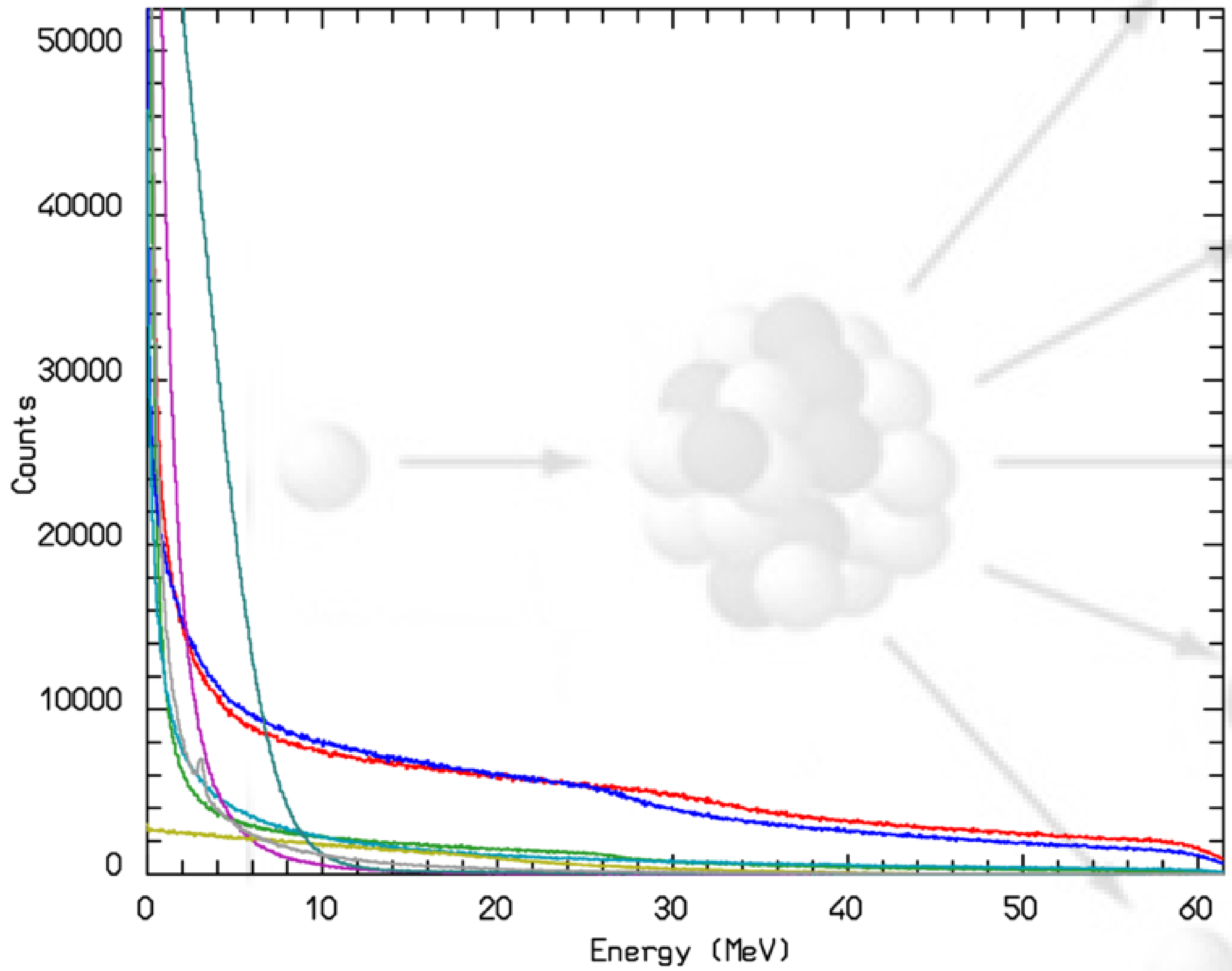
e+e- and photons

Pulse height response to 50 MeV neutrons (res:no,quen:no)



Color coding:
All particles
Protons from elastic recoils
All protons
Deuterons
Alphas
Charged pions
Other heavies
e+e- and photons

Pulse height response to 500 MeV neutrons:



Color coding:

All particles

Protons from elastic recoils

All protons

Deuterons

Alphas

Charged pions

Other heavies

e+e- and photons

Quick (rough) check of the result:

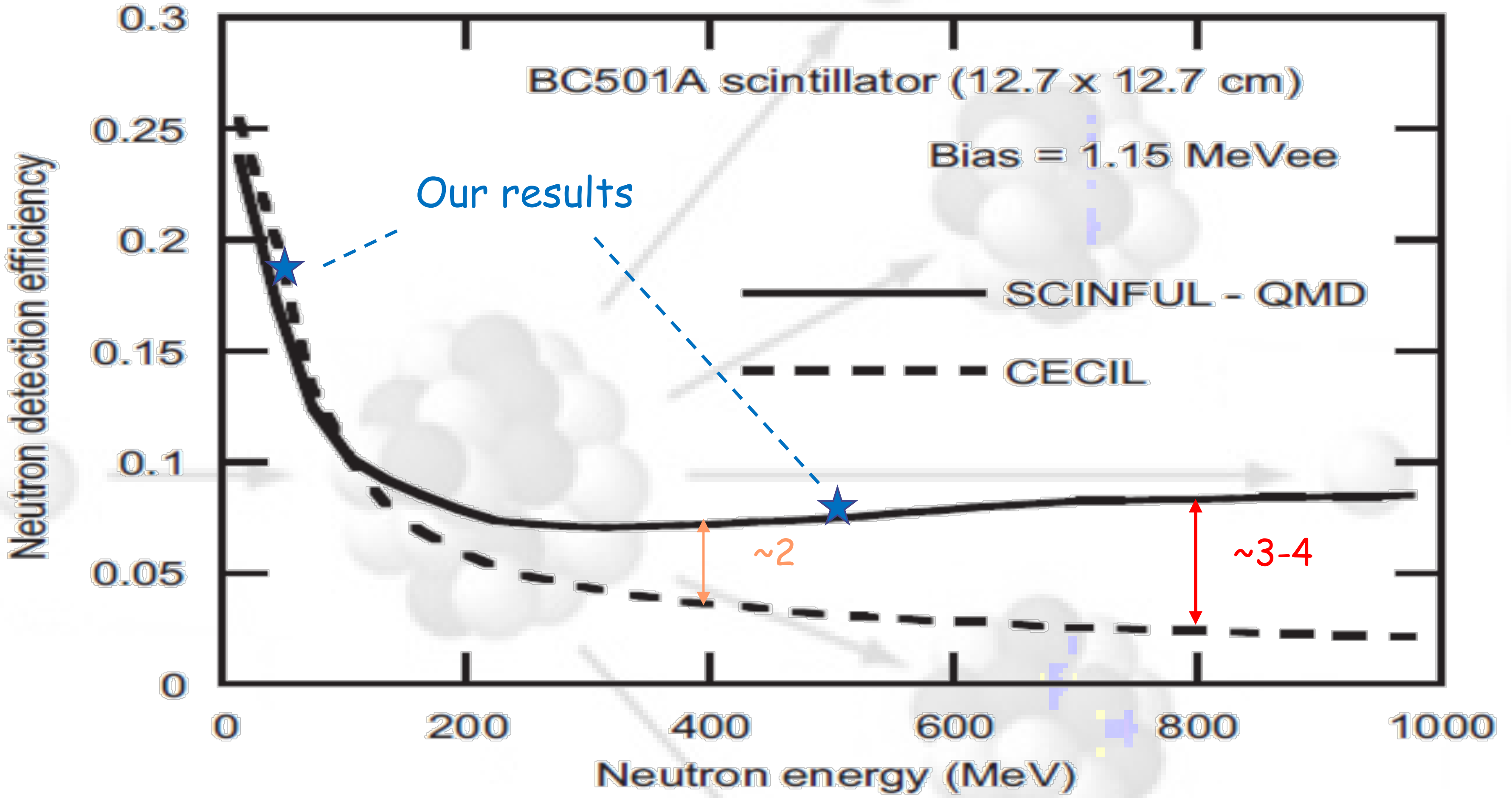


Fig. 1. Neutron-detection efficiency of a BC501A-type liquid organic scintillator with bias of 1.15 MeVee. Solid and dashed lines indicate the calculation results of SCINFUL-QMD and CECIL, respectively. The escaping proton events were eliminated in both calculations.

Simulations for activation detectors:

Folding with known cross sections:

Pros:

- ✓ As precise as available cross sections
- ✓ … and computed fluences
- ✓ Very efficient CPU usage

Cons:

- ➢ Cross sections sometimes not available at all
- ➢ … or available for a limited energy range
- ➢ … or available only for a limited number of projectiles (eg issues with competing/background reactions)

Computing directly isotope production with models:

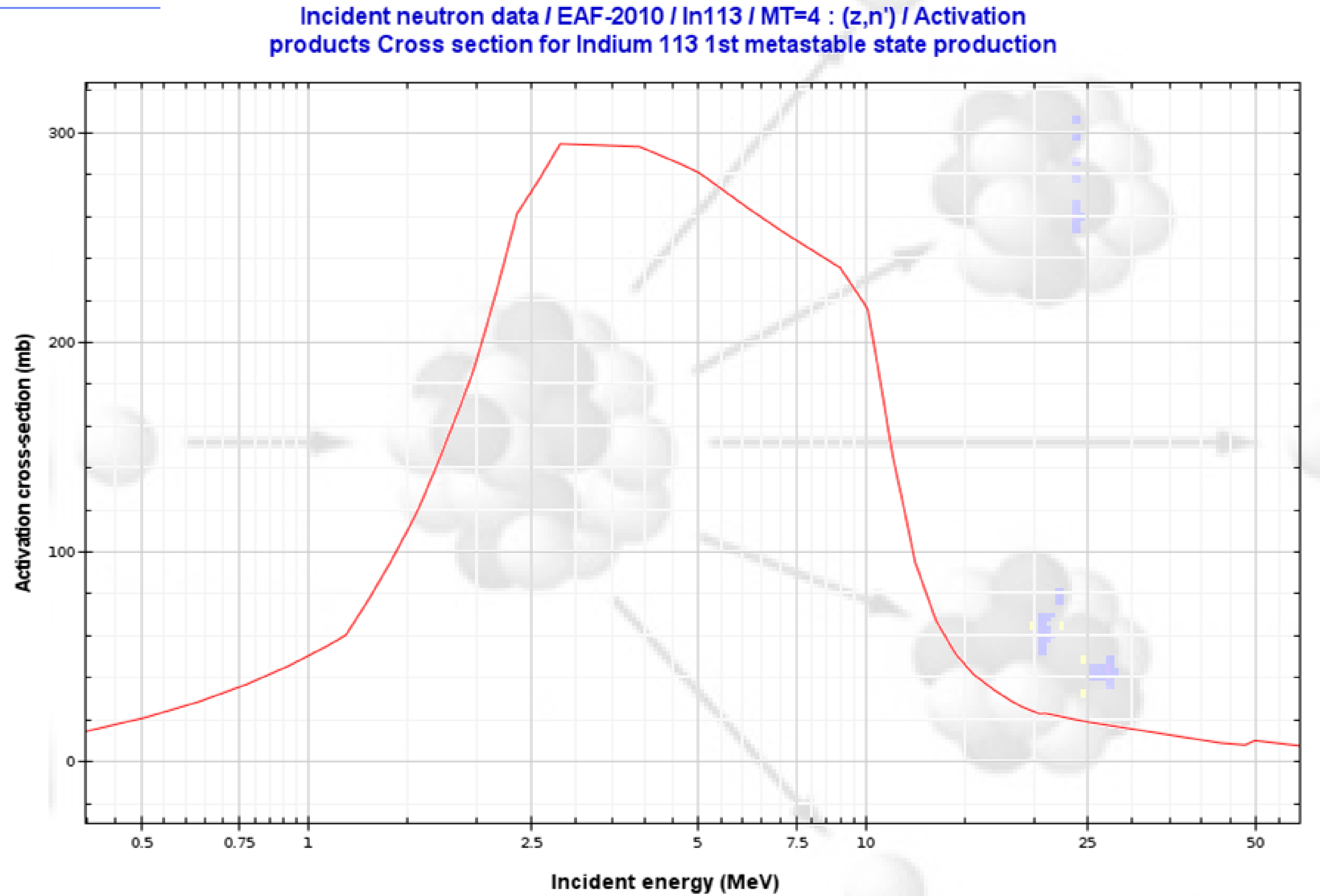
Pros:

- ✓ Available for whichever projectile,
- ✓ … target …
- ✓ … and energy

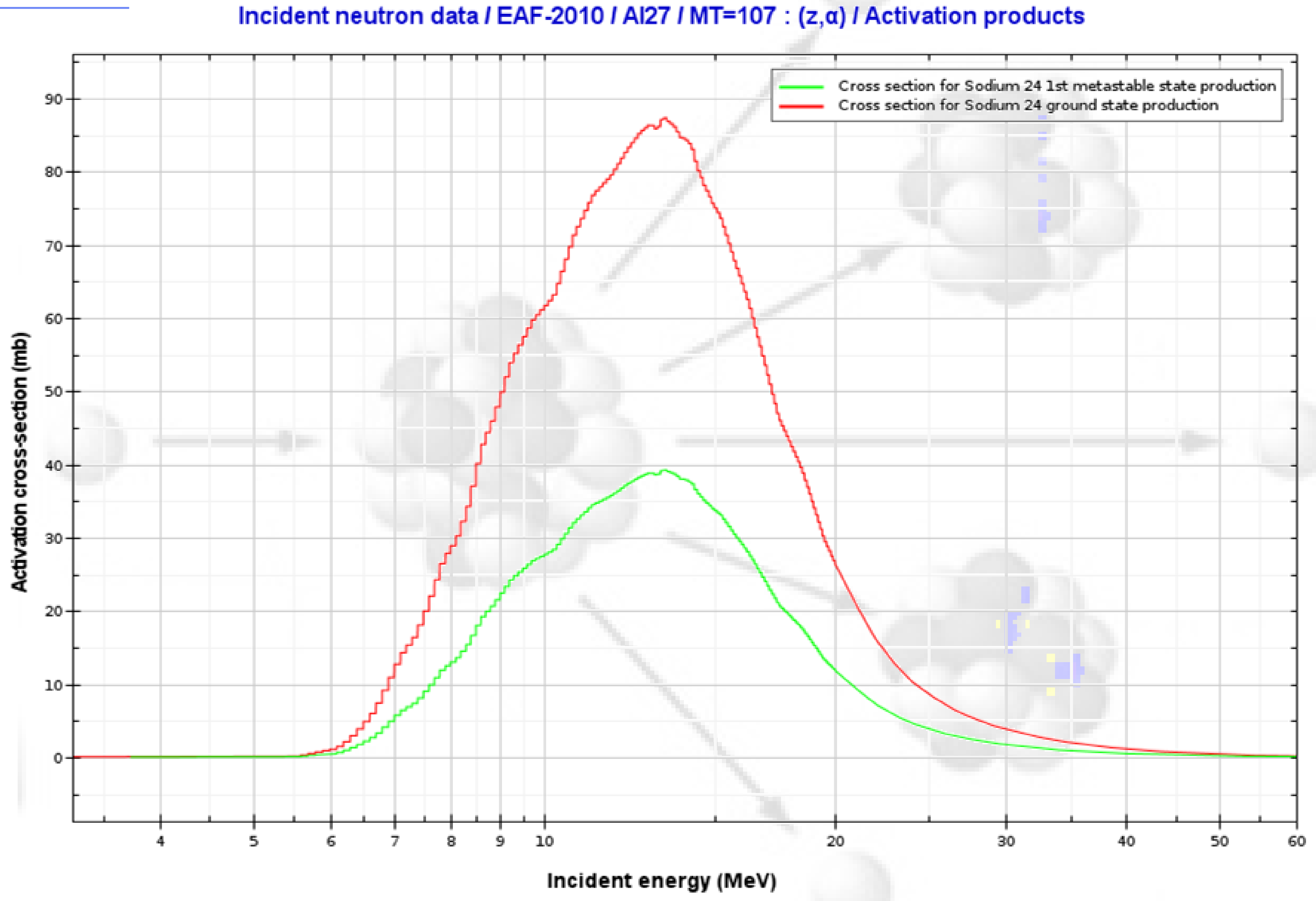
Cons (a lot…):

