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SOME TOPICS OF RECENT DEVELOPMENT ON MONTE CARLO COMPUTATION OF TARGET SYSTEMS IN JAPAN

Motoharu Kimura
Laboratory of Nuclear Science, Tohoku University
Sendai, 982 Japan

Abstract

NMTC code was refined by Nakahara of JAERI to make workable up to 250 of mass number. The code was used to explain the experimental results of high energy fission C.S. and the shoulder of spallation neutron spectra measured by KfK and LANL. Tsukada gave a theoretical basis for it assuming 10% ∿ 50% longer MFP of proton and neutron in nuclei.

Kimura made extensive computer simulation experiment of Monte-Carlo calculation, expecting possible cut down of computation cost, introducing James-Stein-Estimator (JSE). JSE proceedure will be useful for the data of large statistical fluctuation in general.

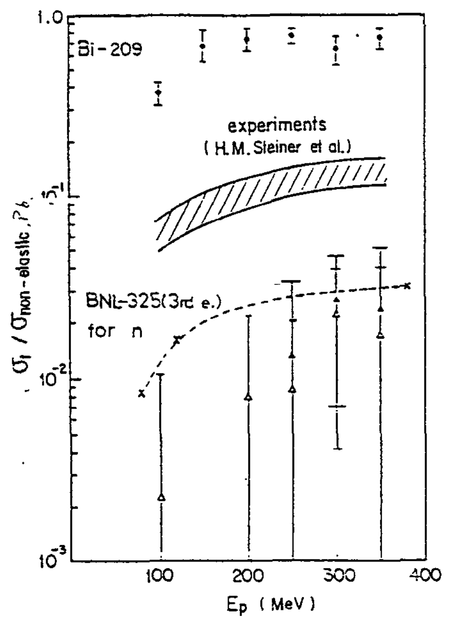
Introduction

Accelerator based neutron beams were used for condensed matter research for more than 15 years in Japan, and Accelerator breeder system is being studied systematically for 5 or more years now.

I would like to talk on some related topics recently developed by our study group.

On hadron transport Code

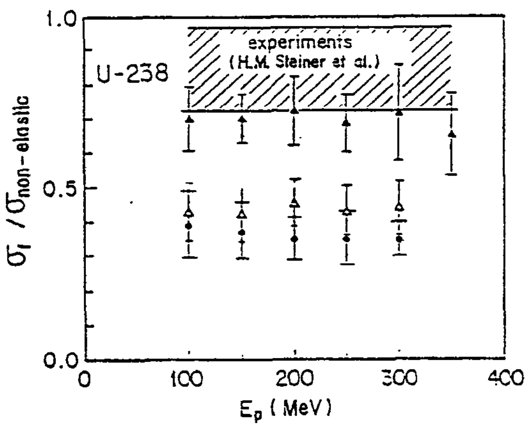
Nakahara et al[1] refined the NMTC/JAERI code which takes into account the high energy fission. He tried various cases of chosing formulae and parameter values related to the high energy fission and compared with the experimental results[2]. Mass dependence of the calculated nonelastic cross sections is also shown in comparison with the experimental data[3]. I will show just a small part of their results in the following three view graphs. The first view graph shows the comparison of their results with the experiments of Steiner et al[2] on the proton induced fission cross sections for Bi^{209}. Here, A_f and A_n are level density at Saddle point and equil. deformation. Ordinate is $\sigma_f(Bi)/\sigma_{non-el}(Pb,Bi)$. It is not clear yet if there is a real physical meaning in the discrepancy between proton and neutron bombardments. In Fig 2, for ^{238}U, comparison between Il'inov's [4] and Kupriyanov's[5] idea of double humped structure of fission barrier was made.



Monte Carlo calculations :

- • a_f / a_n (Vandenbosch – Huizenga), a_n (Le Couteur)
- ▲ a_f / a_n (Il'inov et al.), $a_n = A/10$.
- △ a_f / a_n (Il'inov et al.), $a_n = A/20$.

Fig1 Proton induced fission on ^{209}Bi



Monte Carlo calculations :

- ▲ Weisskopf - Bohr - Wheeler theoery with a_f / a_n due to Il'inov et al. and $a_n = A/10$.
- △ Same as the case ▲ except $a_n = A/20$.
- • Kupriyanov et al's model (Double humped)

Fig 2 Proton Induced Fission on ^{238}U

Fig 3 is for ^{232}Th.

A ≦ 250 made possible.

Nakahara made possible to handle mass number up to 250 which is needed to study actinide incineration and other problems.

On Energy Spectra of Spallation Neutrons

The evidence of slight shoulder near 100 MeV in the energy spectrum of spallating neutrons bombarded by high energy protons on heavy nuclei was explained by Tsukada[6] assuming longer mean free path of nucleons in the nuclear matter. Nakahara, using NMTC/JAERI code[1] calculated the energy spectra of neutrons for the case of Pb and U cylinder of 60 cm in length and 10 cm dia, bombarded axially by 590 or 800 MeV protons, obtained results which suggest the existence of such a shoulder. The KfK[7] and LANL[8] groups performed extensive measurements at different emerging angles of neutrons from various targets and the shoulder becomes more conspicuous for smaller emerging angles.

Both the NMTC or HETC calculational results ever obtained assuming free nucleon interaction cross sections have never given such shoulders, irrespective of the inclusion of high energy fission process or not.

