

EVENT-BY-EVENT

**MONTE CARLO TRACKING OF
NEUTRON-NUCLEUS COLLISIONS
IN NEUTRON DETECTORS**

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**UNIVERSITY OF
SURREY**

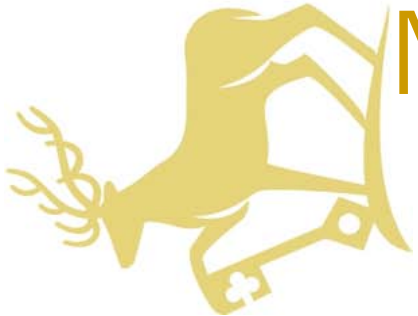
A
VERY
SIMPLE
EXPERIMENT

THERMAL
NEUTRONS IN
BORON-10

- ONE ENERGY
- ONE MATERIAL
- ONE CELL

TWO
INDEPENDENT
MONTE CARLO
CODES

- MCNPX
- FLUKA





WHEN EVERYONE'S BUSY MODELLING VERY COMPLEX PROBLEMS

THE EXTREME ...

OR AT LEAST ...



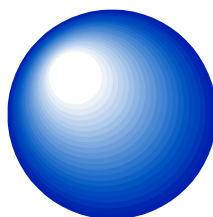
LARGE H

TO SEE THINGS
WE WOULDN'T
OTHERWISE SEE

T DOSE
et al 2006
Computing

WHY SHOULD WE SIMULATE

SIMPLE SPHERE



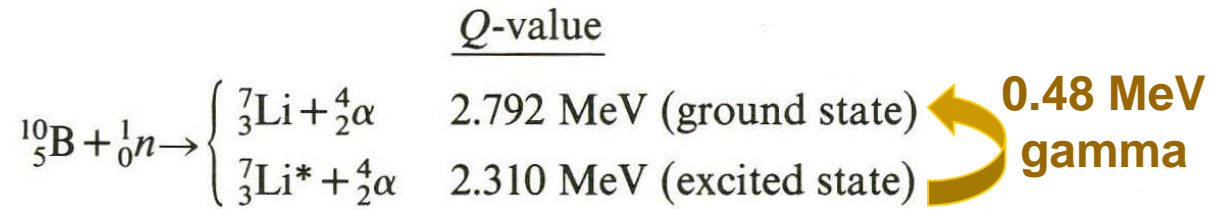
MONOENERGETIC BEAM

SINGLE NUCLIDE

SINGLE PARTICLE TYPE

A. The $^{10}\text{B}(n,\alpha)$ Reaction

Probably the most popular reaction for the conversion of slow neutrons into directly detectable particles is the $^{10}\text{B}(n,\alpha)$ reaction. The reaction may be written:



from each reaction

we expect either

NO GAMMA

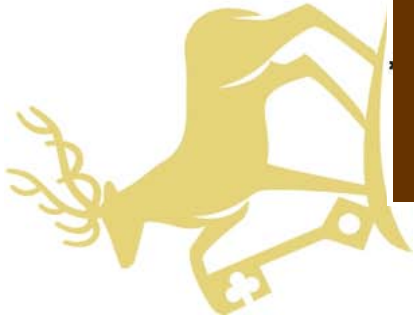
**6%
OF THE TIME**

or

ONE 0.48 MeV GAMMA

**94%
OF THE TIME**

... be left either in
neutrons (0.025 eV)
... lead to the
... either case, the
... compared with the
... to the reaction
... the incoming
... reaction energy,
... ginal value. Also,
... reaction products



MCNPX WOULD QUITE
HAPPILY GIVE US
ONE, TWO, THREE, ...

from each reaction

we expect either

NO GAMMA

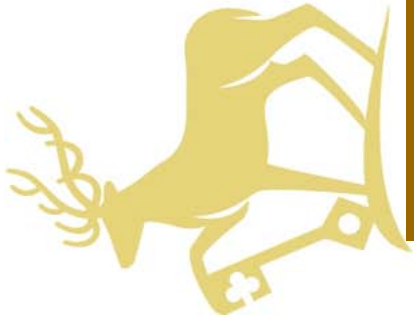
6%
OF THE TIME

or

ONE 0.48 MeV GAMMA

94%
OF THE TIME





MCNPX WOULD QUITE
HAPPILY GIVE US
ONE, TWO, THREE, ...

MCNPX SIMULATION

SOURCE: 0.025 eV NEUTRONS

NUMBER OF HISTORIES: 10 MILLION

MEDIUM: ^{10}B

OUT OF 10 MILLION NEUTRONS STARTED

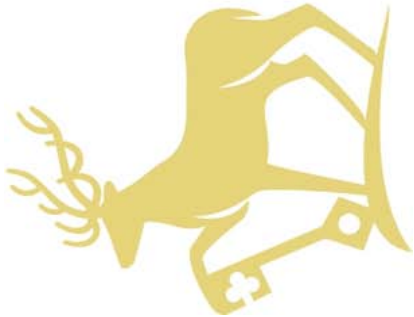
632,665 COUNTS OF ZERO GAMMA PER NEUTRON

9,362,277 COUNTS OF 1 GAMMA PER NEUTRON

5,053 COUNTS OF 2 GAMMAS PER NEUTRON

5 COUNTS OF 3 GAMMAS PER NEUTRON

VIOLATES THEORETICAL EXPECTATION



YET ...

ISI Web of KnowledgeSM [Access the new version!](#) CrossSearch

[CrossSearch](#)

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Search Results

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topic= **MCNP or MCNPX**
Databases=WCI, Web of Science, ISI Proceedings; Timespan=All Years

1,955 results found (1,000 shown)