- ➢ Individual $\sigma(A,Z)$ hardly predicted much better than a factor ~1.5-2
- ➢ Issues with isomers
- ➢ Systematics hard to evaluate

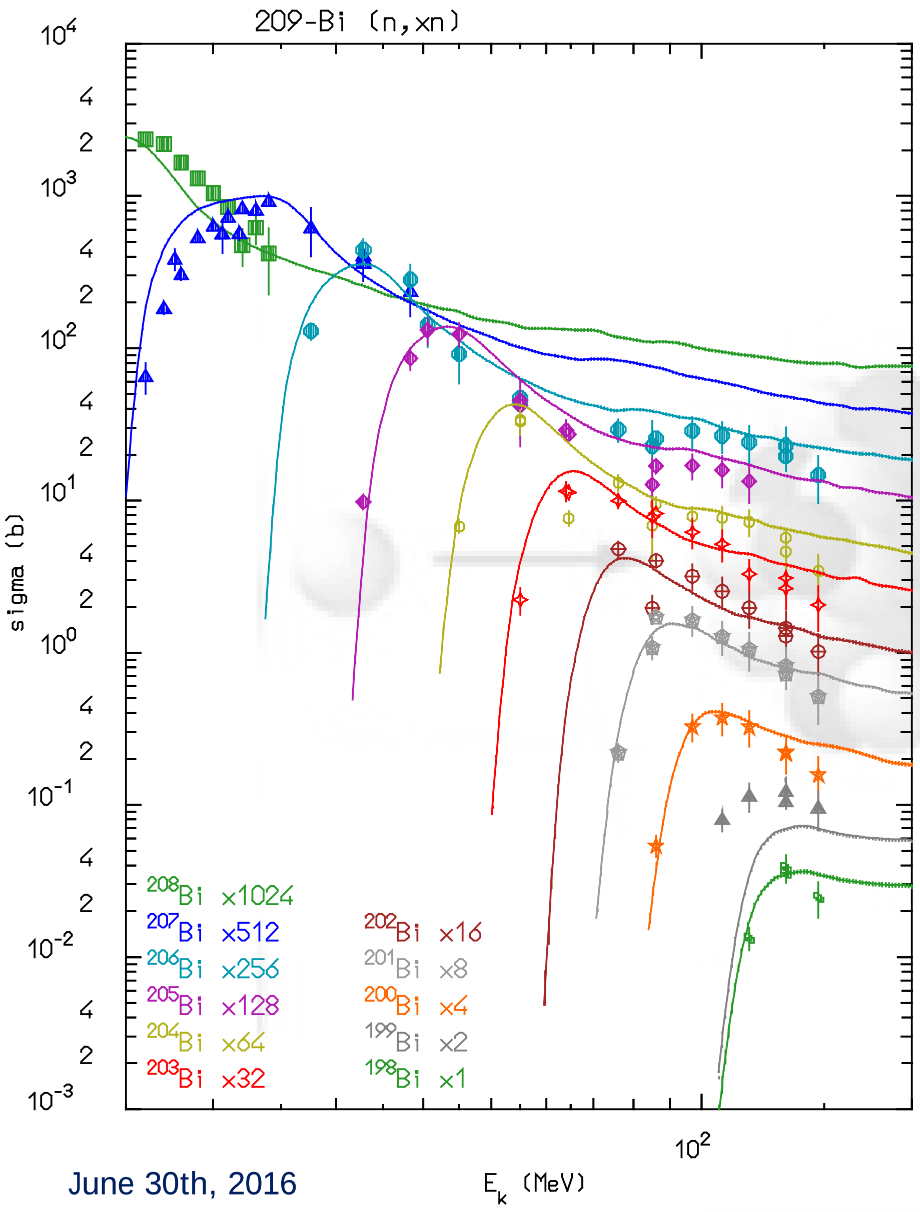
Activation cross section for folding (from EAF10): $^{113}In(n,n')^{113m}In$



Activation cross section for folding (from EAF10): $^{27}Al(n,\alpha)^{24m/24}Na$



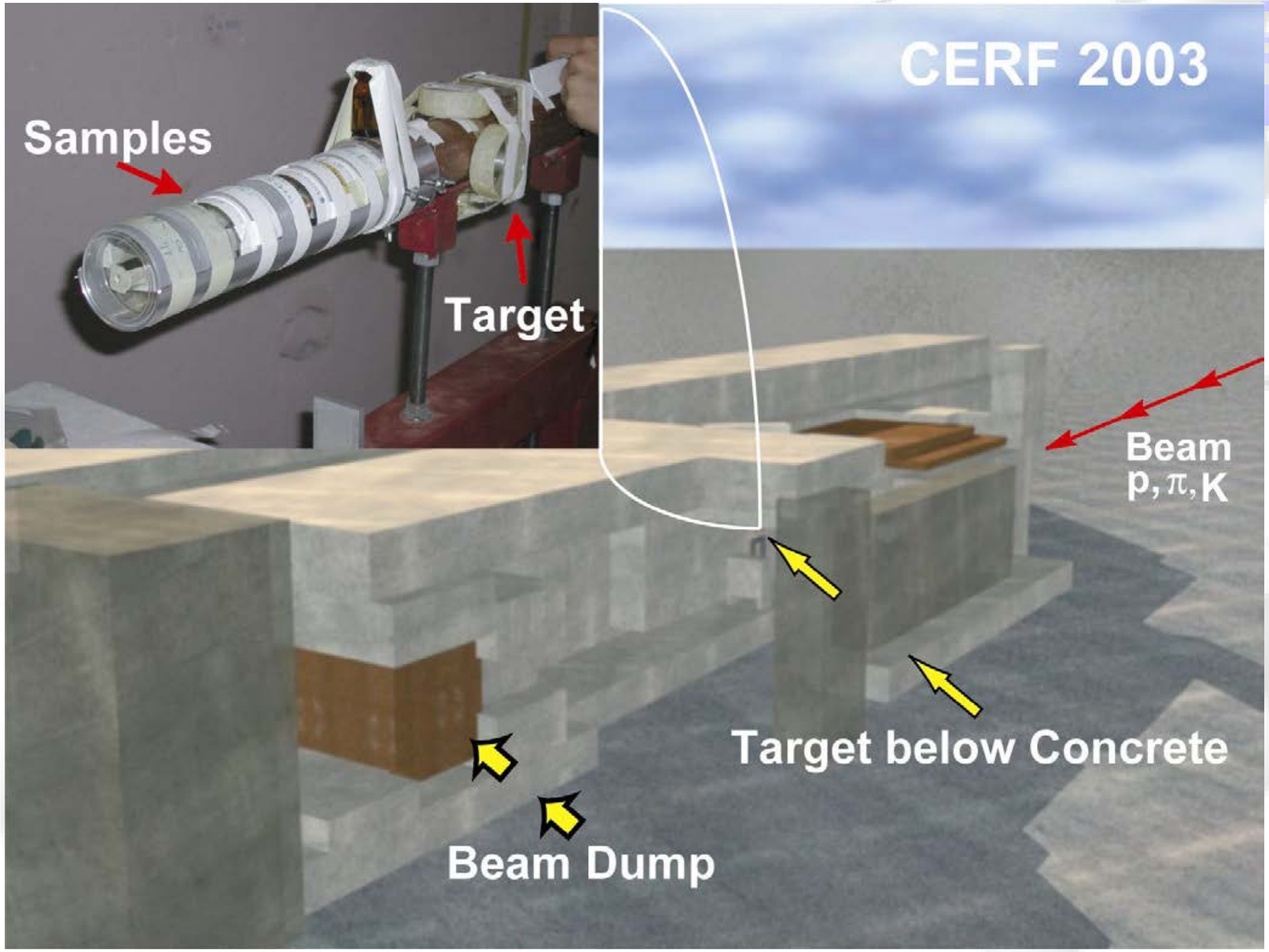
Isotope production for ^{209}Bi(n,xn):



Examples of computed isotope production versus exp.data: FLUKA (lines with dashing) vs exp. data (symbols).
Data: CSISRS database, NNDC
(Actually NSE129, 209, (1998))

These reactions have been proposed as suitable ~step-like reactions for detecting high energy neutrons

CERN-EU High-Energy Reference Field (CERF) facility



Location of Samples:

Behind a 50 cm long, 7 cm diameter copper target, centred with the beam axis
Beam: 120 GeV/c hadrons

Activation: Stainless Steel

Table 1: Stainless Steel, cooling times 1d 6h 28m, 17d 10h 39m

Isotope	$t_{1/2}$	Exp Bq/g	± %	OLD FLUKA/Exp	± %	FLUKA/Exp	± %
Be 7	53.29d	0.205	24	0.096	34	1.070	30
Na 24	14.96h	0.513	4.3	0.278	8.6	0.406	13
K 43	22.30h	1.08	4.6	0.628	8.7	0.814	11
Ca 47	4.54d	0.098	25	0.424	44	(0.295	62)
Sc 44	3.93h	13.8	4.8	0.692	5.8	0.622	6.2
mSc 44	58.60h	6.51	7.1	1.372	8.1	1.233	8.6
Sc 46	83.79d	0.873	8.3	0.841	9.1	0.859	9.5
Sc 47	80.28h	6.57	8.2	0.970	9.7	1.050	13
Sc 48	43.67h	1.57	5.2	1.266	8.4	1.403	11
V 48	15.97d	8.97	3.1	1.464	3.8	1.354	4.8
Cr 48	21.56h	0.584	6.7	1.084	11	1.032	12
Cr 51	27.70d	15.1	12	1.261	13	1.231	13
Mn 54	312.12d	2.85	10	1.061	10	1.060	11
Co 55	17.53h	1.04	4.6	1.112	7.7	0.980	10
Co 56	77.27d	0.485	7.6	1.422	9.0	1.332	10
Co 57	271.79d	0.463	11	1.180	12	1.140	12
Co 58	70.82d	2.21	5.9	0.930	6.3	0.881	6.9
Ni 57	35.60h	3.52	4.5	1.477	6.5	1.412	8.2

M. Brugger, *et al.*, Proceedings of the Int. Conf. on Accelerator Applications (AccApp'05), Venice, Italy, 2005

Simulations for fission detectors:

Folding with known cross sections:

- Standard method for low energies and/or known isotopes/cross section
- Not available for not yet measured isotopes

Computing directly fission cross sections from models

- Last resort if no exp. cross section known (eg high energies, "exotic" projectiles…)
- Obvious uncertainties related to model use

A few important remarks:

- Just above the Coulomb barrier fission is available also for p, π^+ (even at rest for π^-)
- Above a few tens of MeV fission progressively opens also for Bi, Pb, Au, W, Ta…
- … and with increasing energy it becomes less and less well defined wrt nuclear fragmentation

Simulati…

Folding with … …ly fission cross … …dels

- Standar… and/or k… …exp. cross section known … "exotic" projectiles…)
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A fe…
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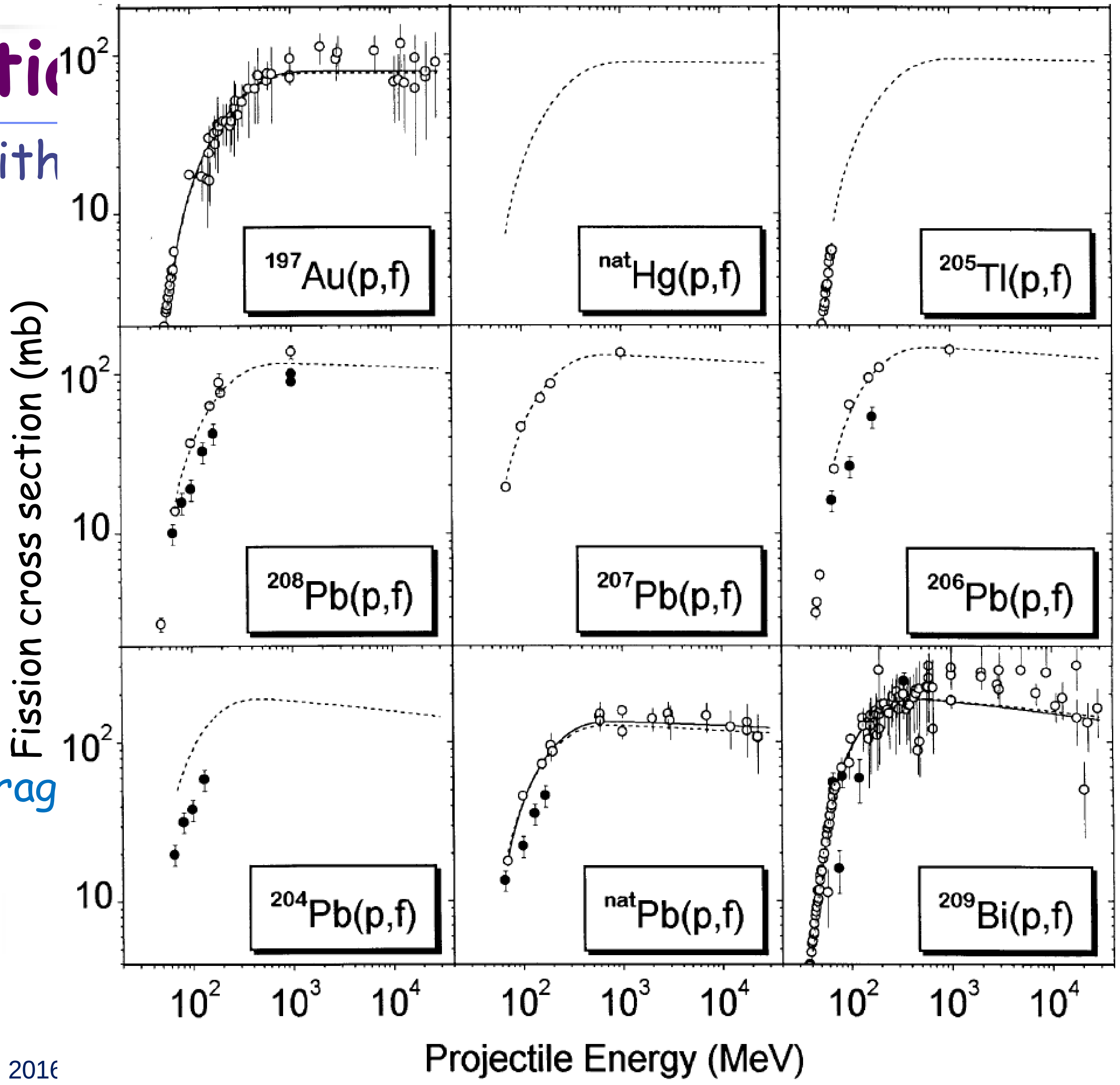