Tsukada, therefore, assumed smaller interaction, that is, longer MFP of nucleon-nucleon collisions inside the nucleus. This will enhance the leakage of high energy neutrons from the nucleus and the number of evaporating neutrons will be suppressed.

Fig 4 is a NMTC/JAERI results assuming 10% and 50% increase of MFP. Even though the statistics is not yet very good, we can see a slight bamp in the energy spectrum at about 100 MeV.

However, Nakahara found decrease of the total neutron yield as shown in Fig 5.
It seems a good compromize may exist at about 10% increase of MFP. However, if the target dimension is much larger than the one of KfK experiment, total yield may be larger independent of MFP.

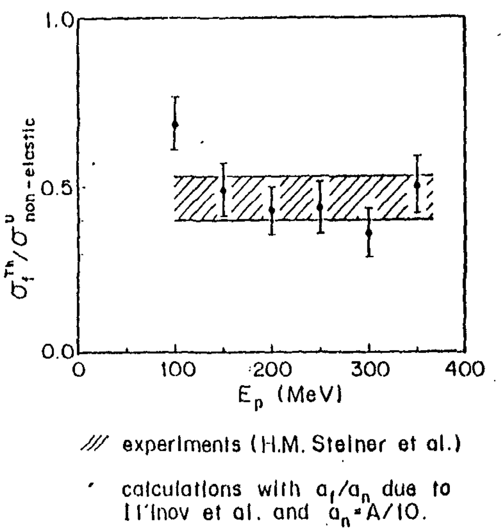


Fig 3 Proton induced fission on ^{232}Th

Tsukada carefully analysed the spectra and suggested existence of the third component as shown in Fig 7 and Fig 8. He assumed exponential forms like

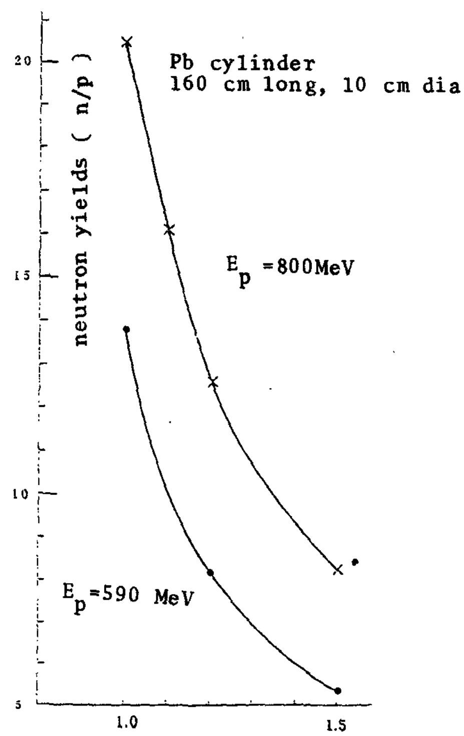
$$A_i(E/E_{0i})\exp(-E/E_{0i})$$
$$i = 1, 2, 3$$

for the evaporation part, high energy tail and also for the third component.

The third component, that is, of intermediate energy of around 20 MeV may correspond to the pre-equilibrium component as suggested by Nakai et al.[9] This component is included in the cascade calculations of Nakahara.

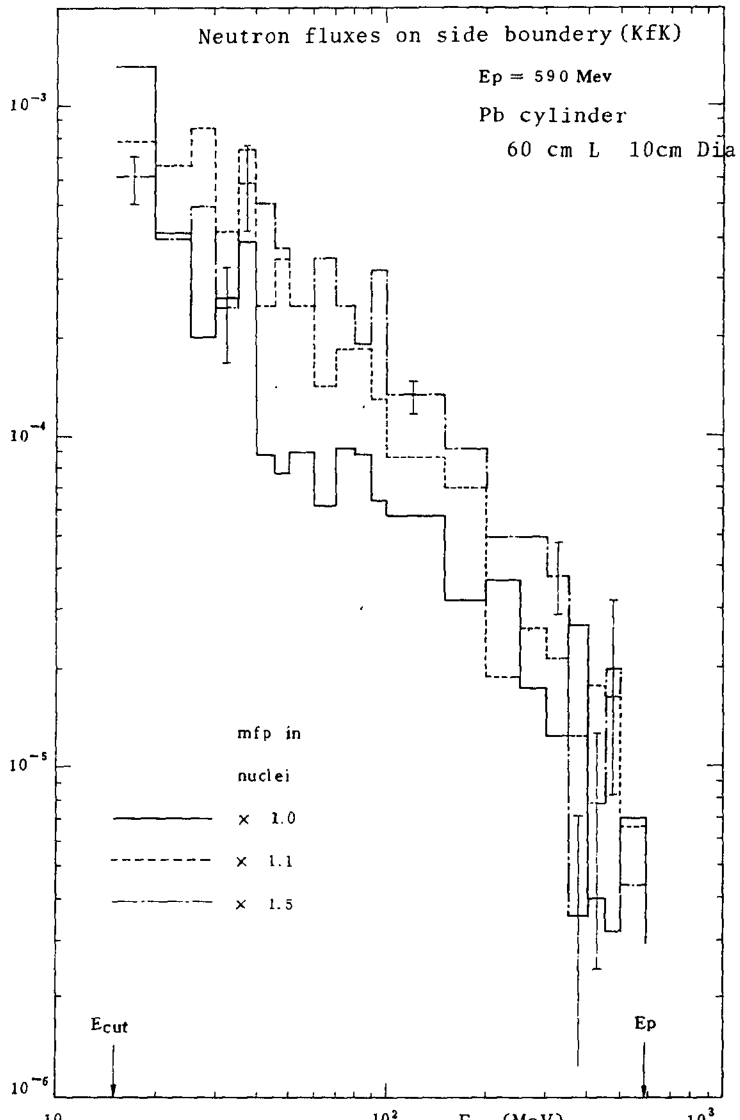
Molten salt target Molten salt of $LiF\text{-}BeF_2\text{-}UF_4$, for example, looks very promising, with many advantagious features. A molten salt accelerator breader system is being proposed by Furukawa et al.