Records 1 -- 10 |<<< [1 | 2 ... >>>

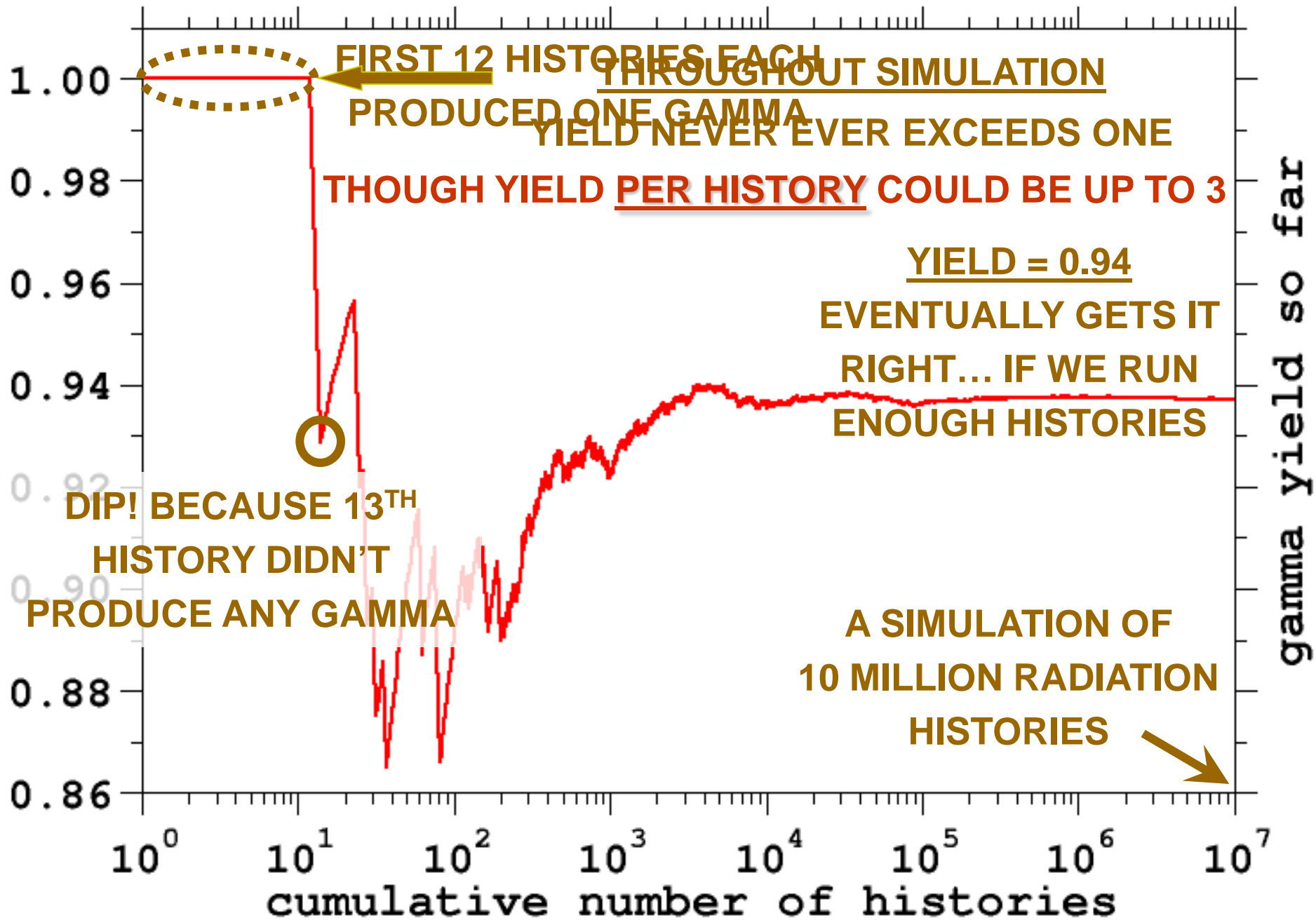
CAN'T BE THAT
WRONG AFTER ALL

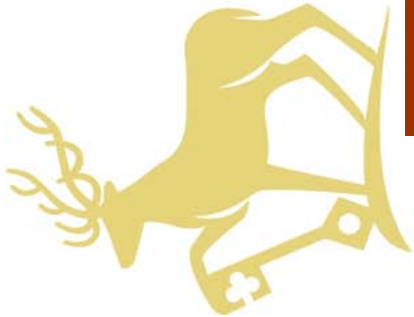
USED WORLDWIDE

TO SOLVE A WIDE RANGE OF PROBLEMS

OVER THE YEARS

VIOLATES THEORETICAL EXPECTATION





THIS HAS ALWAYS BEEN IN
MCNP/MCNPX

NOT A BUG, BUT
A DESIGN FEATURE

NOT NEW, JUST THAT
MOST USERS ARE UNAWARE

DOESN'T MATTER IN MOST CASES
AFFECTS EXCEPTIONS ONLY

VIOLATES THEORETICAL EXPECTATION

MCNP-PoliMi: a Monte-Carlo code for correlation measurements

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Department of Nuclear Engineering, Polytechnic of Milan, Via Ponzio 34/3, Milan 20133, Italy

Nuclear Instruments and Methods in Physics Research A 513 (2003)

deviation from physical reality: the emission of secondary gamma rays from neutron collisions. In fact, in MCNP secondary photons are sampled independently from the type of neutron collision. For example, it is possible for a neutron in a collision with uranium to generate fission photons in the course of an elastic scattering. This technique provides correct answers when we consider the average outcome of a large number of histories, and it is well suited for biased calculations, but it fails when considering the single history [2]. This is a severe drawback in the simulation of correlation measurements in which the experimental quantity of interest is the delay between particles emitted by a single event [1,3].

In this paper we describe the MCNP-PoliMi

of the standard MCNP code. A major deviation to the standard code is introduced by inverting the order of photon production and neutron production.

The MCNP-PoliMi code implements a new particle tracking. This means that the weight is equal to one to each of the particles produced from the source and to each of the particles produced at a collision. With this method, particles have weight equal to one, whether they escape or are absorbed, and the process is simpler to model.

The modifications to the standard MCNP transport can be grouped in two main concerns: first concerns secondary particles, whereas the second concern

A. The $^{10}\text{B}(n,\alpha)$ Reaction

Probably the most popular reaction for the conversion of slow neutrons into α particles. This reaction may be written as

LOOKS NICE & CLEAN

IN THE TEXTBOOKS

BUT IF WE REALLY START

THERMAL NEUTRONS

IN ^{10}B WE'LL GET

CAPTURE GAMMAS

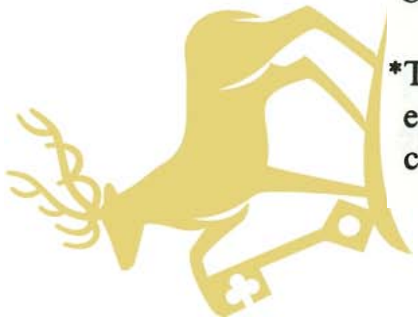
AS WELL

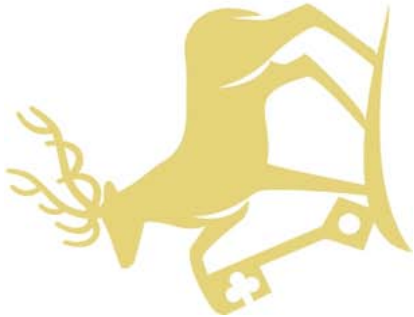
0.48 MeV
gamma



may be left either in its ground state or in an excited state. In either case, the reaction energy, compared with the binding energy of the reaction products, is sufficient to ensure that the reaction products are emitted with kinetic energy. Also, the reaction products may be left either in their ground state or in an excited state. In either case, the reaction energy, compared with the binding energy of the reaction products, is sufficient to ensure that the reaction products are emitted with kinetic energy.

*The reaction products are emitted with kinetic energy. The ground state with the emission of a 0.48 MeV gamma ray. We will assume that this photon always escapes and does not contribute to the response of the detector.





THERMAL NEUTRONS IN ^{10}B

WHAT DO WE EXPECT OF
THE GAMMA SPECTRUM?

What do we get from a
FLUKA[‡] simulation?