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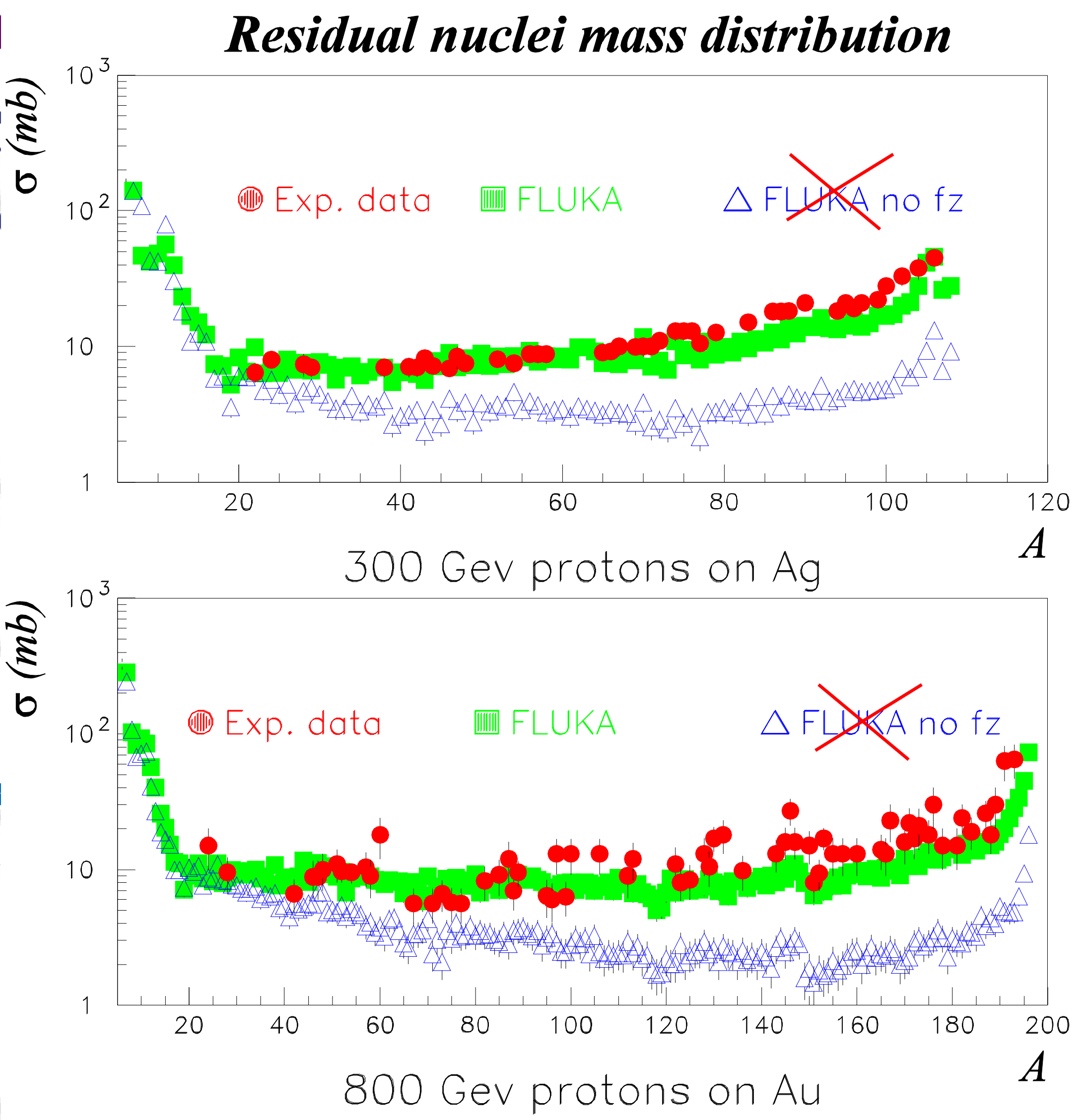

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*However when explicit **generation** and **transport** of the **fission fragments (FF)** for E_n in the evaluated data file range is required (eg fission/alpha discrimination etc) **ad-hoc models** must be developed, since the evaluated data files only contain the **uncorrelated FF yields** for each A/Z , also codes suitable for **low energy heavy ion transport** should be used*

Capture measurements/detectors:

Capture gamma cascades are not correlated in the evaluated nuclear data files

- Standard MC codes are not able to produce correlated gamma cascades for capture, except for a few "hand-written" cases, however ***statistical gamma cascade*** models can/should be used for the continuum/unresolved part of the spectrum
- $\rightarrow$ if photon-to-photon correlations are important for the capture detector/experiment under consideration, an ad-hoc model must be built and implemented (eg combining known discrete transitions with statistical model generated continuum)

Possible detectors:

- Ge or similar spectroscopy
- C_6D_6 "total" energy measurements
- 4π calorimeters

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No further comments, Peter tomorrow will nicely explain how they work!

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Possible detecto

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- C_6D_6 "total" energy measurements
- 4π calorimeters

In order to compute reliably response functions (particularly critical for C_6D_6) Monte Carlo with precise EM physics are required (many! EGSnrc, FLUKA, GEANT4, MCNP, PENELOPE…)

Example of statistical γ de-exc. models:

Z. Phys. C 71, 75–86 (1996)

The production of residual nuclei in peripheral high energy nucleus-nucleus interactions

A. Ferrari[1], J. Ranft[2], S. Roesler[3], P.R. Sala[1]

[1] INFN, Sezione di Milano, Via Celoria 16, I-20133 Milano, Italy
[2] Departamento de Fisica de Particulas, Universidade de Santiago de Compostela, E-15706 Santiago de Compostela, Spain
[3] Universität Siegen, Fachbereich Physik, D-57068 Siegen, Germany

Received: 9 March 1996

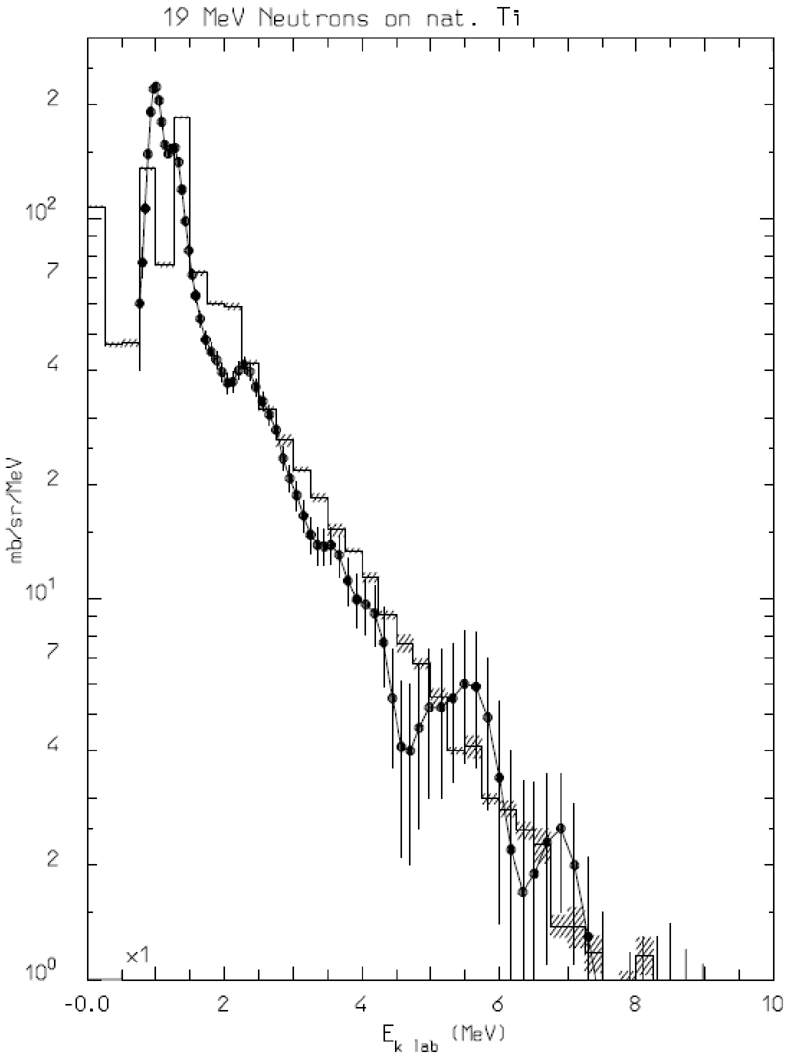

Fig. 1. Photon spectrum resulting from the reaction Ti(n,x) at 19 MeV. The dashed histogram represents PEANUT results with errors. Dots are experimental data from [34]

Example of statistical γ de-exc. models:

Z. Phys. C 71, 75–86 (1996)

The production
in peripheral hi

A. Ferrari[1], J. Ranft[2], S. Ro

[1] INFN, Sezione di Milano, Via Ce
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[3] Universität Siegen, Fachbereich F

Received: 9 March 1996

19 MeV Neutrons on nat. Ti

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Nuclear Instruments and Methods in Physics Research A 417 (1998) 434–449

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH
Section A

Dicebox

Simulation of γ cascades in complex nuclei with emphasis on assessment of uncertainties of cascade-related quantities

F. Bečvář[a,b,*]

[a] *Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, CZ-180 00 Prague 8, Czech Republic*
[b] *Institut Laue-Langevin, F-38042 Grenoble, France*

Received 24 March 1998; received in revised form 26 June 1998

Abstract

A new simulation of nuclear γ cascades by the Monte Carlo method is described. It makes it possible to generate artificially individual events of the γ-cascade decay of an isolated, highly excited initial level in a medium and heavy nucleus. A broad class of quantities, associated with the process of γ-cascade de-excitation, can be modelled. The main

10

x) at 19 MeV.
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Example of statistical γ de-exc. models:

Z. Phys. C 71, 75–86 (1996)

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Received: 9 March 1996

Dicebox

Simulatio
assessm

[a] *Faculty of M*

Abstract

A new simulation
artificially individual
nucleus. A broad clas

19 MeV Neutrons on nat. Ti

Nuclear Instruments and Methods in Physics Research B 325 (2014) 35–42

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

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BEAM INTERACTIONS WITH MATERIALS AND ATOMS

Development of gamma de-excitation model for prediction of prompt gamma-rays and isomer production based on energy-dependent level structure treatment

CrossMark

T. Ogawa[a,*], S. Hashimoto[a], T. Sato[a], K. Niita[b]

[a] *Research Group for Radiation Protection, Division of Environment and Radiation Sciences, Nuclear Science and Engineering Directorate, Japan Atomic Energy Agency, Shirakata-Shirane, Tokai, Ibaraki 319-1195, Japan*
[b] *Research Organization for Information Science and Technology, Shirakata-shirane, Tokai, Ibaraki 319-1188, Japan*

ARTICLE INFO

Article history:
Received 16 July 2013
Received in revised form 4 February 2014
Available online 3 March 2014

Keywords:
Prompt gamma-rays
Isomers
De-excitation
Total angular momenta
Parity
Excitation energy

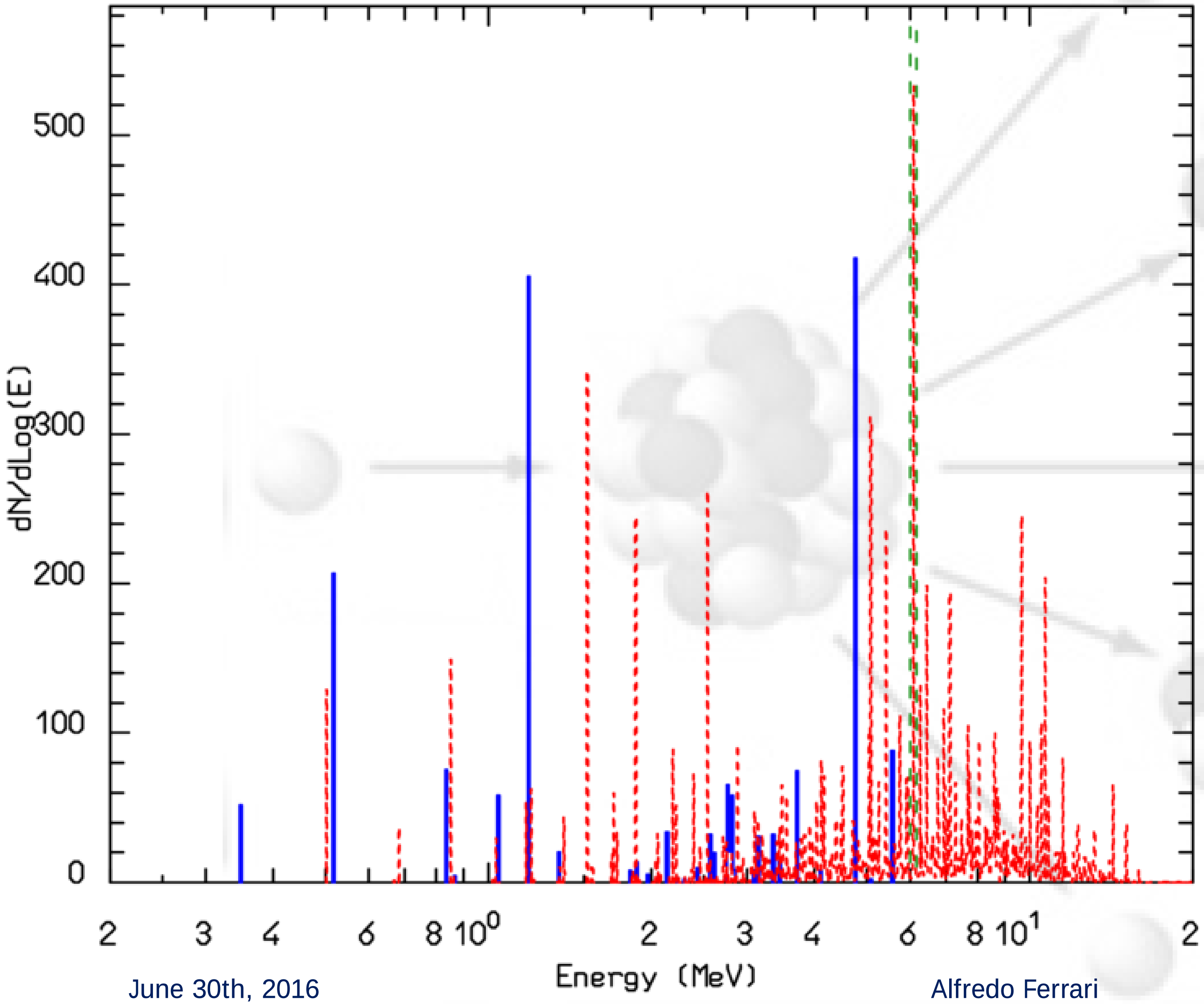
ABSTRACT

A new theoretical model to simulate gamma de-excitation of excited nuclei, EBITEM (ENSDF-Based Isomeric Transition and isomEr production Model), is developed based on the Evaluated Nuclear Structure Data File (ENSDF), supplementary evaluated data tables, and theories. In the model, reaction products after nucleon evaporation were de-excited by using theoretical calculations if the excitation energy was higher than 3000 keV and the mass number was greater than 40 amu. Otherwise, the nuclei were de-excited based on the scheme provided in the ENSDF. Thus by tracking nuclear de-excitation, production of prompt gamma-rays and isomers was simulated.