Our study group for A.B. system proposes to construct an 800 MeV × 500 μa proton synchrotron, GEMINI, as the first step to the 1 GeV × 300 ma proton linac which will be the final demostration machine of A.B. system. We hope it will be realized in the early 2000's. On GEMINI, Sasaki talked yesterday. We think we need at least 2∿3 more accelerators as the intermediate test machine of rather low energy but of high current. This is needed for the R & D of target system for the final design.



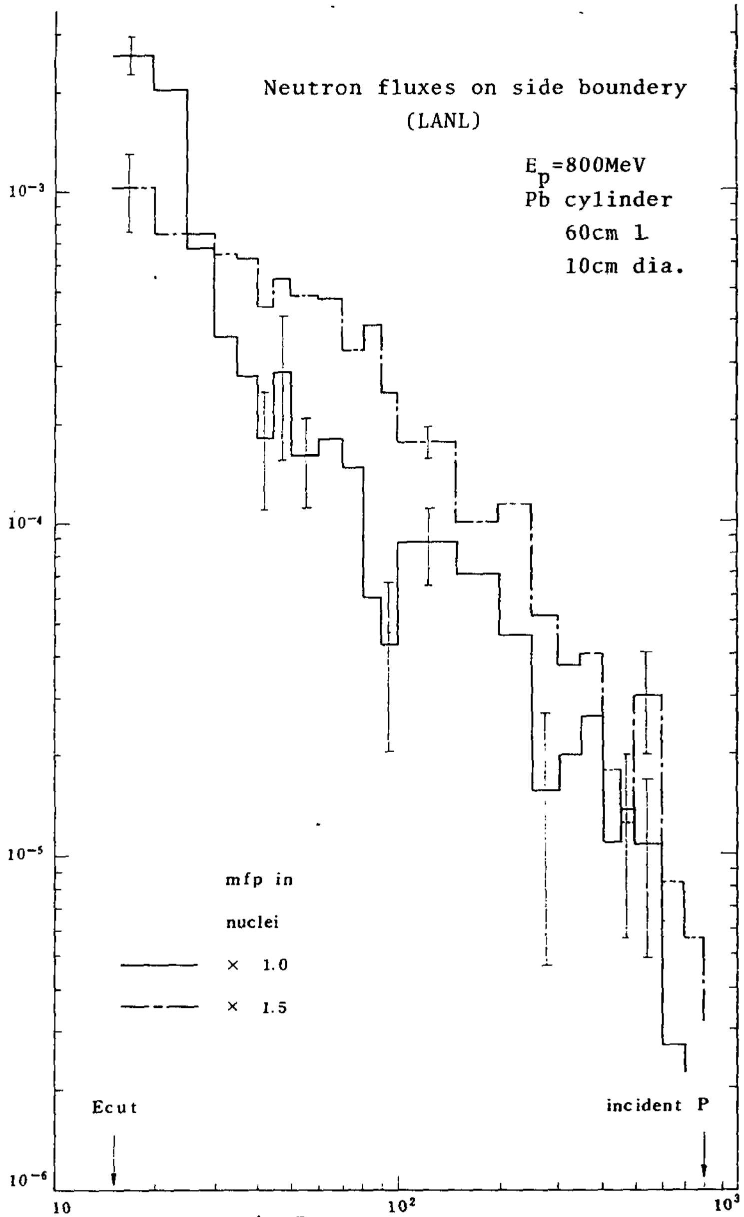
Multiplier to MFP in Nuclei

Fig 6



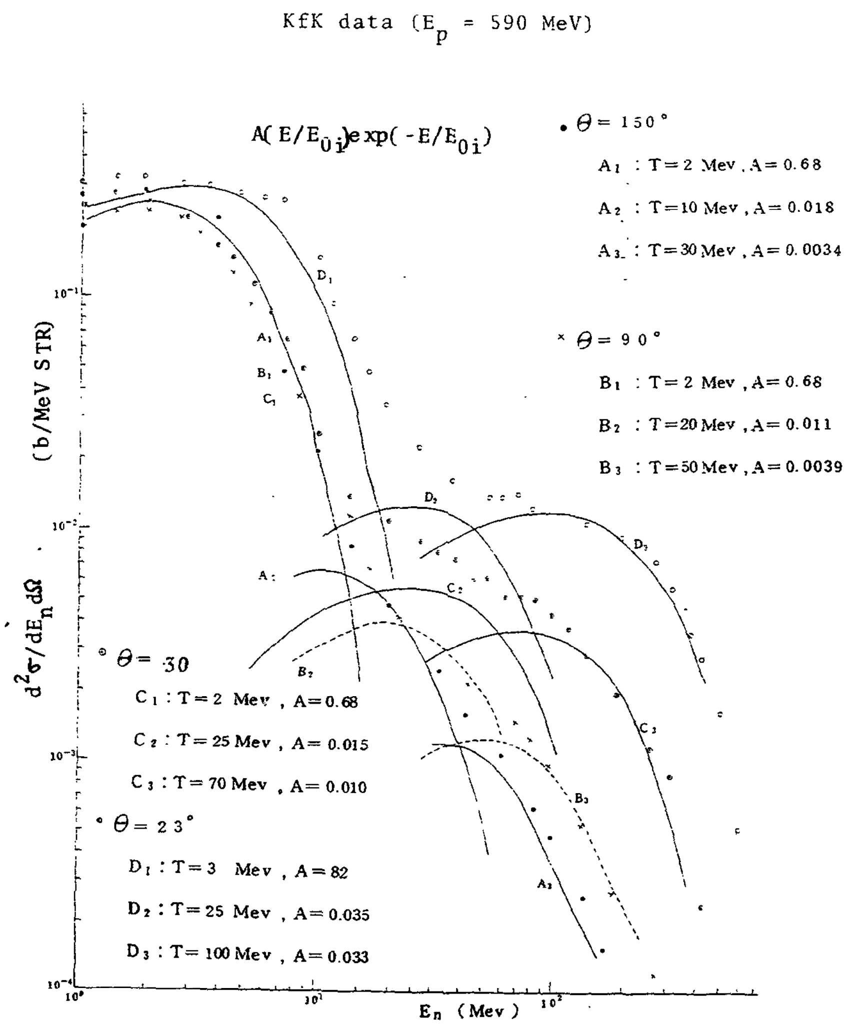
Neutron fluxes on side boundery (KfK)
Ep = 590 Mev
Pb cylinder
60 cm L 10cm Dia
mfp in
nuclei
× 1.0
× 1.1
× 1.5