[‡] *developed by INFN & CERN*

OBSERVATION #1

NO BACKGROUND/CONTINUUM

COZ THESE ARE GAMMAS
CREATED, NOT GAMMAS

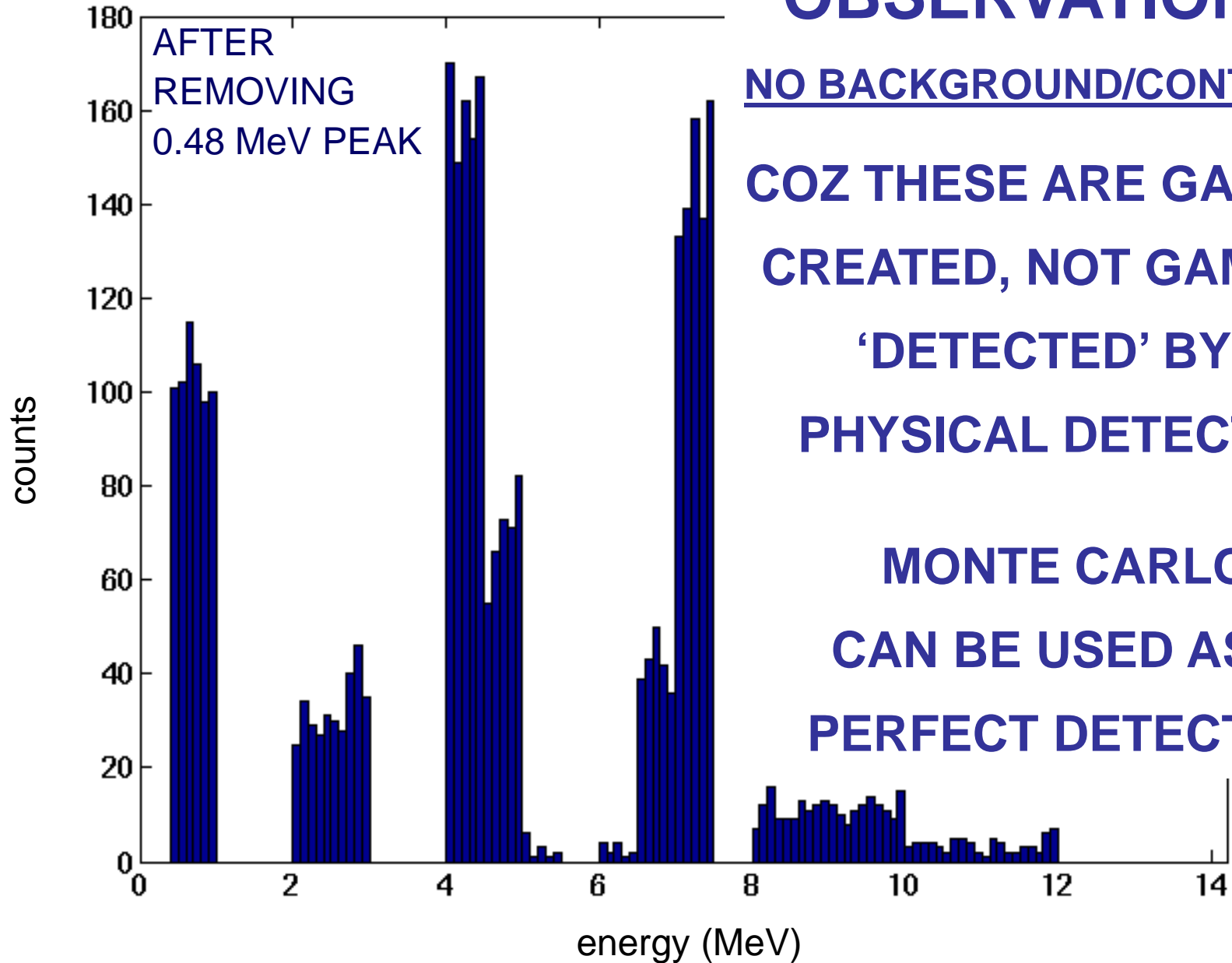
‘DETECTED’ BY A

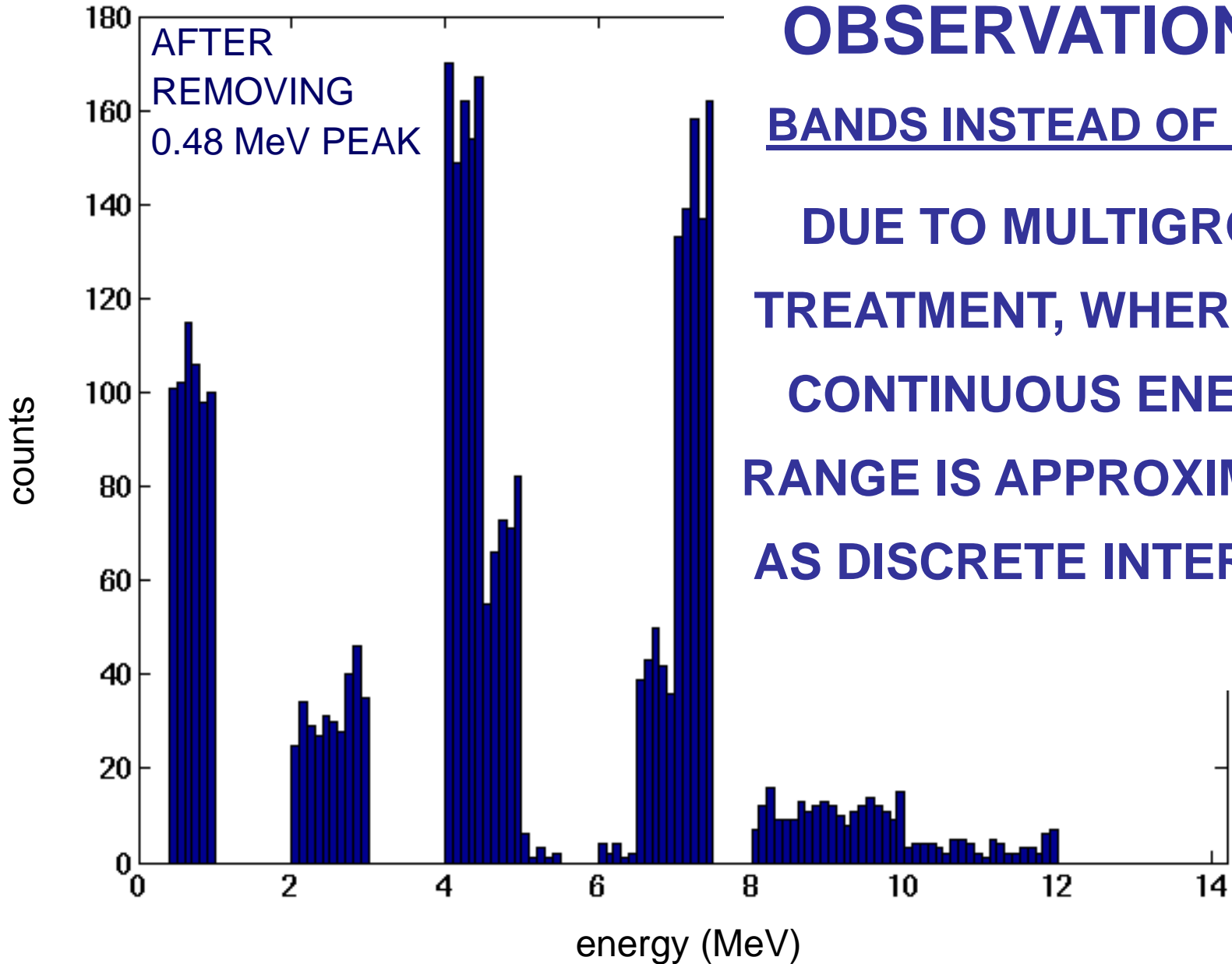
PHYSICAL DETECTOR

MONTE CARLO

CAN BE USED AS A

PERFECT DETECTOR





OBSERVATION #2

BANDS INSTEAD OF LINES