The model is applicable for neutron capture products and spallation products of 1071 nuclear species from Li to Bk. Except for some of the light nuclei with discrete level structure, simulated isomer production and prompt gamma-ray spectra agree generally within 40% and a factor of 3, respectively.

experimental data from [34]

(Un)correlated capture γ cascades: $^{40}Ar(n,\gamma)^{41}Ar$

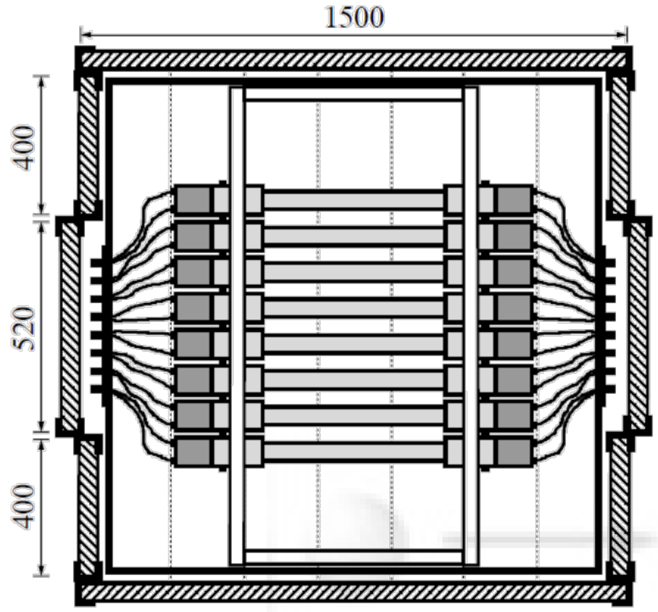


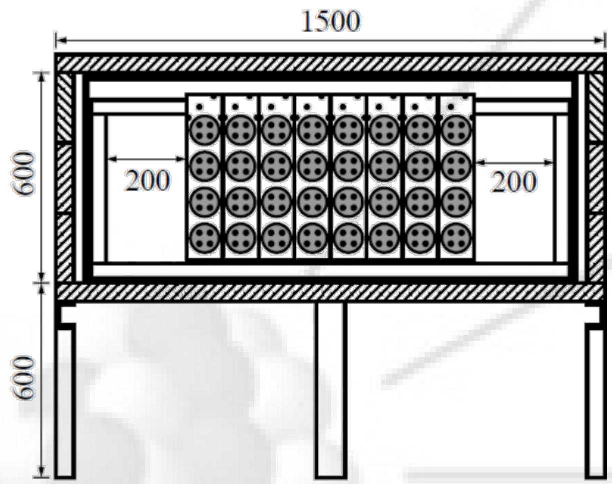
Liquid Argon experiment are popular for neutrino physics. Icarus @LNGS was supposed to measure also solar ν's and the main background was neutron capture by ^{40}Ar

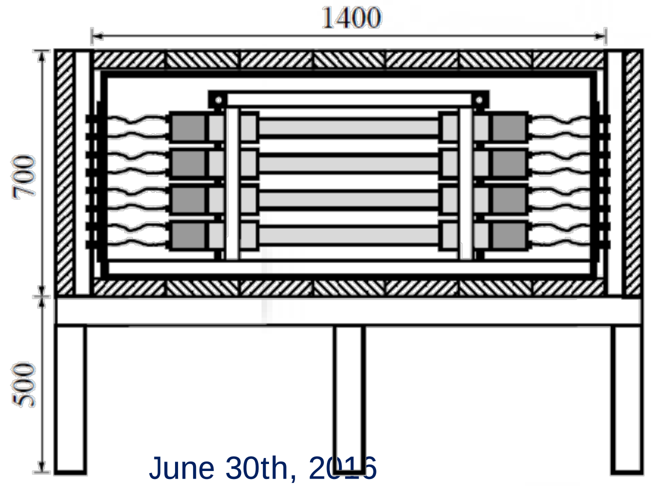
$^{40}Ar(n,\gamma)^{41}Ar$:

- Capture γ spectrum
- Q for corr. cascades (6.10 MeV)
- Q distribution for uncorr. cascades

Background neutron detector for LNGS



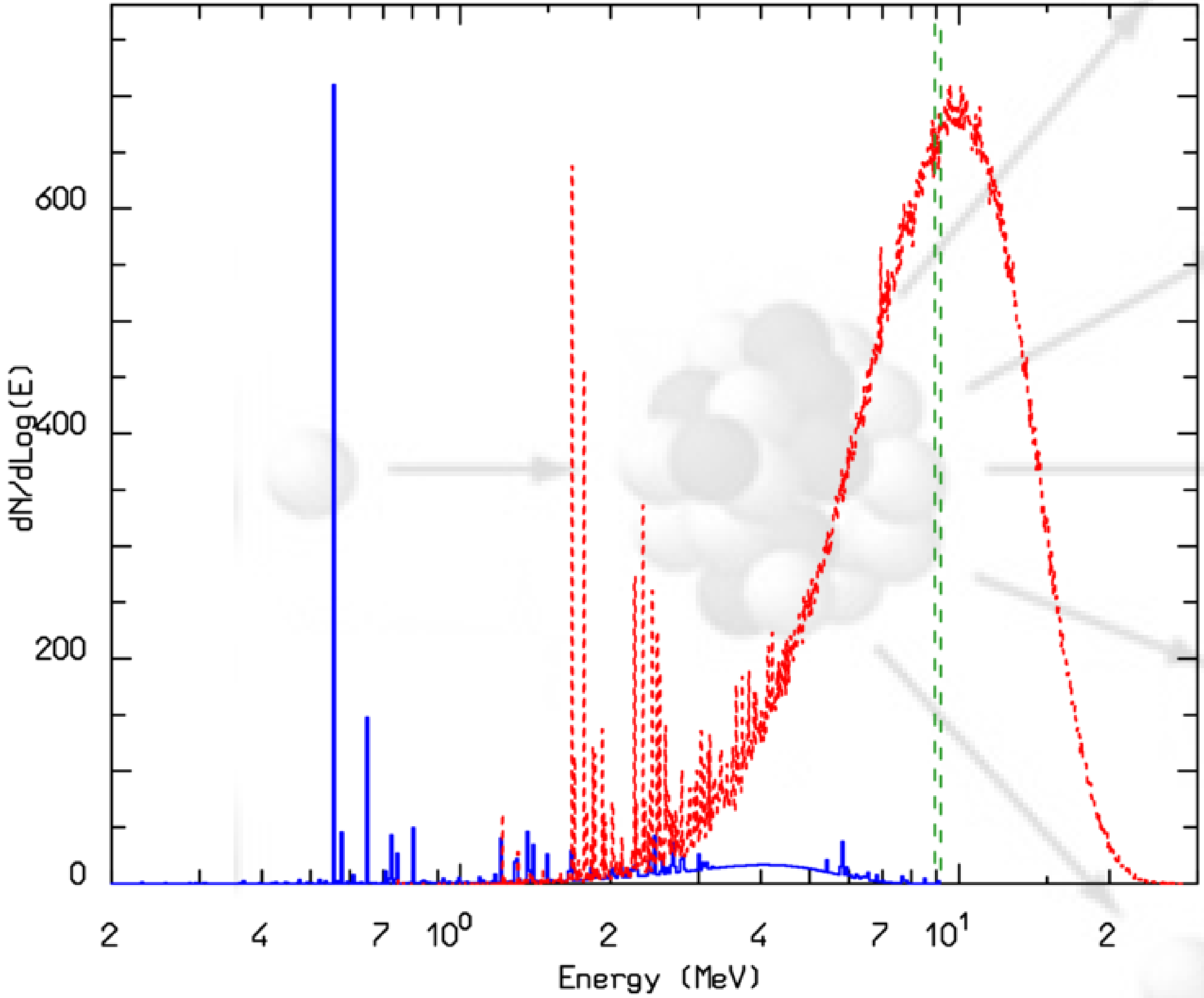




The neutron ***background*** at LNGS is ***very weak*** (~0.5 10^{-6} $cm^{-2}s^{-1}$, E > 1MeV), while the γ one is "normal" $\rightarrow$ a very large discrimination required. Achieved by using 32, 1 liter, liquid scintillator (BC501A) detectors, each one wrapped in Cadmium, and using both PSD and delayed coincidence of the fast neutron proton recoils with capture γ's $\rightarrow$ then unfolding

Efficiency vs energy completely dependent on simulations $\rightarrow$ development of an ad hoc nuclear model for correlated emission of Cd capture γ's

(Un)correlated capture γ cascades: $^{113}Cd(n,\gamma)^{114}Cd$



$^{113}Cd(n,\gamma)^{114}Cd$:

- Capture γ spectrum
- Q for corr. cascades (9.03 MeV)
- Q distribution for uncorr. cascades

General purpose MC codes:

EM + HAD codes:

- FLUKA: http://www.fluka.org
  - coupled HAD+EM+A. 1 keV – 100000 TeV EM, 0-10000 TeV HAD
  - Language: Fortran. Systems: Linux/Unix/Windows (virtual machine)
- GEANT4: http://geant4.web.cern.ch/geant4
  - coupled HAD+EM+A.
  - Language: C++. Systems: Linux/Unix/Windows/MAC
- MARS: http://www-ap.fnal.gov/MARS
  - coupled HAD+EM+A. 1 keV – 100 TeV EM, 0-100 TeV HAD
  - Language: Fortran.
- MCNP(6/x): http://mcnp(x).lanl.gov/
  - "nearly all particles, nearly all energies"
  - Language: Fortran90. Systems: Linux/Unix/Windows
- PHITS: http://phits.jaea.go.jp/
  - coupled hadronic+EM+A. 1 keV – 1 GeV EM, 0-200 GeV HAD
  - Language: Fortran
- …

Statistical Uncertainties:

- Can be calculated for single histories, or for batches of several histories each
- Distribution of scoring contributions by single histories can be very asymmetric (many histories contribute little or zero)
- Scoring distribution from batches tends to be Gaussian for $N \rightarrow \infty$, provided $\sigma^2 \neq \infty$ (thanks to Central Limit Theorem)
- The standard deviation of an estimator calculated from batches or from single histories is a (stochastic) estimate of the standard deviation of the actual distribution ("error of the mean")
- How good is such an estimate depends on the type of estimator and on the particular problem (but it converges to the true value for $N \rightarrow \infty$)

Statistical Uncertainty (batch statistics):

The variance of the mean of an estimated quantity *x* (e.g., fluence), calculated out of *N* batches, is:

$$\sigma^2_{<x>} = \frac{1}{N-1}\left[\frac{1}{n}\sum_{i=1}^{N} n_i x_i^2 - \frac{1}{n^2}\left(\sum_{i=1}^{N} n_i x_i\right)^2\right]$$

where:

- n_i is the number of histories in the i^{th} batch
- $n = \sum n_i$ is the total number of histories in the N batches
- x_i is the average of x calculated in the i^{th} batch: $x_i = \sum_{j=1}^{n_i} x_{ij} / n_i$ where x_{ij} is the contribution to x of the j^{th} history in the i^{th} batch
- In the limit $N = n$, $n_i = 1$, the formula applies to single history statistics

Reduce variance or CPU time ?

Computer cost:

A Figure of Merit

Computer cost of an estimator $= \sigma^2 \cdot t$

(σ^2 = Variance, t = CPU time)

- Some biasing techniques are aiming at reducing σ^2, others at reducing t
- Often reducing σ^2 increases t and viceversa
- Therefore minimizing $\sigma^2 \cdot t$ means reducing σ at a faster rate than t increases or *viceversa*
- ⇒The choice depends on the problems, and sometimes the combination of several techniques is the most effective
- Bad judgment, or excessive "forcing" on one of the two variables, can have catastrophic consequences on the other one, making computer cost "explode"

σ^2 is converging like 1/N, while t is obviously proportional to N

Statistical uncertainties, systematic errors, and... mistakes

Statistical uncertainties, due to sampling (in)efficiency

Relative error	Quality of Estimator/Tally *(from an old version of the MCNP Manual)*
50 to 100%	Garbage
20 to 50%	Factor of a few
10 to 20	Questionable
< 10%	Generally reliable

- Why does a 30% σ mean an uncertainty of a "factor of a few"?
  Because σ in fact corresponds to the sum (in quadrature) of two uncertainties: one due to the fraction of histories which don't give a zero contribution, and one which reflects the spread of the non-zero contributions, and anyway it cannot exceeds 100% by construction
  Further, σ is itself a stochastic variable, usually harder to converge than the mean
- The MCNP guideline is empirically based on experience, not on a mathematical proof. But it has been generally confirmed to work well in practical experience
- Small penetrations and cracks are very difficult to handle by MC, because the "detector" is too small and too few non-zero contributions can be sampled, even by biasing

Statistical uncertainties, systematic errors, and... mistakes

Systematic errors, due to code weaknesses

Apart from the statistical uncertainties, which other factors affect the accuracy of MC results?

- physics: different codes are based on different physics models/data. Some models/data are better than others. Some models are better in a certain energy range. Model quality is best shown by benchmarks at the microscopic level (e.g. thin targets)
- artifacts: due to imperfect algorithms, e.g., energy deposited in the middle of a step, inaccurate path length correction for multiple scattering, missing correction for cross section and *dE/dx* change over a step, etc. Algorithm quality is best shown by benchmarks at the macroscopic level (thick targets, complex geometries)
- data uncertainty: an error of 10% in the absorption cross section can lead to an error of a factor 2.8 in the effectiveness of a thick shielding wall (10 attenuation lengths). Results can never be better than allowed by available experimental/evaluated/model data!

Statistical uncertainties, systematic errors, and... mistakes

Systematic errors, due to user ignorance

- Missing information:
  - ***material composition*** not always well known. In particular concrete/soil /steel composition (how much water content/Co? Can be critical for backgrounds)
  - ***beam losses***: most of the time these can only be guessed. Close interaction with engineers and designers is needed
  - Presence of ***additional material***, not well defined (cables, supports, surrounding environment...)
  - Is it worth to do a very detailed simulation when some parameters are unknown or badly known?