Ecut
Ep
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10
10^{2}
E_n (MeV)
10^{3}

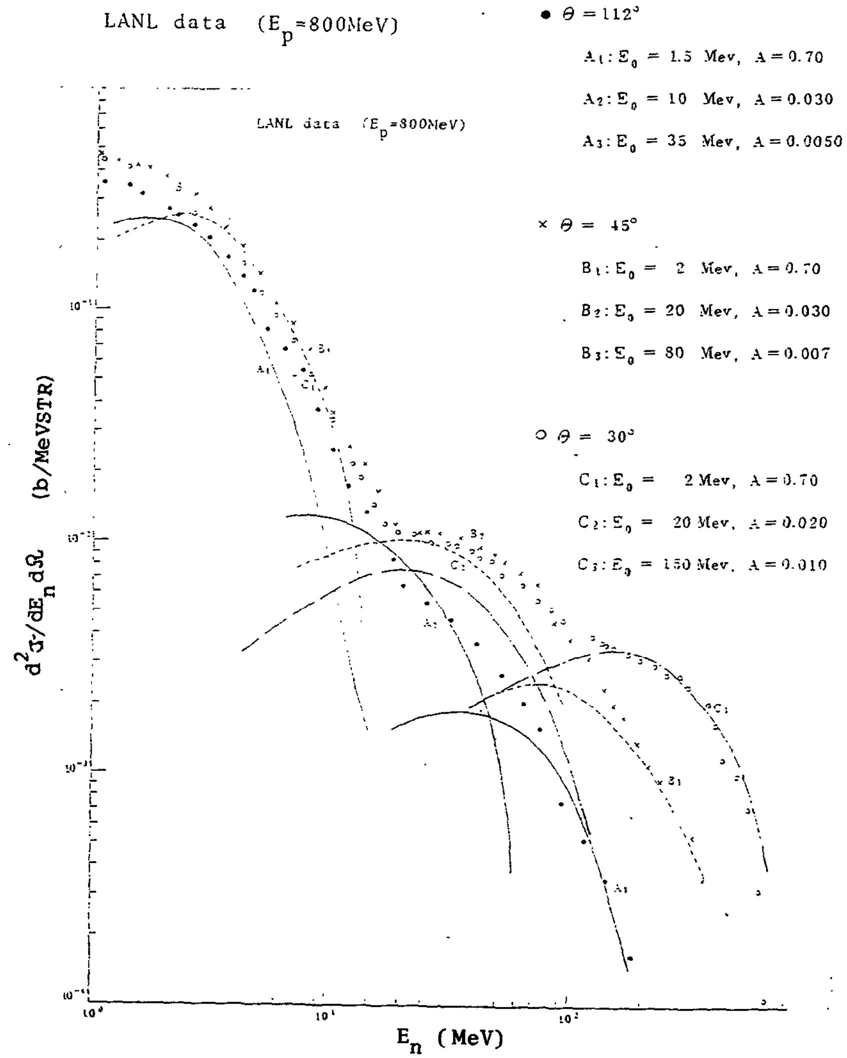
Fig 4



Neutron fluxes on side boundery
(LANL)
E_p=800MeV
Pb cylinder
60cm L
10cm dia.
mfp in
nuclei
× 1.0
× 1.5
Ecut
incident P
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10
10^{2}
10^{3}

Fig 5


KfK data (Ep = 590 MeV)
A(E/E0i)exp(-E/E0i)
θ = 150°
A1 : T=2 Mev, A=0.68
A2 : T=10 Mev, A=0.018
A3 : T=30 Mev, A=0.0034
θ = 90°
B1 : T=2 Mev, A=0.68
B2 : T=20 Mev, A=0.011
B3 : T=50 Mev, A=0.0039
θ = 30
C1 : T=2 Mev, A=0.68
C2 : T=25 Mev, A=0.015
C3 : T=70 Mev, A=0.010
θ = 23°
D1 : T=3 Mev, A=82
D2 : T=25 Mev, A=0.035
D3 : T=100 Mev, A=0.033
d2σ/dEndΩ (b/MeV STR)
En (Mev)
Fig 7