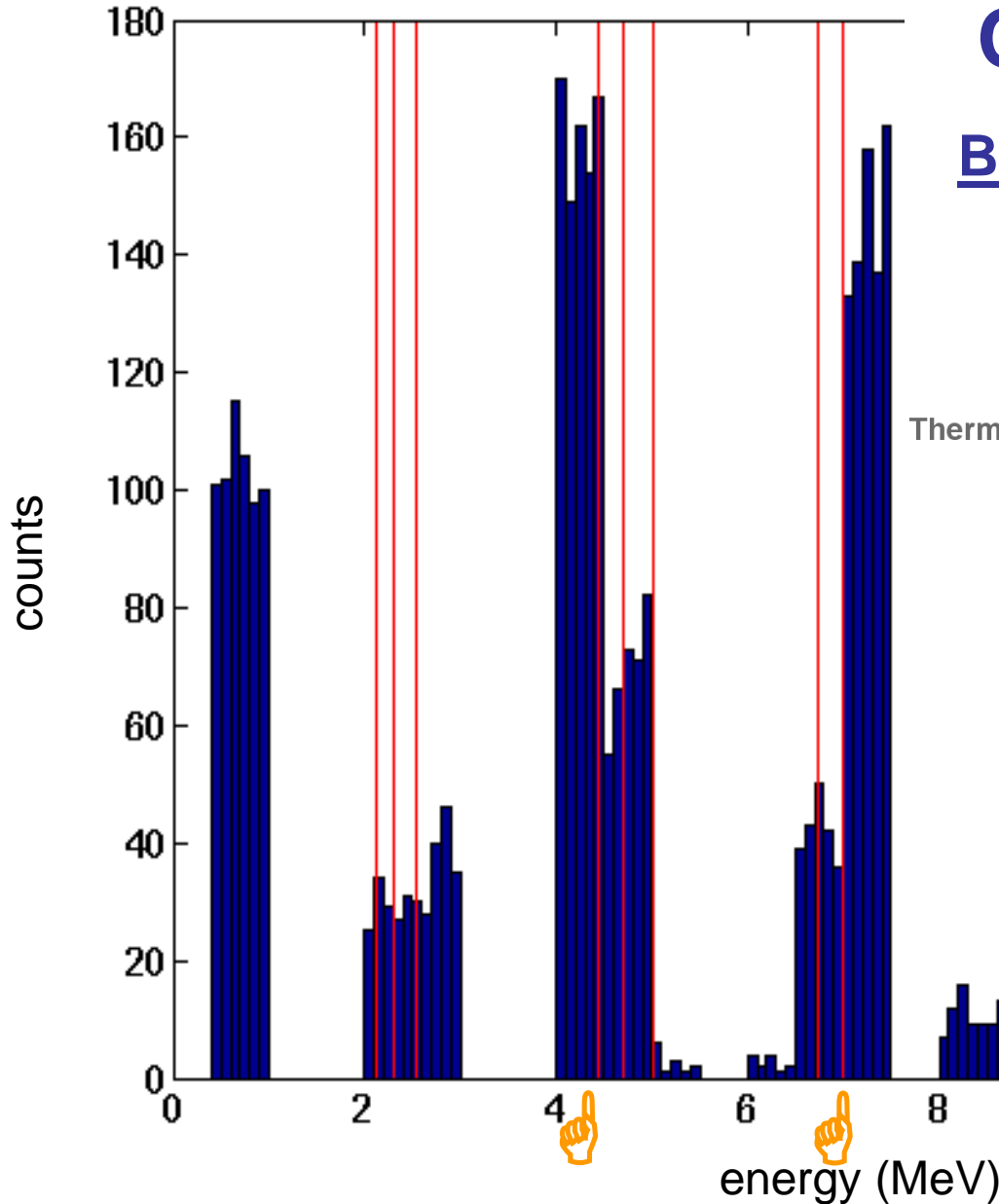
DUE TO MULTIGROUP
TREATMENT, WHERE THE
CONTINUOUS ENERGY
RANGE IS APPROXIMATED
AS DISCRETE INTERVALS

OBSERVATION #2

BANDS INSTEAD OF LINES

MATCH WITH NUCLEAR DATA

Thermal Neutron Capture Gammas — Target Nucleus ^{10}B



Target Nucleus= ^{10}B
Strongest transition $E_\gamma=4444.00\pm 2.00$ keV %I_γunknown