Systematic errors, due to simplification

- Geometries that cannot be reproduced exactly (or would require too much effort)
- Air contains humidity and pollutants, has a density variable with pressure

Statistical uncertainties, systematic errors, and... mistakes

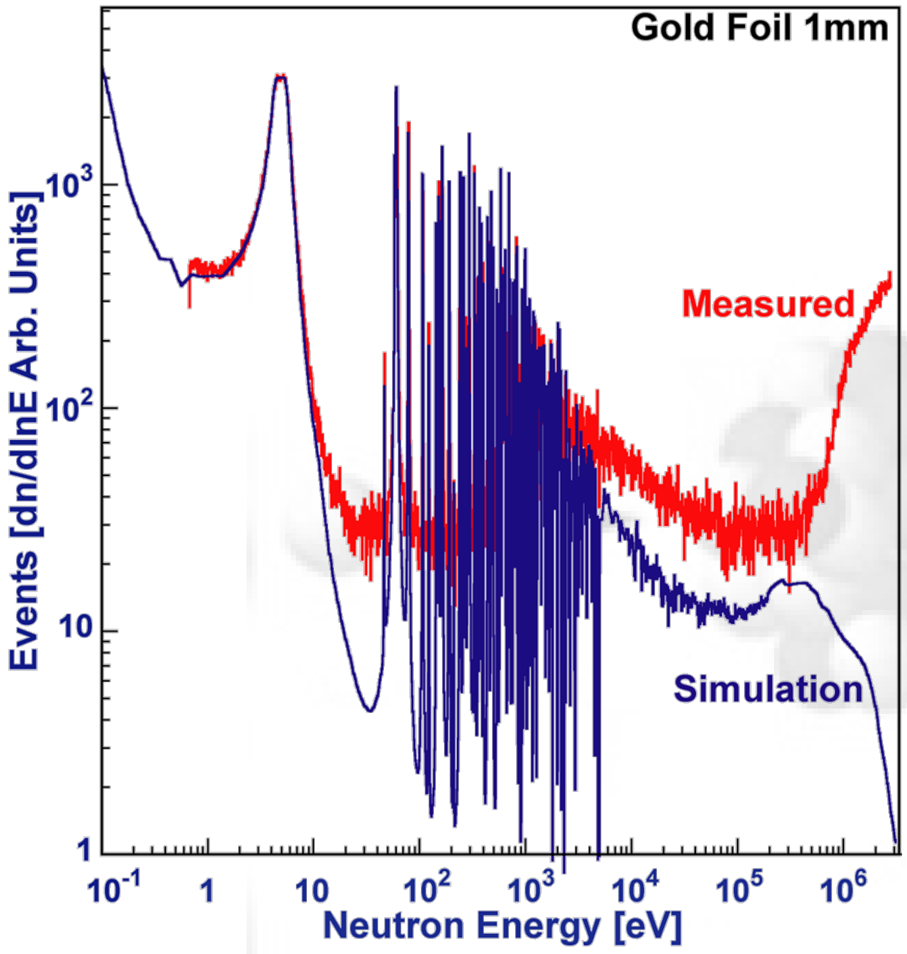
Code mistakes ("bugs")

- MC codes can contain bugs:
  - Physics bugs: I have seen pair production cross sections fitted by a polynomial... and oscillating instead of saturating at high energies, non-uniform azimuthal scattering distributions, energy non-conservation, A < 0 residuals...
  - Programming bugs (as in every other software, of course)

User mistakes

- Errors in the input: cross section choice, $S(\alpha,\beta)$, temperature, models, geometry, … check again and again, it is your final responsibility
- error in user code: use code built-in features as much as possible!
- wrong units
- wrong normalization: quite common and very dramatic!
- unfair biasing: energy/space cuts cannot be avoided, but must be done with much care
- forgetting to check what is available, eg γ production, in the neutron cross sections (e.g. Sb cross sections before)

n_TOF: background June 2001



For more info: CERN/INTC 2001-038

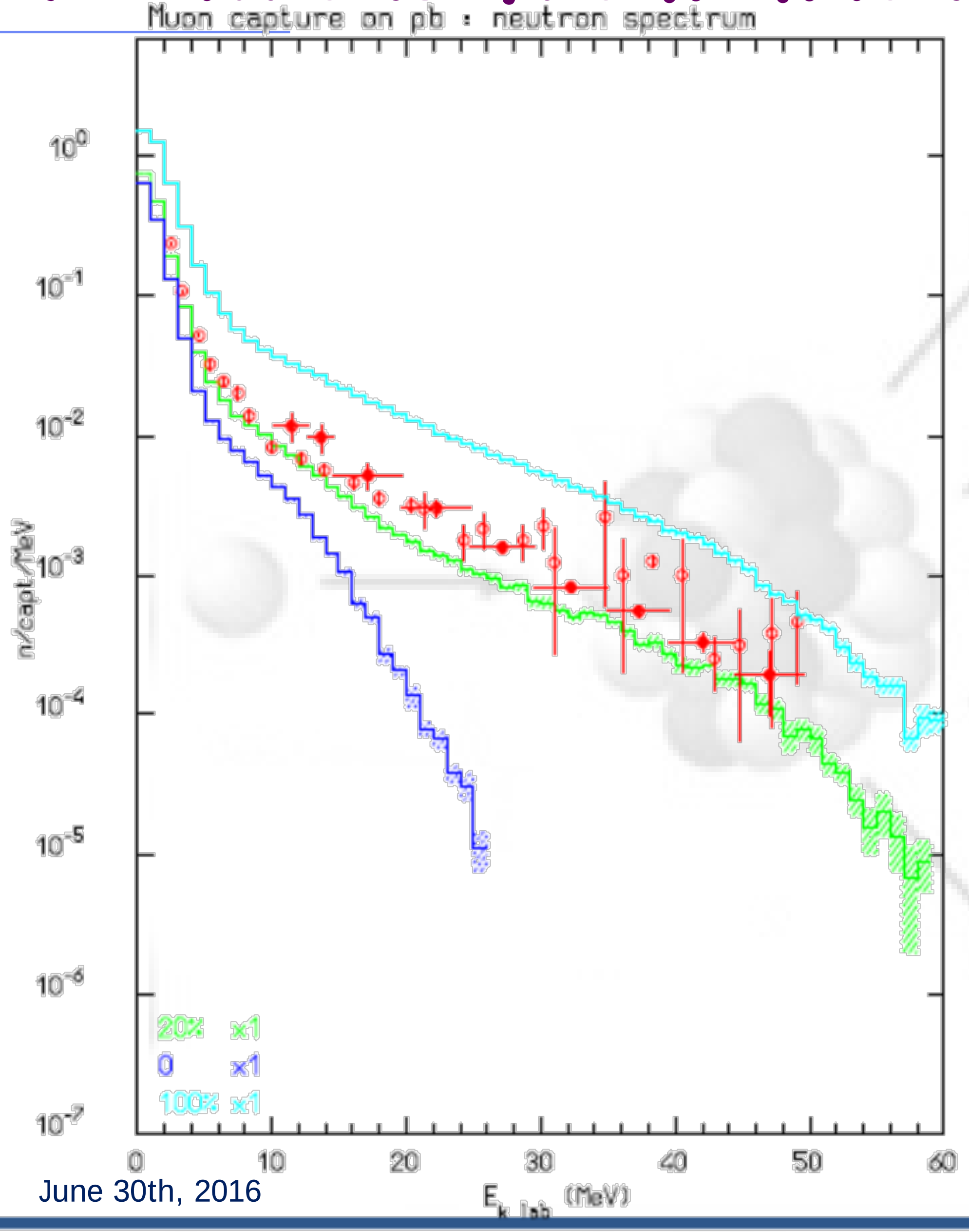
Background Features

- ×50 larger than simulations
- Three time components
  - 400 ns "flash"
  - 20 μs – fast neutrons
  - > 16 ms – thermal neutrons
- Position dependent
- Strong Left-Right asymmetry
- Strong ionization signal
- TLD's scored a signal probably muons
- Not sample related

Possible Sources

- Elements in the neutron Tube
  - Collimators
  - Escape line
- Insufficient concrete shielding in the exp. area
- Charged particles deflected from the magnet
- High energy neutrons leaking from the target area
- *Negative muon capture*
- …

Neutrons from muon capture



Neutron spectra following muon capture on Lead

Dots: experimental data histograms: FLUKA calculations

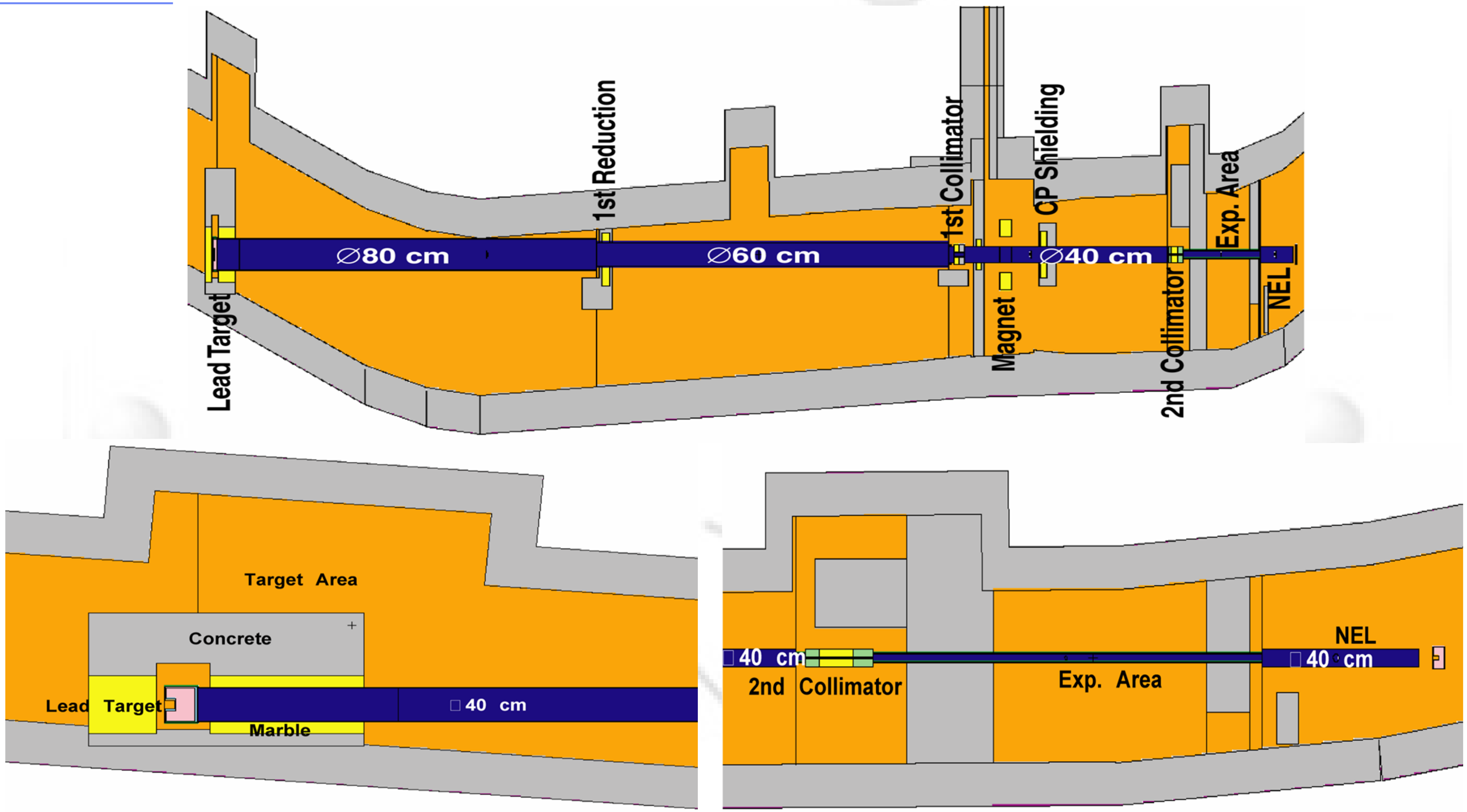
The three curves correspond to a percentage of 2-body absorption of 0, 20%, and 100% .

Emitted:

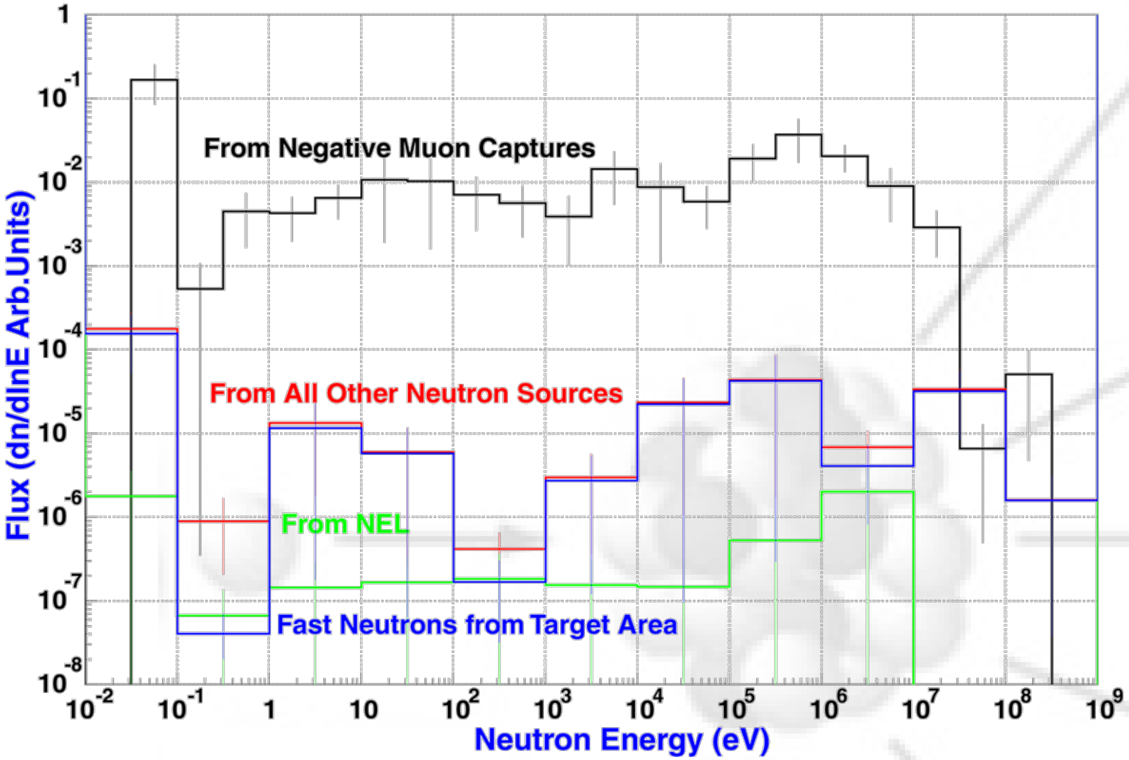
1.7 neutrons/capture

0.002 protons/capture

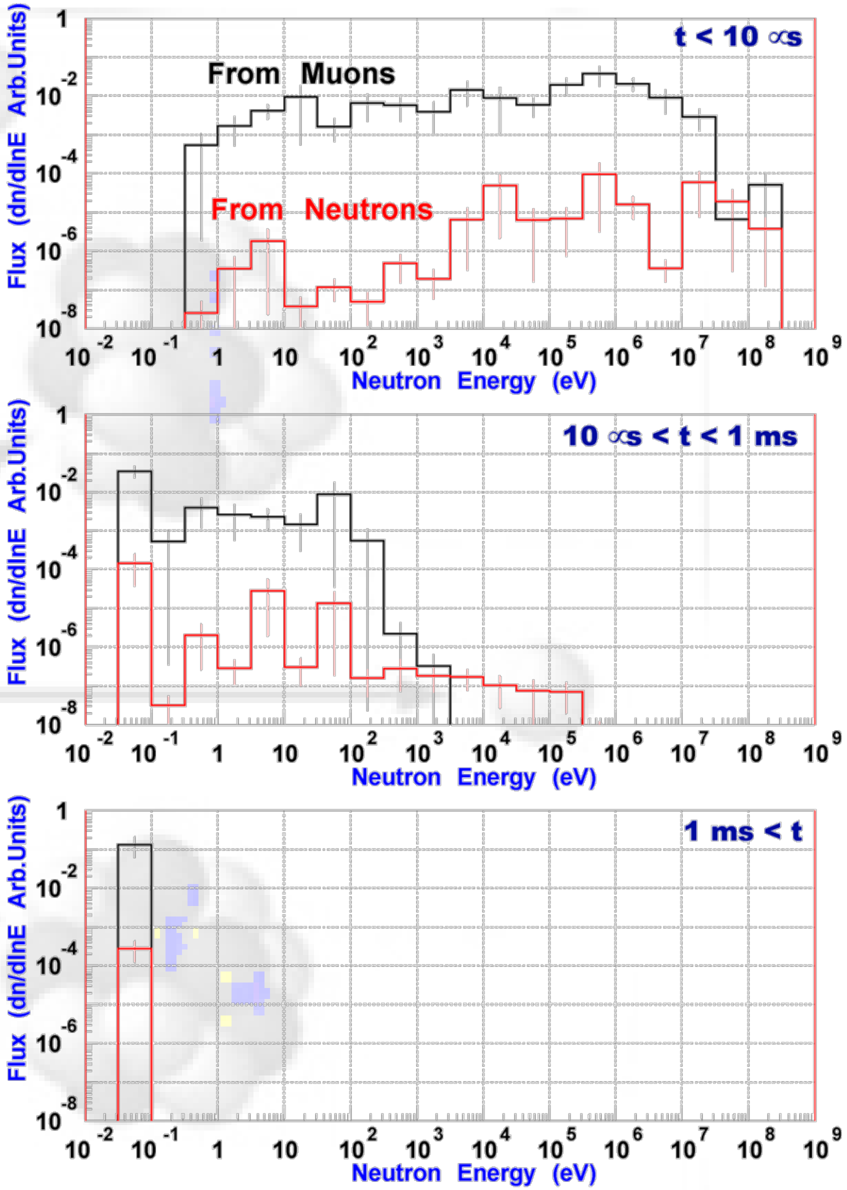
n_ToF Tunnel Geometry



Neutron Fluence in EAR



Neutron Fluence in the experimental area divided into the various sources



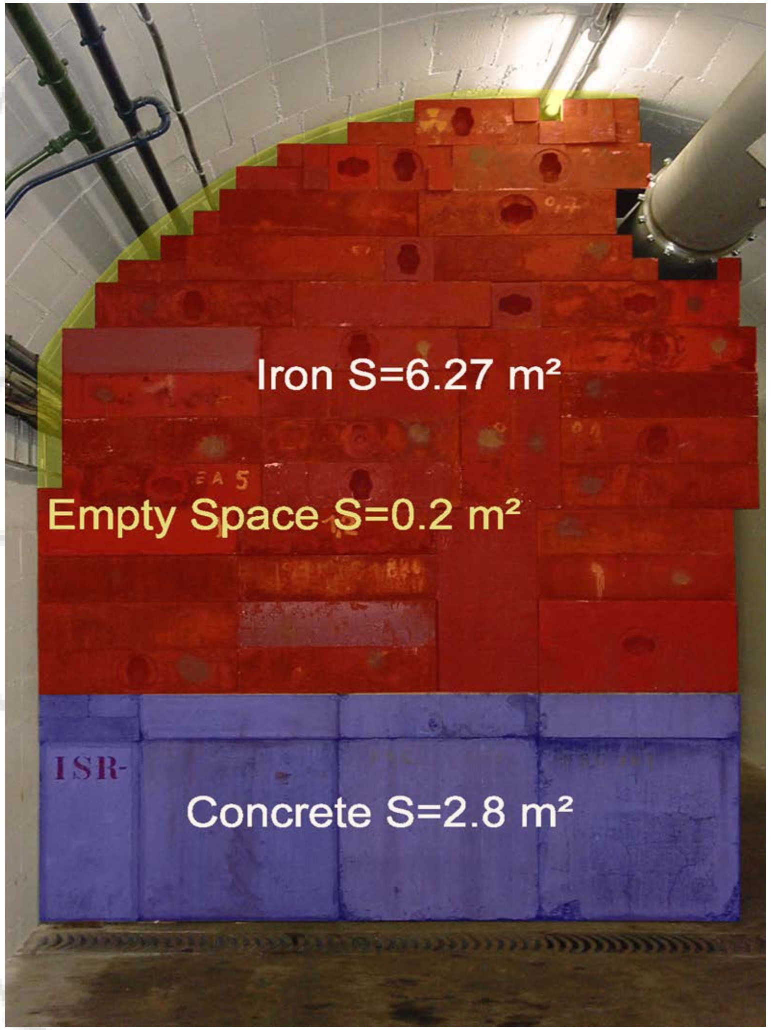
Neutron Fluence in the experimental area for a some time windows

We reconstructed these plots from the TAG information that was associating each particle that entered in the experimental area.

The 3m Iron Wall

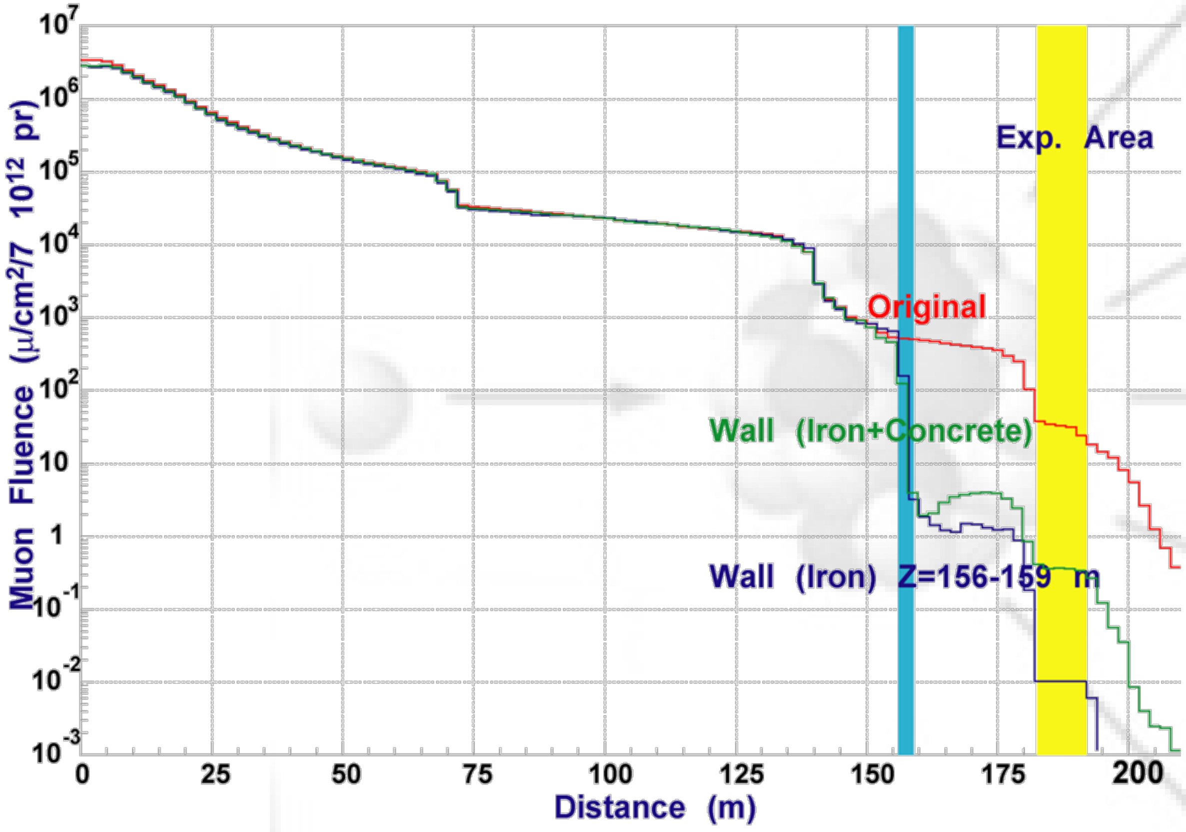
- The simulation results have clearly demonstrated the ineffectiveness of a possible wall close to the target area:
  - 50% of parent pions are still in the tube at the exit of the target shielding
  - 10% of muons/parent pions are still in the tube as far as 60 m from the target
- Therefore a suitable shielding should be located where the fraction of muons/pions in the pipe is minimal or just after the sweeping magnet

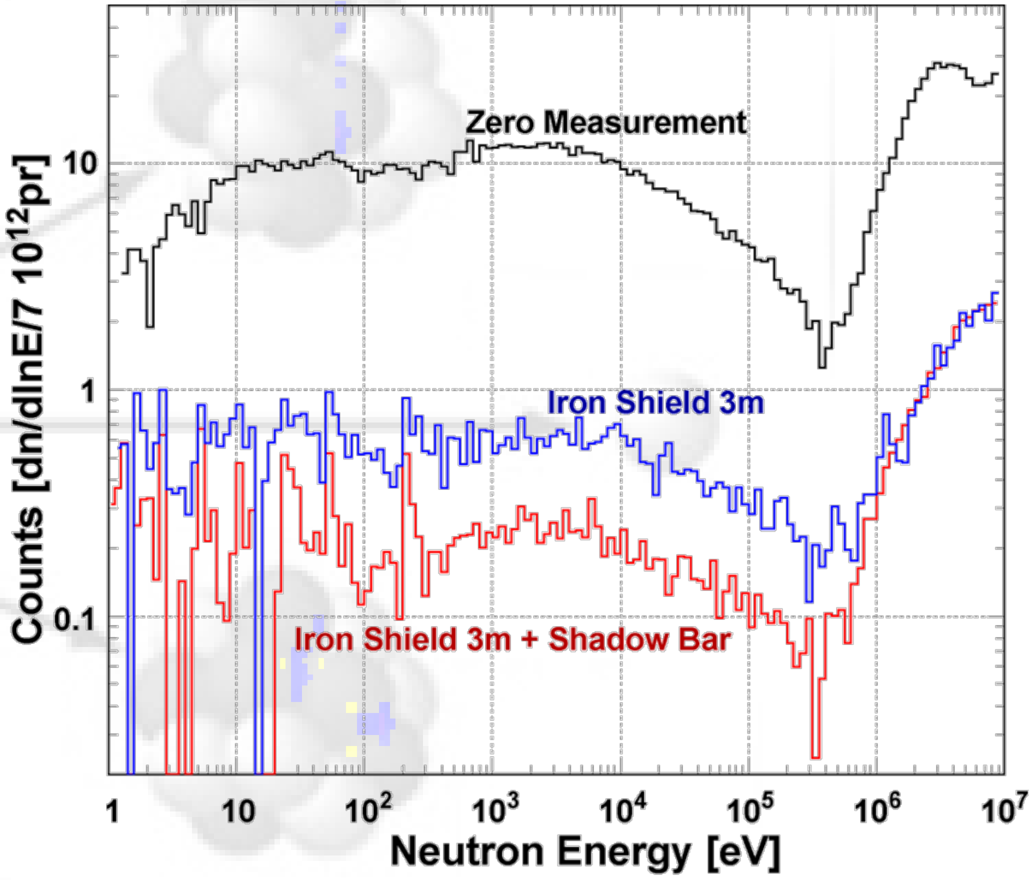
3 m of Iron will lower the muon energy by 3.5 GeV