LANL data (Ep=800MeV)
θ = 112°
A1: E0 = 1.5 Mev, A=0.70
A2: E0 = 10 Mev, A=0.030
A3: E0 = 35 Mev, A=0.0050
θ = 45°
B1: E0 = 2 Mev, A=0.70
B2: E0 = 20 Mev, A=0.030
B3: E0 = 80 Mev, A=0.007
θ = 30°
C1: E0 = 2 Mev, A=0.70
C2: E0 = 20 Mev, A=0.020
C3: E0 = 150 Mev, A=0.010
d2σ/dEndΩ (b/MeVSTR)
En (MeV)
Fig 8

<u>Possible Application of James-Stein Estimator to cut Monte-Carlo Computation Cost.</u>

This is a study done mainly by Kimura with a help of Matsubara, a mathematical statistician. J.M. Carpenter noticed the theory of James-Stein Estimater may work.

<u>What is James-Stein-Estimator.</u> The notion of James-Stein Estimator was first introduced on 1960 by C. Stein[10] who pointed out the possibility of improving the usual estimator in the case of multivariate normal (Gaussion) mean.

<u>Simplest example.</u> Suppose we have k test pieces, designated as j = 1, 2, ··· k, of various metals whose length were measured by a certain person using a certain instrument. The length depends on the temperature X. Suppose the results are shown by A_{ij} in Fig 9. It is not possible to know the true length f_{ij}. We usually take the estimate Y_{ij} by the least square fitting against X.

The measurement for A_1, for example, is independent of the measurements for A_2, A_3··· and it is quite natural to take separately the least square fitting. We have, however, missed to use other information obtainable from the data of A_2, A_3 ···. By taking into account all the data of all other samples simultaneously, we might be able to shift somewhat the data points like (as shown in Fig 9)

A_{ij} = The original measurements
$A_{ij}^{(1)}$ = A_{ij} shifted vertically in some way
Y_{ij} = The regressed value of A_{ij}
$Y_{ij}^{(1)}$ = The regressed value of $A_{ij}^{(1)}$.

We conjecture that when a proper shifting is applied, then the total "risk" might be less. Here, the risks are defined as follows:

$$\text{RISK } 0 = \sum_{j=1}^{k} \sum_{i=1}^{n} (A_{ij} - f_{ij})^2 \tag{1}$$

$$\text{RISK } 1 = \sum_{j=1}^{k} \sum_{i=1}^{n} (A_{ij}^{(1)} - f_{ij})^2 \tag{2}$$

$$\text{RISK } 2 = \sum_{j=1}^{k} \sum_{i=1}^{n} (y_{ij} - f_{ij})^2 \tag{3}$$

$$\text{RISK } 3 = \sum_{j=1}^{k} \sum_{i=1}^{n} (y_{ij}^{(1)} - f_{ij})^2 \tag{4}$$

If we can observe a tendency

RISK 1 ≦ RISK 0, RISK 3 ≦ RISK 2 (5)

then it may be allowed to say that the shifted data points $A_{ij}^{(1)}$ and their regressed values $y_{ij}^{(1)}$ are closer to the true values. And there does exist such a case actually.

The most essential point to reduce $A_{ij}^{(1)}$ and $y_{ij}^{(1)}$ in this James-Stein proceedure is the introduction of "Shrinkage factor ρ" which plays the central role to take into account the fluctuation of measurement in total.

The "sectioned" data at each X = Xi, that is A_{ij}(j = 1, 2,···k) will be processed by the James-Stein proceedure (called JSE) to give rise to

$$A_{ij}^{(1)} = \bar{\mu}_i + \rho_i (A_{ij} - \bar{\mu}_i) \tag{6}$$

$$\bar{\mu}_i = \text{average of } y_{ij} \text{ over } j = \frac{1}{k} \sum_{j=1}^{k} y_{ij} \tag{7}$$

and ρ_i is given by

$$\rho_i = 1 - \frac{k-3}{k-1} \cdot \frac{\sigma^2 \{\frac{1}{n} + (X_i - \bar{X})^2 / \sum_i (X_i - \bar{X})^2\}}{\sum_j (y_{ij} - \frac{1}{k} \sum_j y_{ij})^2} \tag{8}$$

ρ_i are usually less than 1 and have a function to smear out the fluctuation. A large A_{ij} may have larger chance to have fluctuated to the positive side from the true value and vice versa. In case ρ_i < 0, we should put it equal to 0. σ^2, the true variance, which we can not know, but can be replaced by its estimate S^2 which is the average over j of residual variances S_j^2 from the sample regression lines, (that is as shown in the graph)