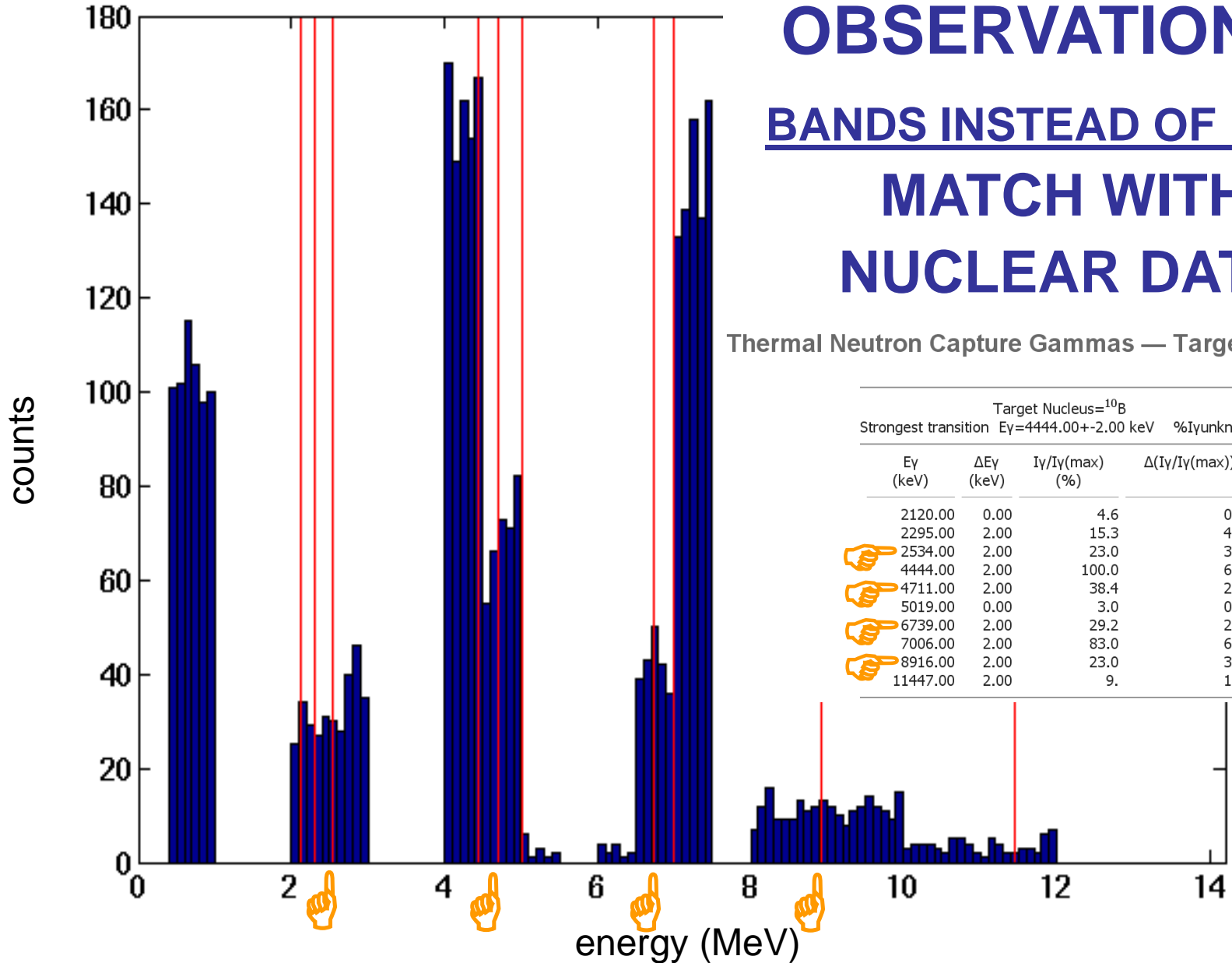
E_γ (keV)	ΔE_γ (keV)	$I_\gamma/I_\gamma(\text{max})$ (%)	$\Delta(I_\gamma/I_\gamma(\text{max}))$
2120.00	0.00	4.6	0.21
2295.00	2.00	15.3	4.67
2534.00	2.00	23.0	3.26
4444.00	2.00	100.0	6.53
4711.00	2.00	38.4	2.35
5019.00	0.00	3.0	0.14
6739.00	2.00	29.2	2.05
7006.00	2.00	83.0	6.00
8916.00	2.00	23.0	3.26
11447.00	2.00	9.	1.60

OBSERVATION #2

BANDS INSTEAD OF LINES

MATCH WITH NUCLEAR DATA

Thermal Neutron Capture Gammas — Target Nucleus ^{10}B



Target Nucleus= ^{10}B
Strongest transition $E_\gamma=4444.00\pm 2.00$ keV %I_γunknown

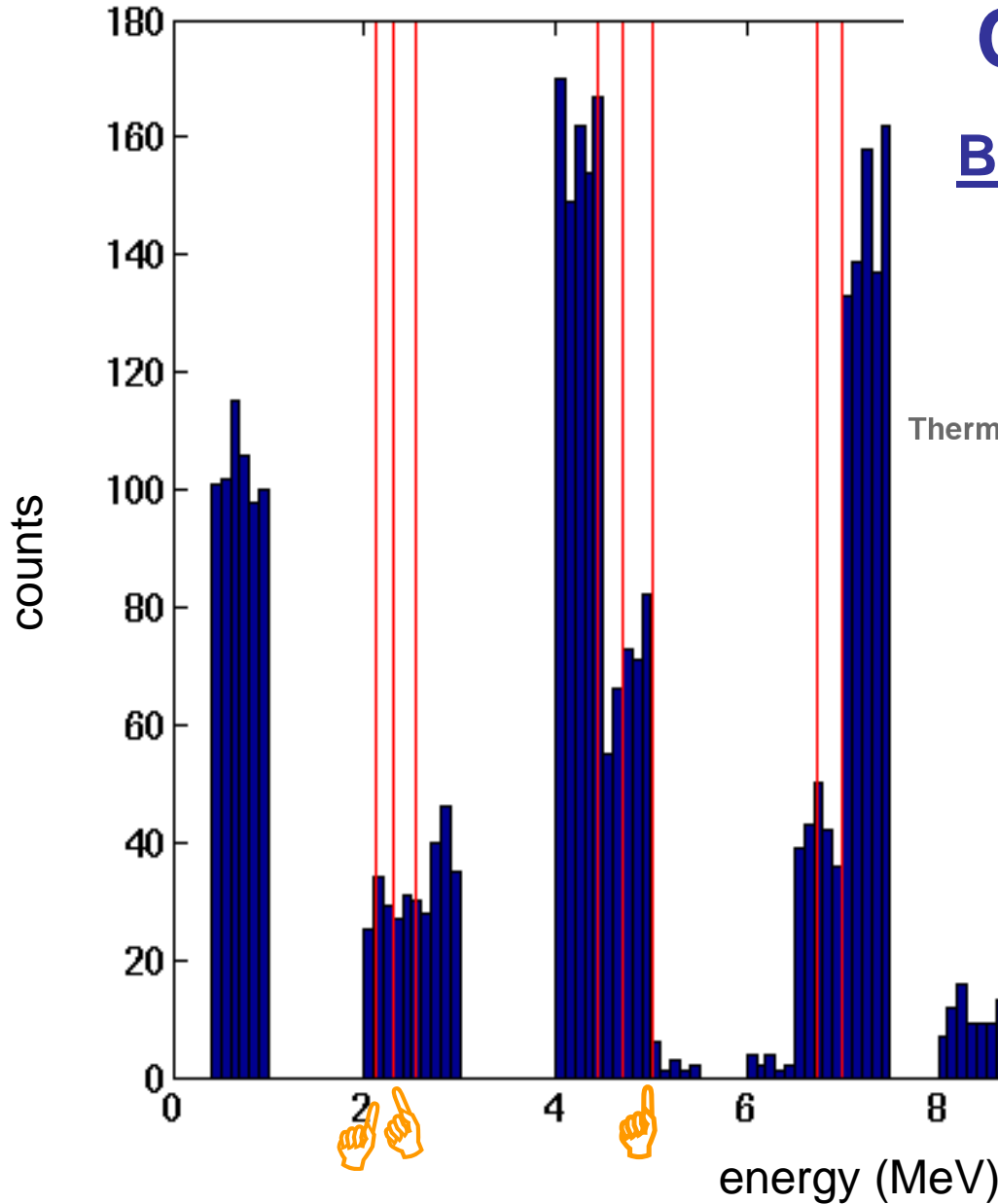
E_γ (keV)	ΔE_γ (keV)	$I_\gamma/I_\gamma(\text{max})$ (%)	$\Delta(I_\gamma/I_\gamma(\text{max}))$
2120.00	0.00	4.6	0.21
2295.00	2.00	15.3	4.67
2534.00	2.00	23.0	3.26
4444.00	2.00	100.0	6.53
4711.00	2.00	38.4	2.35
5019.00	0.00	3.0	0.14
6739.00	2.00	29.2	2.05
7006.00	2.00	83.0	6.00
8916.00	2.00	23.0	3.26
11447.00	2.00	9.	1.60