The 3 m long Iron wall

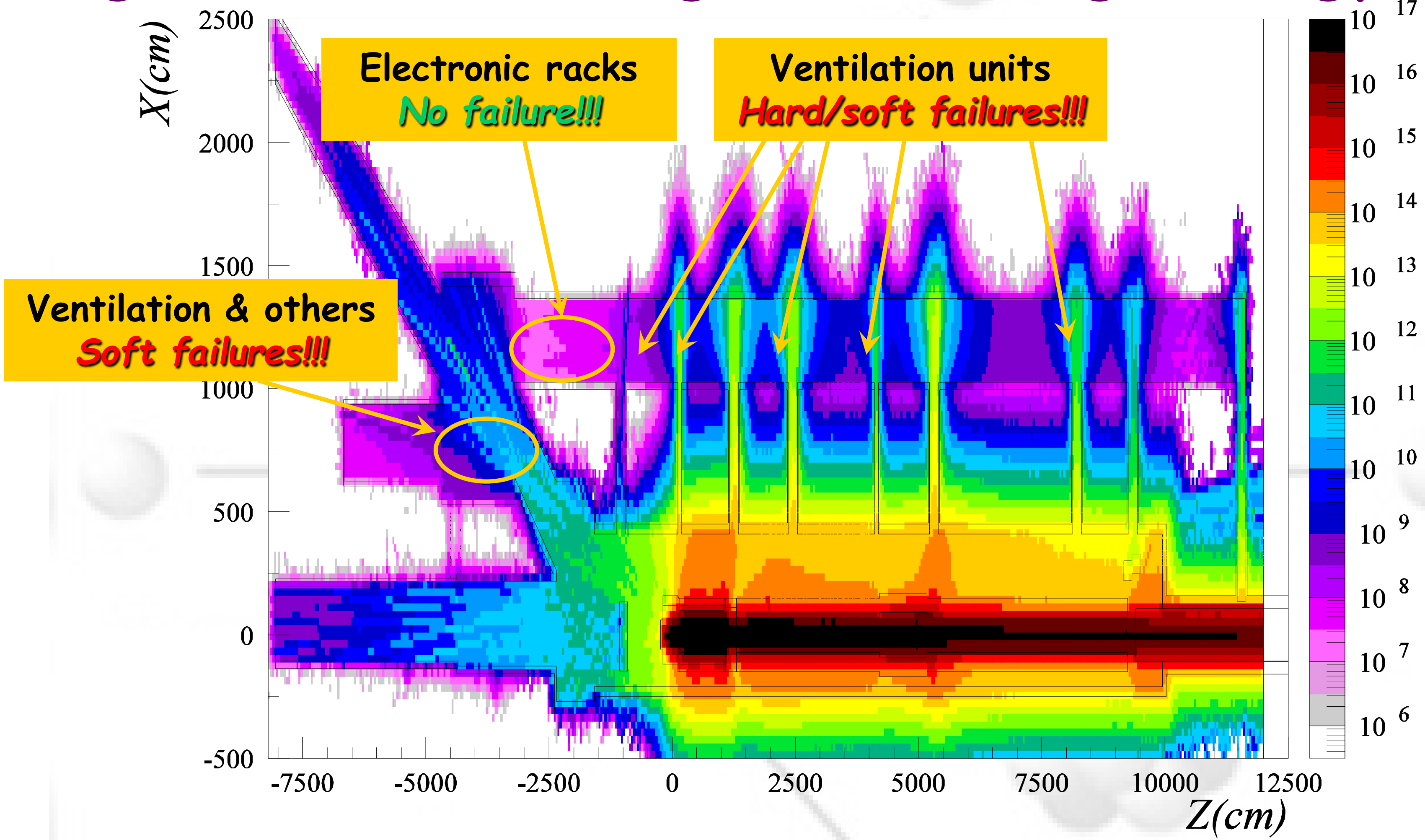
Muon & Neutron Fluence Attenuation





C_6D_6 raw data with various setups

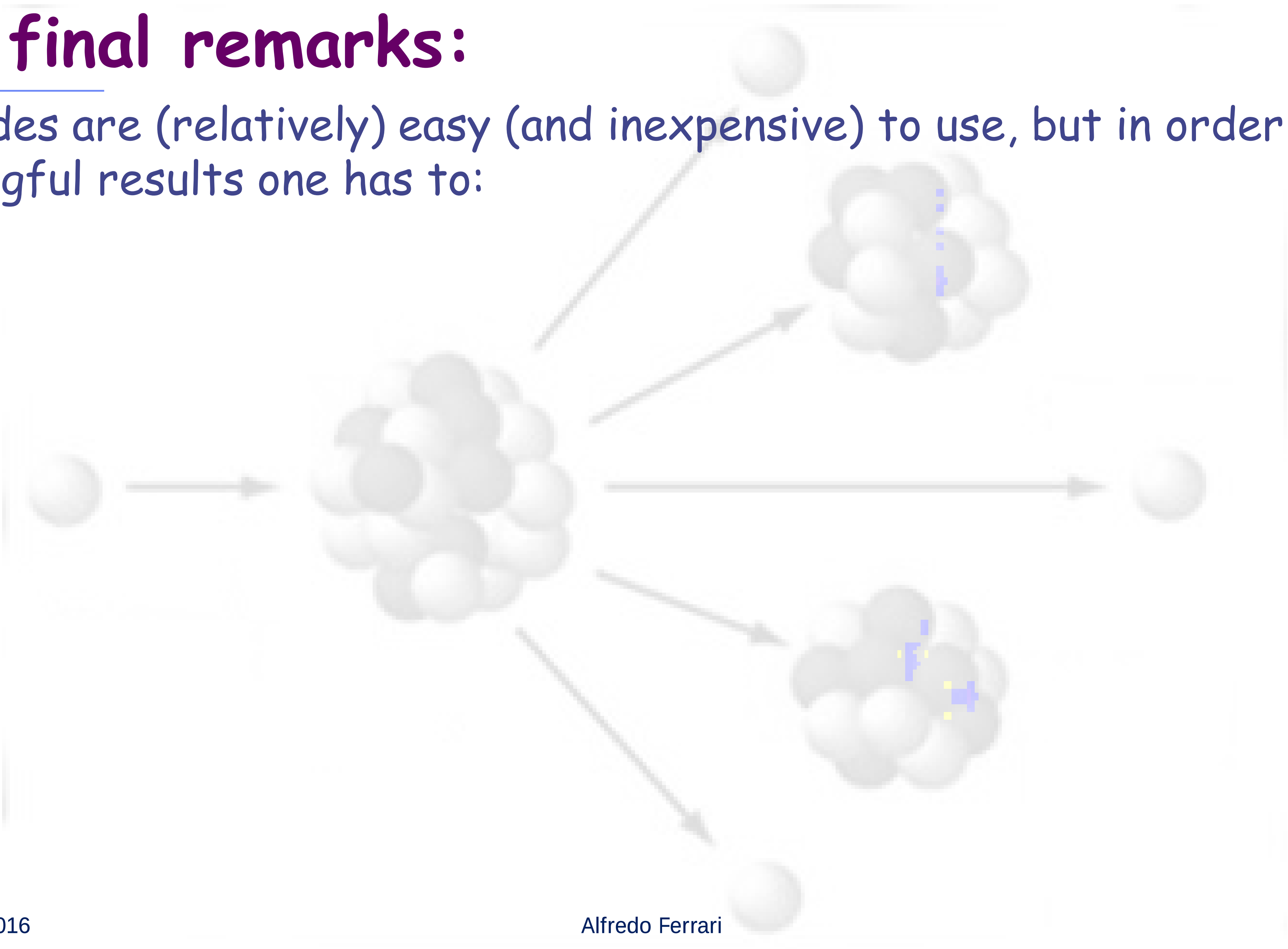
Never forget radiation damage!! CNGS: high energy hadron levels



Energetic (> 20 MeV) hadron fluence (cm^{-2} yr^{-1}) for a nominal CNGS year of 4.5 10^{19} pot *(2007 run: ~8 10^{17} pot)*

Some final remarks:

- MC codes are (relatively) easy (and inexpensive) to use, but in order to get meaningful results one has to:



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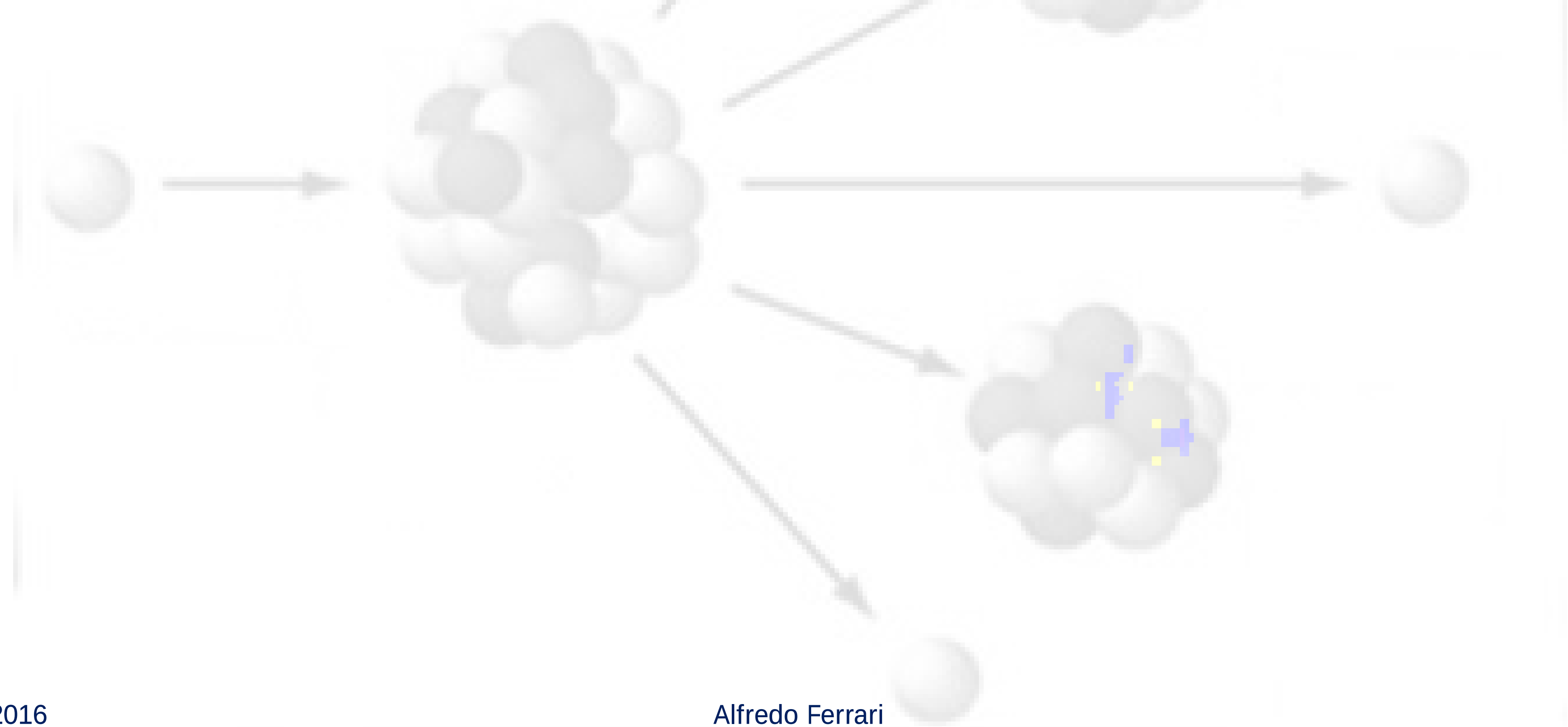

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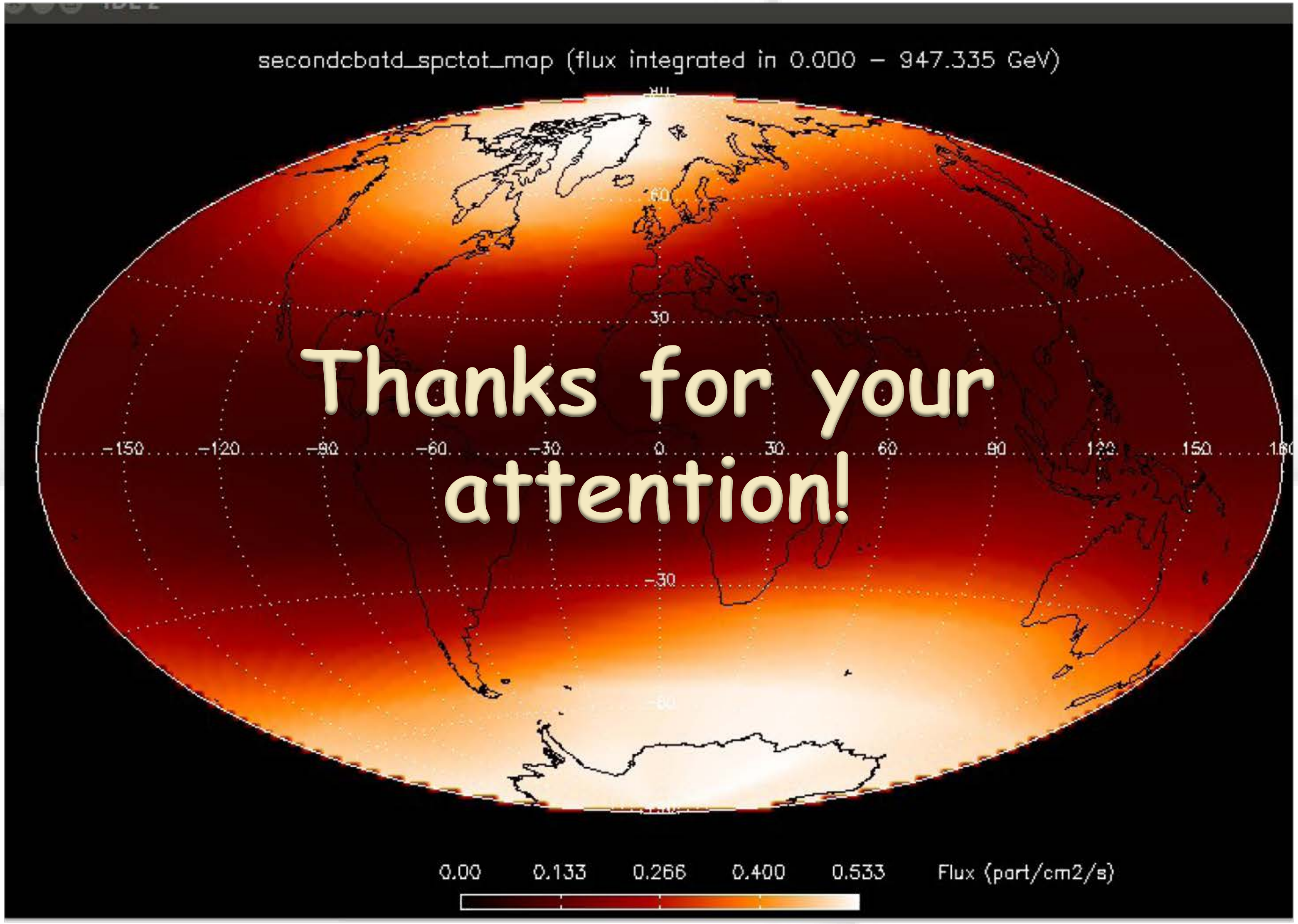
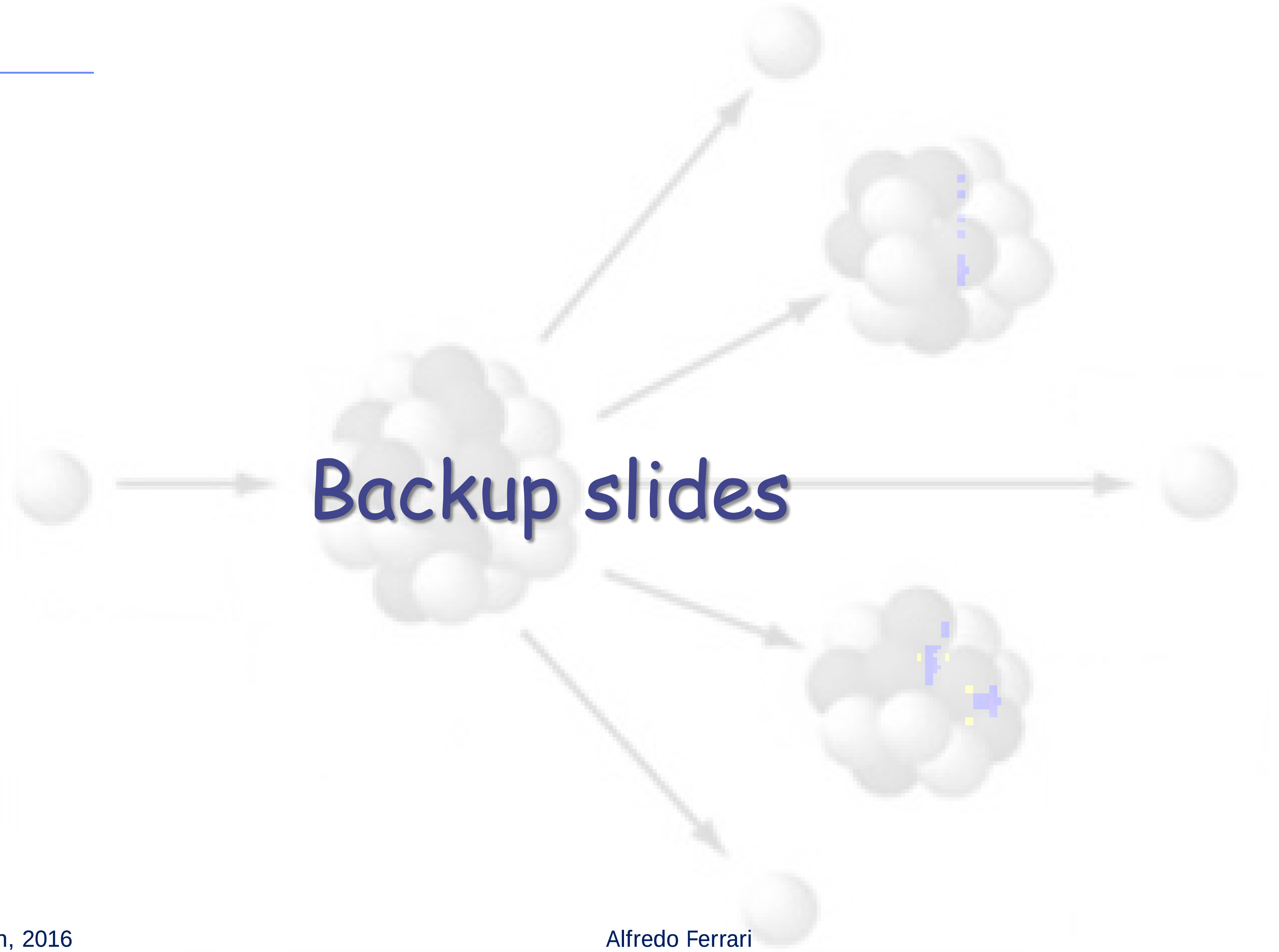
- … and the same applies when the best physicist is using a crappy code!