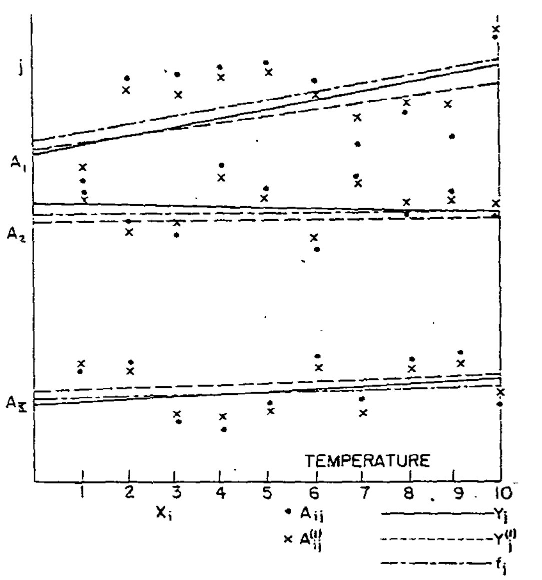


Fig 9

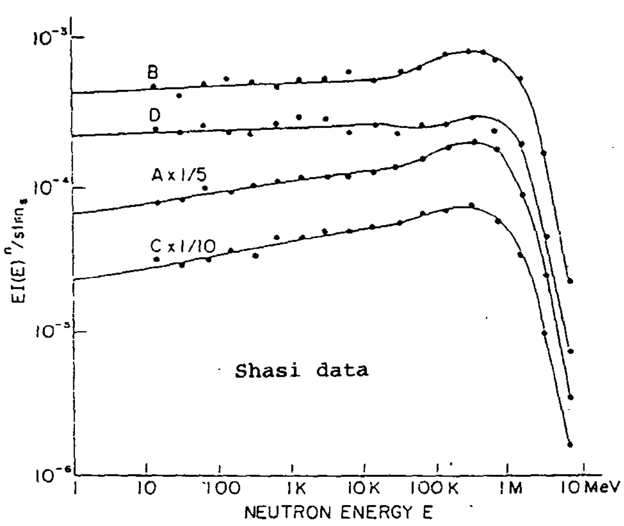


Fig 10

$$S^2 = \frac{1}{k} \sum_j{}^2 S_j^2,$$

$$S_j^2 = \frac{1}{n-2} \left\{ \sum_i (A_{ij}-\bar{y}_j)^2 - \frac{\sum_i (X_i-\bar{X})(A_{ij}-\bar{y}_j)}{\sum_i (X_i-\bar{X})^2} \right\} \quad (9)$$

$$y_j = \frac{1}{n} \sum_i y_{ij}$$

Thus we can calculate $A_{ij}^{(1)}$ and $y_{ij}^{(1)}$. We define the Figures of Merit(FOM) as follows:

$$\begin{aligned} \text{FOM 1} &= \text{RISK 0/RISK 1} \\ \text{FOM 2} &= \text{RISK 2/RISK 3} \end{aligned} \quad (10)$$

FOM 1 and FOM 2 may be of some measure how much the data were improved. FOM 1 and FOM 2 are generally larger than 1 and tend to 1 when the measurement of A_{ij} is more accurate.

Shashi data.[11] This is the raw data of neutron spectra from target-reflector-moderator system of various configurations for the intense pulsed neutron source (IPNS) of Argonne. A, B, C and D correspond to different neutron beams. We will limit our interest to the 10 eV ∿ 10 KeV region, where log E vs log (EI) have straight lines. See Fig10

Hand calculations using above formulae gives the result that all the ρ_i's are very close to 1 and $A_{ij}^{(1)}$ do not differ from A_{ij} more than 0.5% or so. This is because the fluctuation of all the data are rather small and there remains not much room to shift the regression lines. The Monte-Carlo results of Shashi are already too accurate to allow the JSE proceedure work substantially. (Table1)

Computer experiments simulating the problem. We have done some computer experiment to understand the problem more systematically.

(1) Number of data k was increased to 12, the first 4 of which are the regression lines of Shashi data, 8 others were arbitrarily created. Each of these 120 points on the 12 straight lines are designated by f_{ij} representing the true values which we can not know. The 12 straight lines have different inclination and average.

As a reference, we created another data set, which is consisted of 12 identical horizontal lines of the same height, that is f_{ij} = 0.5000, i = 1, 2 ···10, j = 1, ···12, and compared with the result using above data set. An I-number KR(1, 3) was introduced to compute more general way, that is,

KR = 1 : k = 4, Shashi data (A, B, C, D)
KR = 2 : k = 8, A, B, ···H
KR = 3 : k = 12, A, B, ···L.

To simulate the Monte-Carlo out put, we called randon number generator, of Gaussian, Uniform or Poisson type. In the case like Shashi data for neutron spectra, Poisson should be applied, but we also tried to use other subroutines.

The Shashi data possesses a certain amount of variance S^2 which was calculated to be (0.025)^2. We wanted to take the magnitude of S^2 widely changed, covering the one of Shashi data. For this, we introduced another I number NR(1, 9) to cover wide range of standard deviation as follows:

$$\sigma_G = 2^{(n-NR)} \qquad \text{(Ganssian)(10)}$$
NR(1, 9)