OBSERVATION #2

BANDS INSTEAD OF LINES

MATCH WITH
NUCLEAR DATA OK

Thermal Neutron Capture Gammas — Target Nucleus ^{10}B

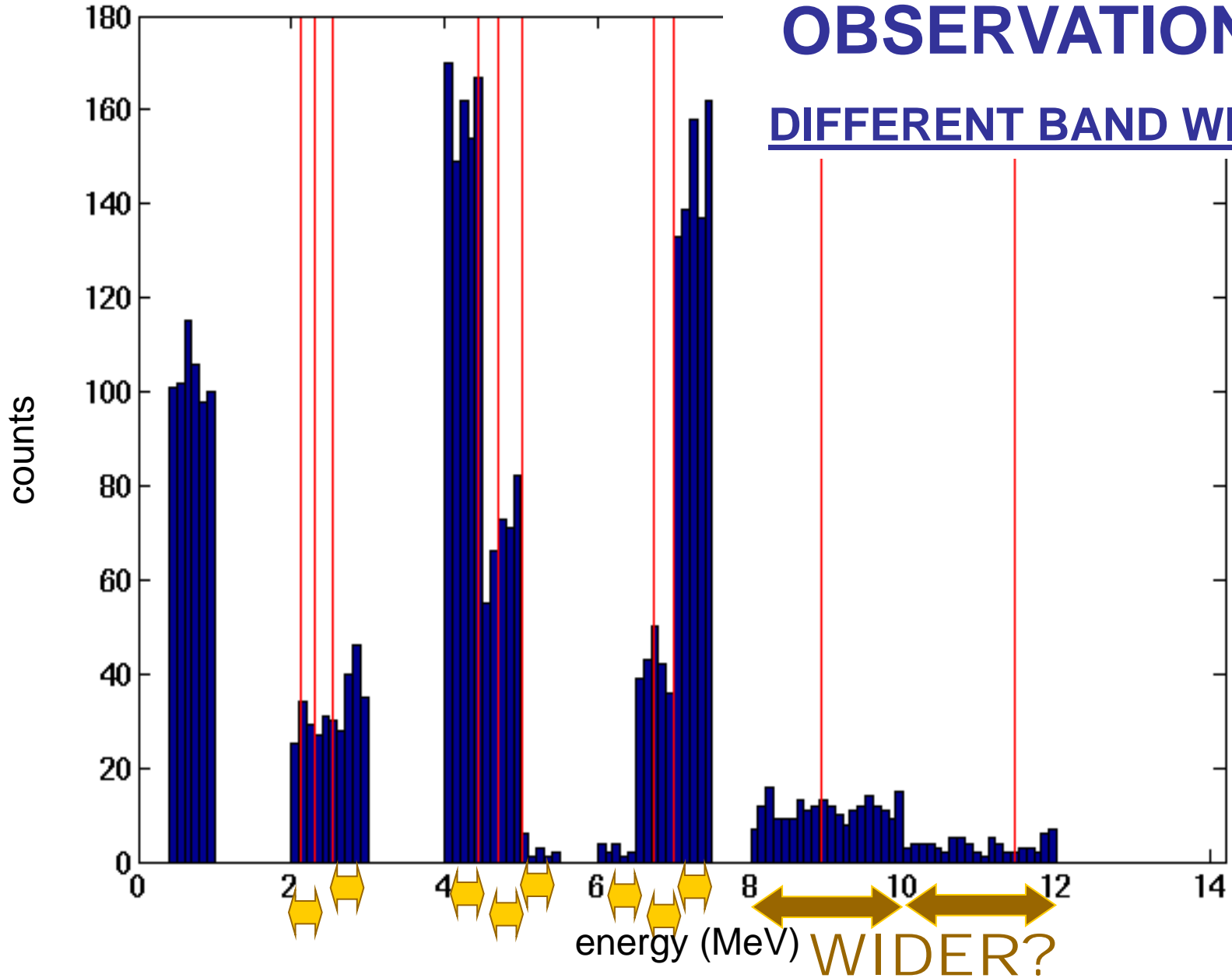


Target Nucleus= ^{10}B
 Strongest transition $E_\gamma=4444.00\pm 2.00$ keV %I_γunknown

E_γ (keV)	ΔE_γ (keV)	$I_\gamma/I_\gamma(\text{max})$ (%)	$\Delta(I_\gamma/I_\gamma(\text{max}))$
2120.00	0.00	4.6	0.21
2295.00	2.00	15.3	4.67
2534.00	2.00	23.0	3.26
4444.00	2.00	100.0	6.53
4711.00	2.00	38.4	2.35
5019.00	0.00	3.0	0.14
6739.00	2.00	29.2	2.05
7006.00	2.00	83.0	6.00
8916.00	2.00	23.0	3.26
11447.00	2.00	9.	1.60