The neutron albedo from GCR's at 400 km altitude



Thanks for your attention!



Backup slides

Central limit theorem

Central limit theorem:

$$\lim_{N\to\infty} P(S_N) = \frac{1}{\sqrt{2\pi\,\sigma_A^2/N}}\exp\left[-\frac{\left(S_N-\overline{A}\right)^2}{2\,\sigma_A^2/N}\right]$$

- For large values of N, the normalized sum of N independent and identically distributed random variables tends to a normal distribution with mean $\bar{A}$ and variance σ^2_A/N

$$\lim_{N\to\infty} S_N = \lim_{N\to\infty}\frac{\sum_{i=1}^{N} A(x_i,y_i,z_i,\ldots)\,f'(x_i,y_i,z_i,\ldots)\,g'(x_i,y_i,z_i,\ldots)\,h'(x_i,y_i,z_i,\ldots)}{N} = \overline{A}$$

Integration efficiency:

- Originally, the Monte Carlo method was not a simulation method, but a device to solve a multidimensional integro-differential equation by building a stochastic process
- Traditional numerical integration methods (Simpson, etc), converge to the true values as $N^{-1/n}$ where N = number of "points" (interval), and n = number of dimensions
- Monte Carlo converges instead as $1/\sqrt{N}$

Number of dimensions	Traditional methods	Monte Carlo	Remark
$n = 1$	$1/N$	$1/\sqrt{N}$	MC not convenient
$n = 2$	$1/\sqrt{N}$	$1/\sqrt{N}$	About equivalent
$n > 2$	$1/\sqrt[n]{N}$	$1/\sqrt{N}$	MC converges faster

A typical particle transport Monte Carlo problem is a 7-D problem!
x, y, z, p_x, p_y, p_z and t !!

Sampling from a distribution:

Sampling from a discrete distribution:

- Suppose to have a *discrete* random variable x, that can assume values $x_1, x_2, \ldots, x_n, \ldots$ with probability $p_1, p_2, \ldots, p_n, \ldots$
- Assume $\sum_i p_i = 1$, or normalize it
- Divide the interval [0,1) in n subintervals, with limits

$$y_0 = 0, \quad y_1 = p_1, \quad y_2 = p_1 + p_2, \ldots.$$

- Generate a uniform pseudo-random number ξ
- Find the interval i^{th} y-interval such that

$$y_{i-1} \leq \xi < y_i$$

- Select $X = x_i$ as the sampled value

Since ξ is uniformly random:

$$P(x_i) = P(y_{i-1} \leq \xi < y_i) = y_i - y_{i-1} = p_i$$

Sampling from a distribution:

Sampling from a generic continuous distribution:

- Integrate the distribution function ***f(x)***, analytically or numerically, and normalize to 1 to obtain the normalized cumulative distribution

$$F(\xi) = \frac{\int_{x_{min}}^{\xi} f(x)dx}{\int_{x_{min}}^{x_{max}} f(x)dx}$$

- Generate a uniform pseudo-random number ξ
- Get the desired result by finding the inverse value $X = F^{-1}(\xi)$, analytically or numerically, i.e. by interpolation (table look-up)

Since ξ is uniformly random:

$$P(a < x < b) = P(F(a) \leq \xi < F(b)) = F(b) - F(a) = \int_a^b f(x)dx$$

Example: the exponential distribution

Take $f(x) = e^{-\frac{x}{\lambda}}$, x ∈ [0,-∞)

Cumulative distribution:

$$F(t) = \int_0^t e^{-\frac{x}{\lambda}} dx = \lambda \times \left(1 - e^{-\frac{t}{\lambda}}\right)$$

Normalized:

$$F'(t) = \int_0^t \frac{e^{-\frac{x}{\lambda}}}{\lambda} dx = 1 - e^{-\frac{t}{\lambda}}$$

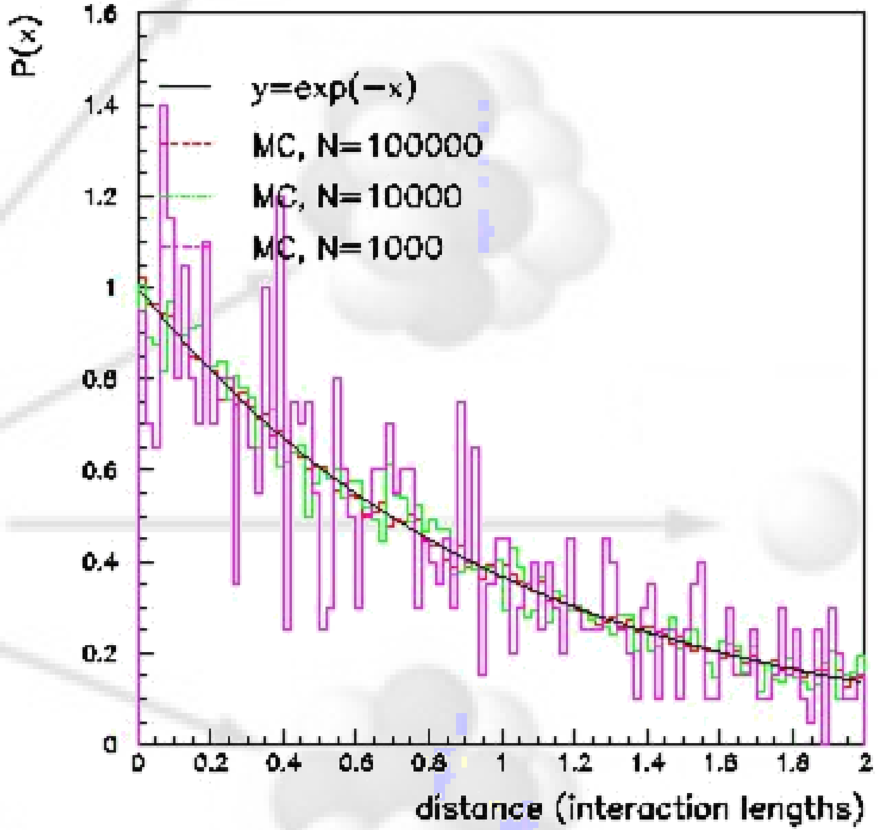
Generate a uniform pseudo-random number ξ ∈ **[0,1)**

Sample **t** by inverting

$$1 - e^{-\frac{t}{\lambda}} = \xi$$

$$t = -\lambda \ln(1-\xi)$$

Repeat N times



Practical rule: a distribution can be sampled directly if and only if its pdf can be integrated and the integral inverted

Sampling from a distribution: rejection technique

Rejection procedure:

- Let be *f′(x)*, a normalized distribution function, which cannot be sampled by integration and inversion
- Let be *g′(x)*, a normalized distribution function, which can be sampled, and such that $Cg'(x) \geq f'(x),\ \forall\ x \in [x_{min}, x_{max}]$
- Sample X from g′(x), and generate a uniform pseudo-random number $\xi \in [0,1)$
- Accept *X* if $f'(X)/Cg'(X) < \xi$, if not repeat the previous step
- The overall efficiency (accepted/rejected) is given by:

$$R = \int \frac{f'(x)}{Cg'(x)} g'(x)\, dx = \frac{1}{C}$$

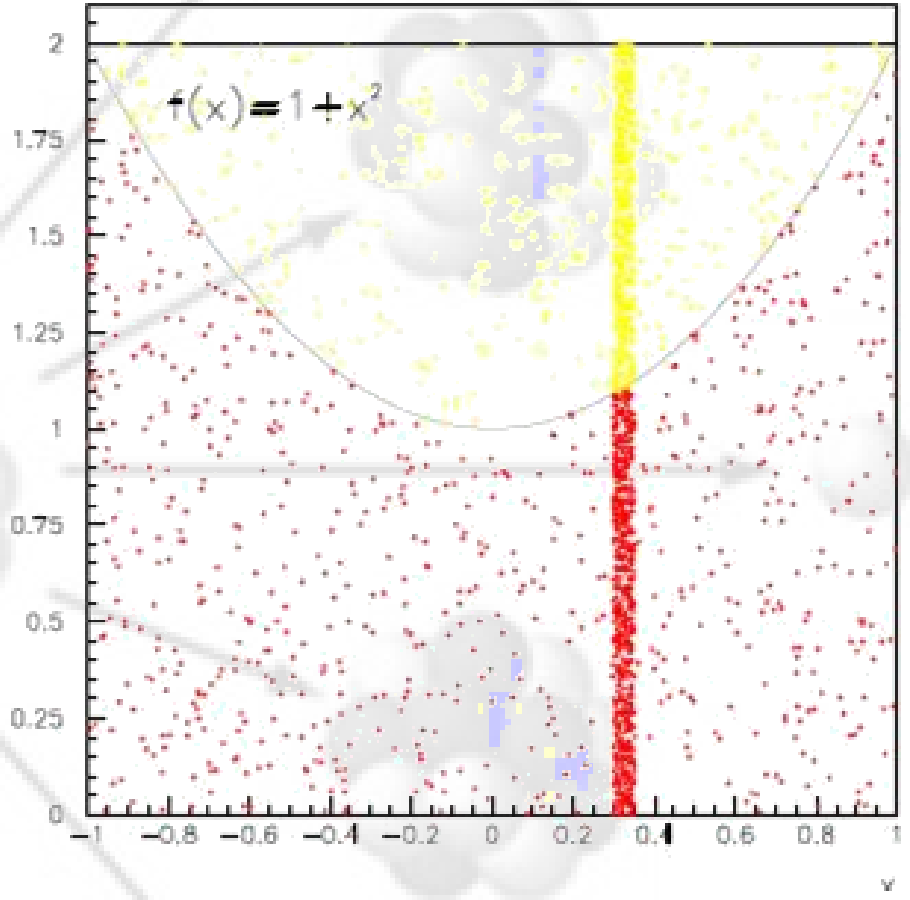
- and the probability that *X* is accepted is unbiased:

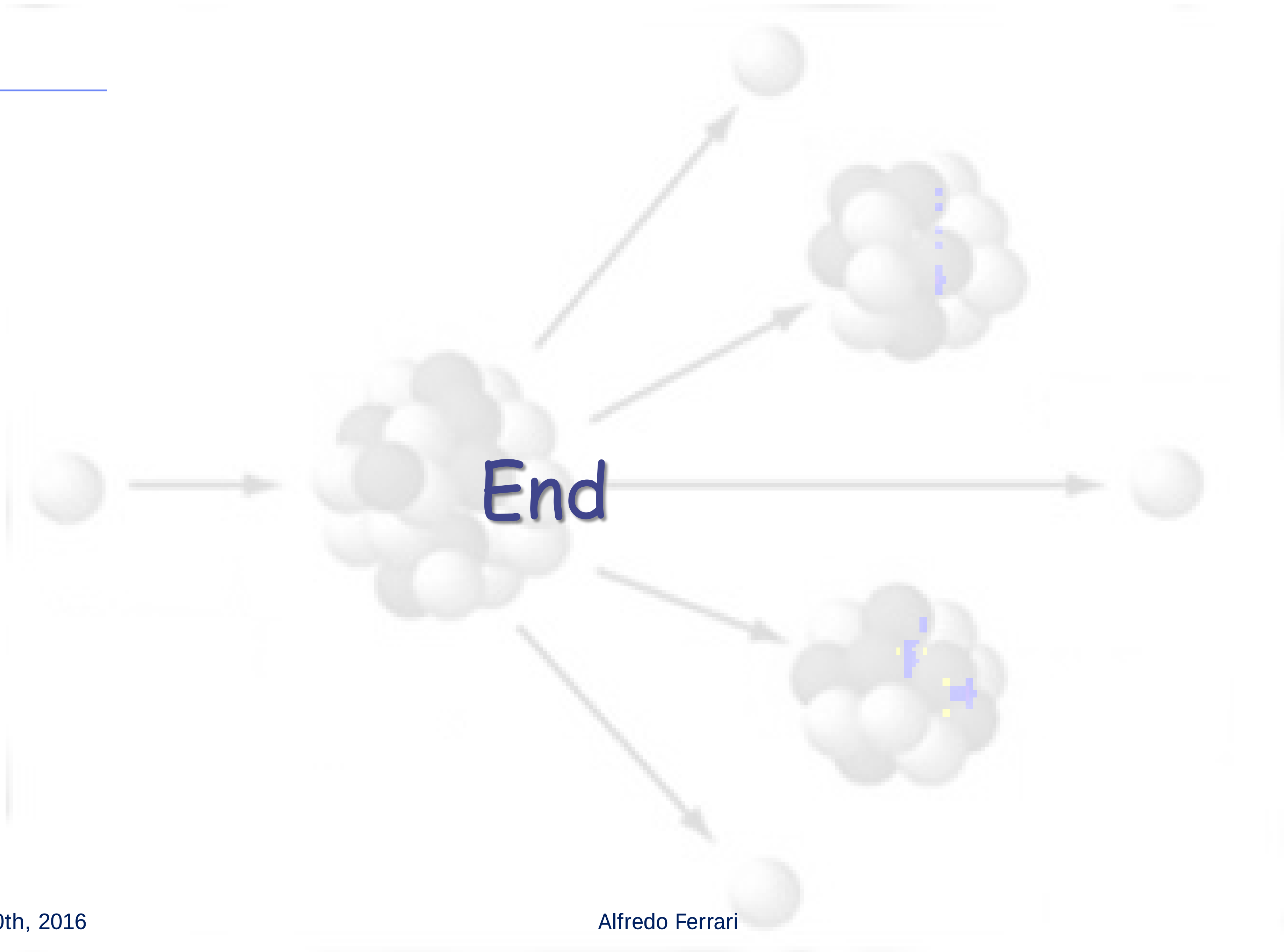
$$P(X)\,dX = \frac{1}{R} g'(X)\,dX \times \frac{f'(X)}{Cg'(X)} = f'(X)\,dX$$

Sampling from a distribution: example

Rejection procedure:

- Let be $f'(x) = A(1+x^2)$, $x \in [-1,1]$, $g'(x)=1/2$, $C=4A$
- Generate two uniform pseudo-random numbers ξ_1, $\xi_2 \in [0,1)$
- Accept $X=2\xi_1-1$ if $(1+X^2)/2 < \xi_2$, if not repeat





End