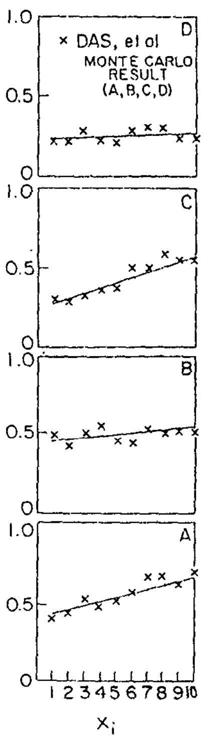


Fig 11a

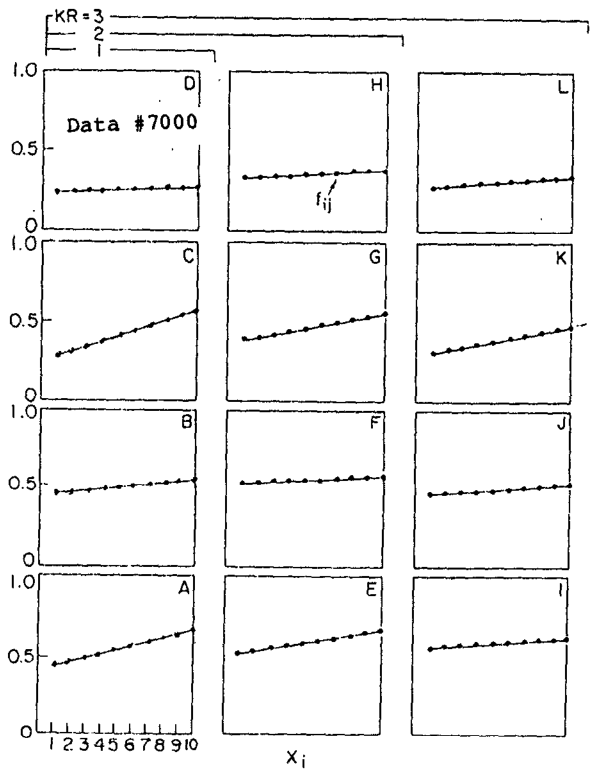


Fig 11b

$$\sigma_U = 2^{(n-NR)/2}\sqrt{f_{ij}(1-f_{ij})} \quad \text{(uniform)} \quad NR(1,\ 9) \qquad (11)$$

$$\sigma_P = \sqrt{f_{ij}/\lambda} = 2^{(n-NR)/2}\sqrt{f_{ij}} \quad \text{(Poisson)} \quad NR(1,\ 7) \qquad (12)$$

with $\lambda = 2^{(NR-n)}$

(n is not the max of i)

n is an integer to shift the range of survey. Usually it is taken 1. We had better taken $\sigma_G = 2^{(n-NR)/2}$ to make the correspondence to the other cases more clearcut. In case of Poisson, we introduced λ to keep the standard deviation independent of absolute number of count of neutrons. In case of uniform, we must call the uniform random number $2^{(NR-n)}$ times and compare it with f_{ij}. Central limit theorem will be applied in the case of σ_U and σ_P.

We obtain from the above 3 equations

$$\ln \sigma_G = (n-NR)\cdot \ln 2 \qquad (13)$$

$$\ln \sigma_U = (n-NR)/2\cdot \ln 2+\frac{1}{2}\ln f_{ij}+\frac{1}{2}\ln(1-f_{ij}) \qquad (14)$$

$$\ln \sigma_P = (n-NR)/2\cdot \ln 2+\ln\sqrt{f_{ij}} \qquad (15)$$

The computer also prints out

$$\sigma_{EX} = \sqrt{RISK\ 0/n\cdot k}, \quad n = 10, \quad k = 4,\ 8 \text{ or } 12. \qquad (16)$$

When the repetition of the computer experiments is increased, σ_{EX} quickly converges into one of above σ's. Therefore, the graphic representation by print out taking the number of lines for NR instead of σ_{EX} is quite adequate. (Fig 12 a, b)

Summary of results. Now, each (*) in Fig 12 a, b is the average of 10 repetitions of rondom number generation. Similar proceedure was repeated 6 times generally, and plotted on the same figure. Fig 13 etc. are plotted the averaged FOM's vs ln σ_{EX}.

Comparison with Shashi data. We must find FOM1 or FOM2 in Fig 14(with Poisson, and for k = 4) corresponding to σ = 0.025 of Shashi's data. Unfortunately, our Poisson subroutine did not work for wide range of NR. It is essentially nothing but a gaussian for small σ_P as 0.025. So, we refer to Fig 13, and find

FOM 1-1 = 0.0054, FOM 2-1 = 0.002.

Thus the application of James-Stein Estimator for Shashi's Monte-Carlo results will improve the data by only 0.5% for FOM1 and 0.2% for FOM2, which are very small, as seen in Table 1 of hand calculation.

Some interesting results. We could find some interesting facts as seen in Figs 12 & 13.

(1) FOM1-1 is larger than FOM2-1 for the same σ_{EX}. This is understandable.
(2) In the normal case, ln(FOM1,2-1) are linear to ln σ_{EX} for wide range, But not exactly of straight lines.
(3) The data points ([illegible]uate very much for FOM1-1 < 0.02 or > 1.0 and also in all region for FOM2.

We can not cxplain these facts just now.

Another data set #4190. We have tried another data set, that is f_{ij} = 0.500000 for all i, j. (We call this #4190. The enlarged data set including Shashi's is called #7000.) We also tried many other data sets between #7000 and #4190, introducing η and ζ, two parameters to approach to #4190 from #7000. The curves of Fig 12a, b gradually go up to higher level and become horizontal, that is, the FOM's become independent of NR or standard deviation, as shown in Fig 15. The fluctuations of FOM's become very large as can be guessed from Fig 12a, b. The total times of calling random number were almost 10^8 to obtain the results as shown in Table 2, in which some FOM's show very large fluctuations due to some capricious results. If we exclude these extremely deviated cases, we obtain (FOM1), (FOM2) or ((FOM1)), ((FOM2)) excluding more cases.

If we are allowed of some conjecture, these numbers may coincide to 10(k-3) and 2(k-3). All are integers in the range of standard deviation, with one exception of the case of KR = 2 and (FOM2) or ((FOM2)).