OBSERVATION #3

DIFFERENT BAND WIDTHS



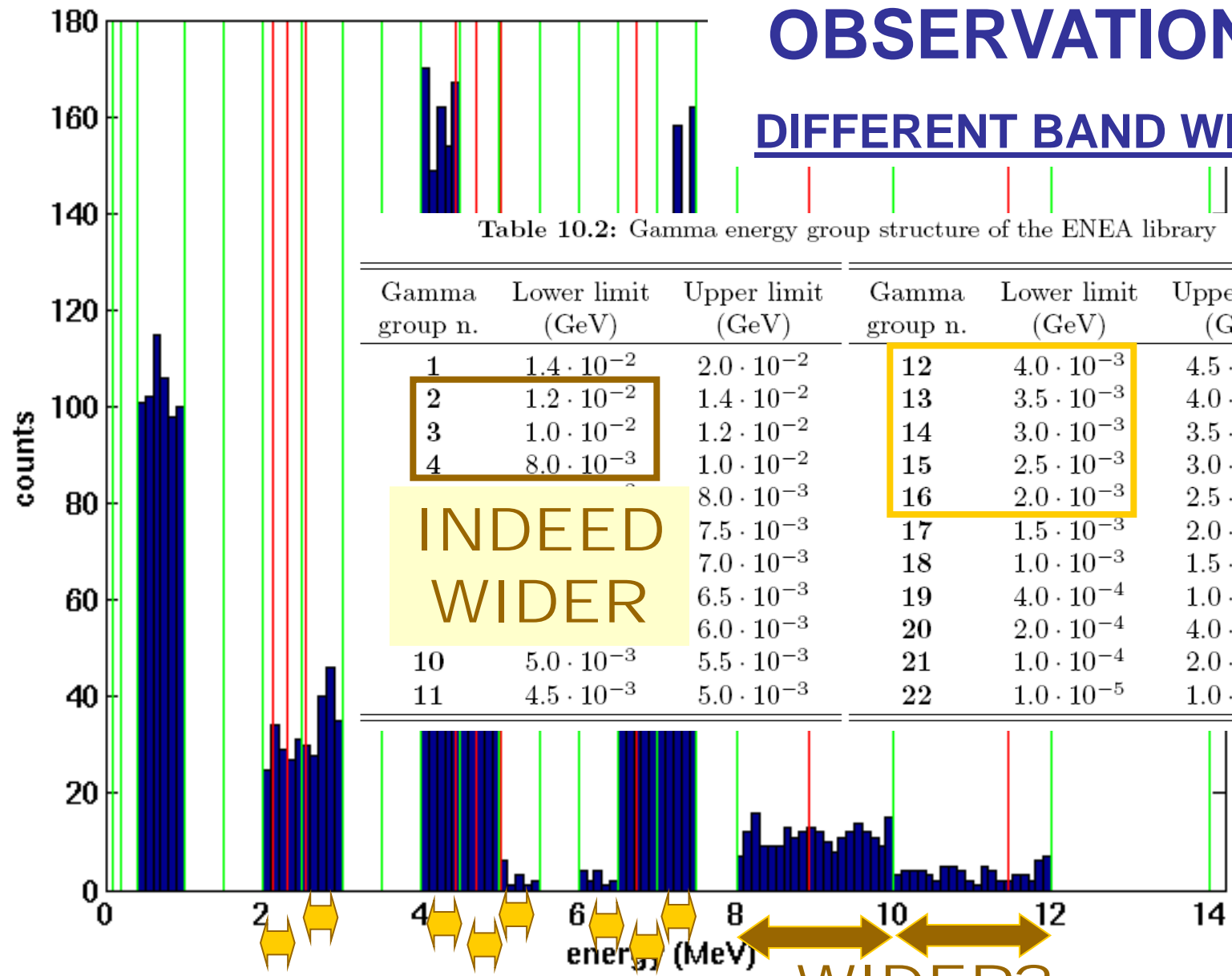
OBSERVATION #3

DIFFERENT BAND WIDTHS

Table 10.2: Gamma energy group structure of the ENEA library

Gamma group n.	Lower limit (GeV)	Upper limit (GeV)	Gamma group n.	Lower limit (GeV)	Upper limit (GeV)
1	$1.4 \cdot 10^{-2}$	$2.0 \cdot 10^{-2}$	12	$4.0 \cdot 10^{-3}$	$4.5 \cdot 10^{-3}$
2	$1.2 \cdot 10^{-2}$	$1.4 \cdot 10^{-2}$	13	$3.5 \cdot 10^{-3}$	$4.0 \cdot 10^{-3}$
3	$1.0 \cdot 10^{-2}$	$1.2 \cdot 10^{-2}$	14	$3.0 \cdot 10^{-3}$	$3.5 \cdot 10^{-3}$
4	$8.0 \cdot 10^{-3}$	$1.0 \cdot 10^{-2}$	15	$2.5 \cdot 10^{-3}$	$3.0 \cdot 10^{-3}$
		$8.0 \cdot 10^{-3}$	16	$2.0 \cdot 10^{-3}$	$2.5 \cdot 10^{-3}$
		$7.5 \cdot 10^{-3}$	17	$1.5 \cdot 10^{-3}$	$2.0 \cdot 10^{-3}$
		$7.0 \cdot 10^{-3}$	18	$1.0 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$
		$6.5 \cdot 10^{-3}$	19	$4.0 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$
10	$5.0 \cdot 10^{-3}$	$5.5 \cdot 10^{-3}$	20	$2.0 \cdot 10^{-4}$	$4.0 \cdot 10^{-4}$
11	$4.5 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	21	$1.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-4}$
			22	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-4}$

INDEED WIDER



WIDER?



Hi Mary,

there are two neutron cut-offs in FLUKA. 1.960E-02GeV is the cut-off for high-energy neutrons, below which the special multigroup treatment starts. With the present version it cannot be changed: it could be changed only when using a different library for low-energy neutrons (one with a different maximum energy). This cut-off is changed with PART-THR, but only when allowed by the low-energy neutron library

The second cut-off, which is changed with LOW-BIAS, is the real cut-off. It is not expressed in energy, but as a neutron group number. Look carefully in the output:

The first cut-off is reported as follows:
Cut-off kinetic energy for NEUTRON transport: 1.960E-02 GeV

And the second cut-off as follows: (here the group cut-off has been set as 73 for regions 1 and 2 - which means no cut-off at all - and group 65 in regions 3 and 4)

Region number	Particle Fluka part.	importances EM part.	RR factor Low en. n.	Cut off group	N.A. abs. group
1	1.0000	1.0000	1.0000	73	72
2	1.0000	1.0000	1.0000	73	72
3	1.0000	1.0000	1.0000	65	72
4	1.0000	1.0000	1.0000	65	72

Here the group cut-off has been set as 73 for regions 1 and 2 - which means no cut-off at all - and group 65 in regions 3 and 4, which means 7.3375E-09 GeV (see energy group structure in the Manual).

Alberto

MULTIGROUP vs POINTWISE TREATMENTS (APPROXIMATION) (CONTINUOUS)

10.2 Pointwise transport

For a few isotopes only, neutron transport can be done also using continuous (pointwise) cross-sections. For ^1H , ^6Li and ^{10}B , it is applied as a user option (above 10 keV in ^1H , for all reactions in ^6Li , and only for the reaction $^{10}\text{B}(n,t\gamma)^4\text{He}$ in ^{10}B). For the reaction $^{14}\text{N}(n,p)^{14}\text{C}$, pointwise neutron transport is always applied.

10.3 Secondary particle production

10.3.1 Gamma generation

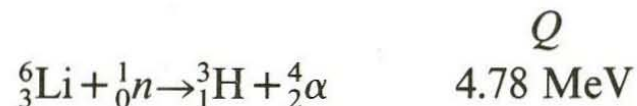
In general, gamma generation by low-energy neutrons (*but not gamma transport*) is treated in the frame of a multigroup scheme too. A downscattering matrix provides the probability, for a neutron in a given energy group, to generate a photon in each of 22 gamma energy groups, covering the range 10 keV to 20 MeV. With the exception of a few important gamma lines, such as the 2.2 MeV transition of Deuterium and the 478 keV photon from $^{10}\text{B}(n,\gamma)$ reaction, the actual energy of the generated photon is sampled randomly in the energy interval corresponding to its gamma group. Note that the gamma generation matrix does not include only capture gammas, but also gammas produced in other inelastic reactions such as (n,n') .

NOT COVERED IN THIS TALK

BUT DETAILED IN *SUMMARY* (ANS TRANS)

B. The ${}^6\text{Li}(n, \alpha)$ Reaction

The next most popular reaction for the detection of slow neutrons is the (n, α) reaction in ${}^6\text{Li}$. Here the reaction proceeds only to the ground state of the product and is written simply as:



Calculation of the reaction product energies for negligible incoming neutron energy yields the following:

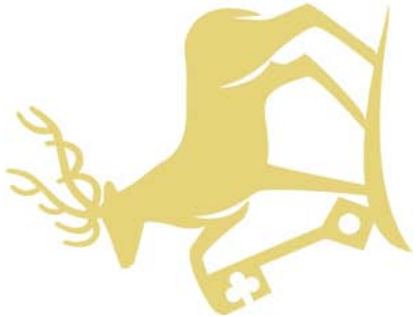
$$E_{3\text{H}} = 2.73 \text{ MeV} \quad E_{\alpha} = 2.05 \text{ MeV}$$

The alpha particle and triton produced in the reaction must be oppositely directed when the incoming neutron energy is low.

The thermal neutron cross section for this reaction is 940 barns. Figure 14-1 shows that the cross section remains below that for the ${}^{10}\text{B}$ reaction until the

EXCERPT FROM G. KNOLL
RADIATION DETECTION & MEASUREMENT





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BEHIND THE SCENES

How we use FLUKA as a perfect detector

Cut-out from \$FLUPRO/usermvax/mgdraw.f

ENTRY USDRAW (ICODE, MREG, XSCO, YSCO, ZSCO)

IF (.NOT. LFCOPE) THEN

LFCOPE = .TRUE.

IF (KOMPOT .EQ. 2) THEN

FILNAM = '/'//CFDRAW(1:8)//' DUMP A'

ELSE

FILNAM = CFDRAW

END IF

OPEN (UNIT = IODRAW

& 'UNFORMATTED')

END IF

IF (JTRACK .EQ. 8 .AND. Np.GT.0) THEN

IF (Np .EQ. 1 .AND. Kpart(1) . EQ. 8) THEN

ELSE

DO I = 1, Np

WRITE (IODRAW) NCASE

& SNGL (Tki(I))

END DO

END IF

END IF

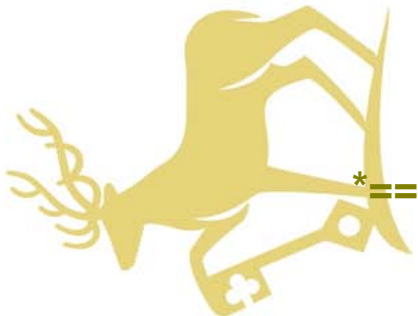
RETURN

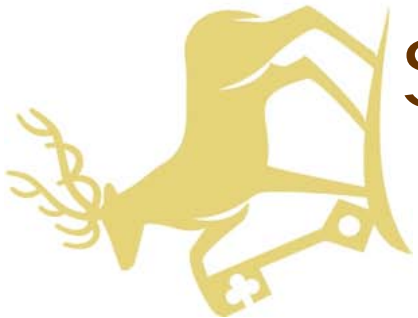
*==== End of subroutine Mgdr

IF NEUTRON, AND
IF THERE ARE SECONDARIES

FILTER OUT ELASTIC
SCATTER TO AVOID FILESIZE
EXPLOSION

LOOP THRU EACH SECONDARY
HISTORY #, TOTAL SECONDARIES
ENERGY OF PARENT
PARTICLE ID OF SECONDARY
ENERGY OF SECONDARY





INFN
+
CERN

LOS
ALAMOS

↓
FLUKA

↓
MCNPX

ANALOG
TRANSPORT



CROSS
SECTION



EVENT-BY-EVENT INVESTIGATIONS

Chin & Spyrou. Monte Carlo simulation of (n, p), (n, d), (n, t), (n, α), (n, γ) activations; a comparison of MCNPX and FLUKA. Int Conf Trends in Activation, Kyoto, 2007.

NEUTRONS

**MCNPX
FLUKA**

Chin & Spyrou. Monte Carlo studies and simulation of proton and deuteron beams for biomedical applications. Energy Systems. Guildford, 2007.

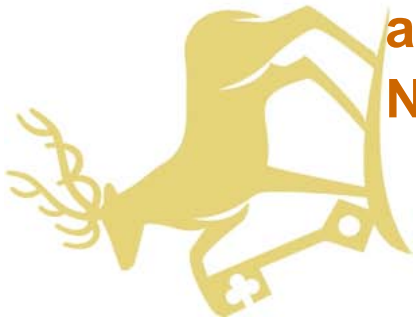
**PROTONS
DEUTERONS**

**GEANT4
MCNPX
FLUKA**

Chin & Spyrou. Monte Carlo investigation of positron annihilation in tissue. Nucl. Instrum. Methods Phys. Res. 2001.

POSITRONS

**EGSnrc
PENELOPE**

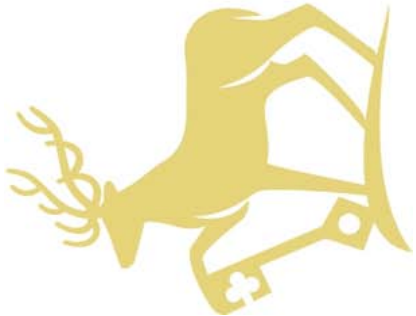


CHOICE OF CODE

WRONG EMPHASIS ON
CONVENIENCE

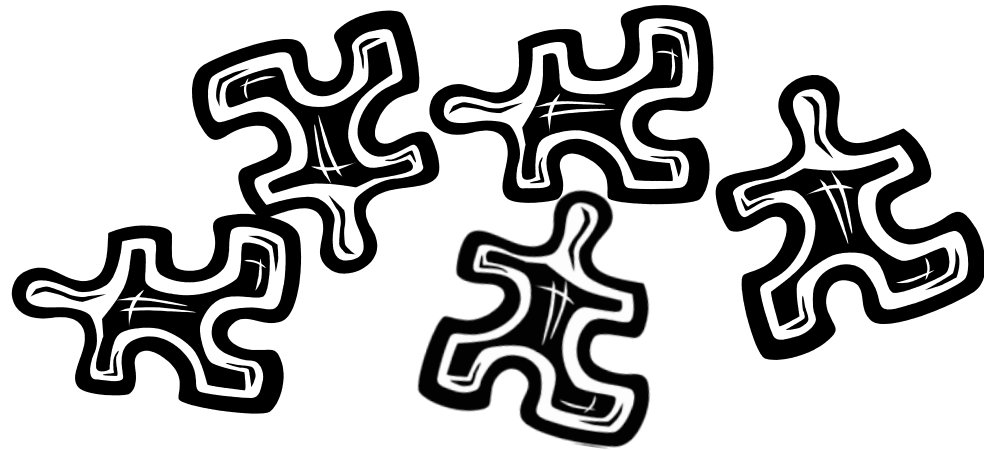
“GEOMETRY CODING IS THE EASIEST
WITH GATE, SO WE USE GATE.”

“OUR GROUP HAS ALWAYS USED
MCNP, SO WE USE MCNP FOR
EVERYTHING.”



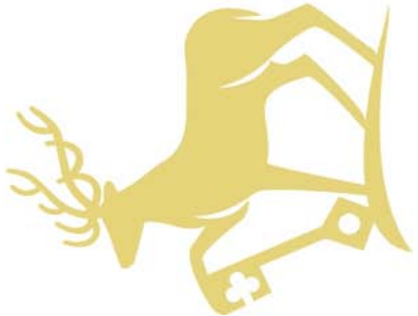
OUR POINT

**Different codes combine to
give the full picture**



We need to understand each code

**Scratching the surface is
not enough**



OUR POINT

**We need different codes
(with independent history
and different philosophy)
so that Monte Carlo results
may be used to
validate each other**