We can not find the reason just now.

Discussion. Finally, I must come back to the first problem, that is : Can we cut the computation cost of Monte-Carlo calculation ?

Suppose we have cut down to 1/100 of what Shashi had spent, the standard deviation may be 10 times larger. It may be allowed to say that the amount of information contained will be proportional to the inverse of standard deviation squared, generally. Fig 13 shows that the degree of improvement (FOM1-1 or FOM2-1) are almost proportional to σ^2. Does this fact mean that the saving of expenses to 1/100 will result in the improvement of reliability by JSE proceedure but, inevitably accompanied by the decrease of usefulness to 1/100 ? In other words, does the JSE processing give nothing good ? It is not so. The increase of standard deviation is the results of saving cost to 1/100, but the size of standard deviation did not change very much by JSE processing itself.

JSE proceedure will not be vary powerful when the raw data are enough accurate. If the raw data are consisted of sevaral (> 4) regression lines considered as distributed in multi-variate normal distribution, the JSE application will be recommendable, especially when the counting rate, for example, is very low and can not be measured again.

Table 1 Hand Calculated Results

i = 1: $X_i = \log E_i = 1.197$

A	= 3.830×10^{-4}	B	= 4.800×10^{-4}
$A^{(1)}$	= 3.828 "	$B^{(1)}$	= 4.390 "
C	= 3.056 "	D	= 2.388 "
$C^{(1)}$	= 3.060 "	$D^{(1)}$	= 2.397 "

Similar results are obtained for i = 2, ···10.

Table 2

FOM 1 and FOM 2 of #4190 averaged NR=(1,9)

KR=	1	2	3
FOM 1	12.3+4.4	98.8+135	101.2+27.2
FOM 2	2.1+0.1	13.3+ 12.6	18.6+ 2.6
(FOM 1)	11.2+1.7	47.9+2.0	89.9+ 7.6
(FOM 2)	2.07+.04	8.9+0.5	17.9+ 1.6
((FOM 1))	9.53+0.8	47.9+2.0	89.9+ 1.6
((FOM 2))	2.06+0.03	8.9+0.04?	17.9+ 1.6
k	4	8	12
k-3	1	5	9
10(k-3)	10	50	90
2(k-3)	2	10 ?	18

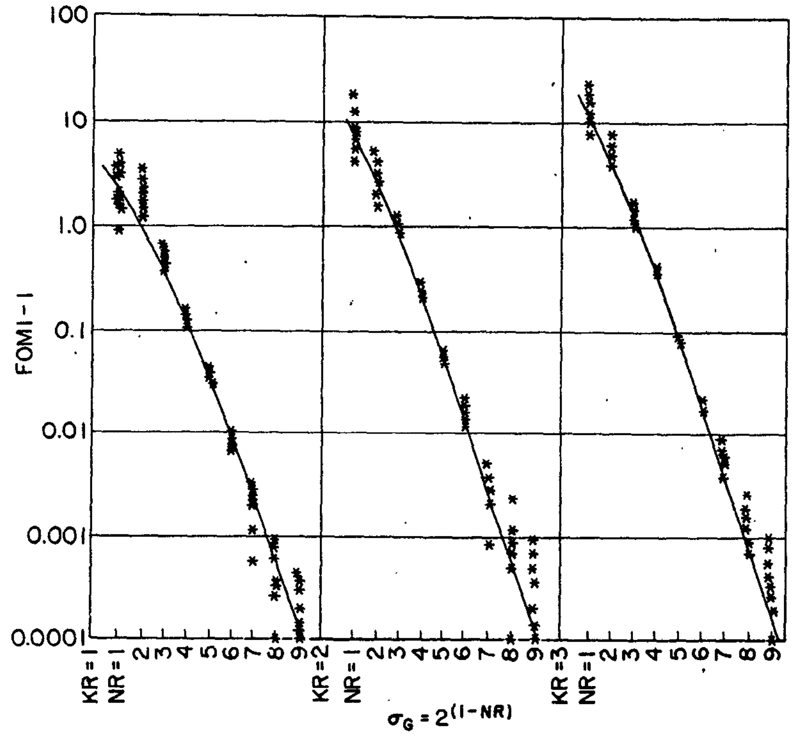


Fig 12a

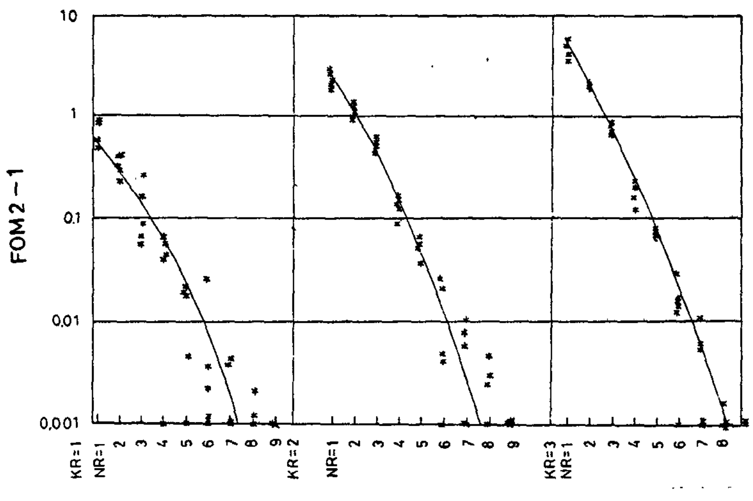


Fig 12b

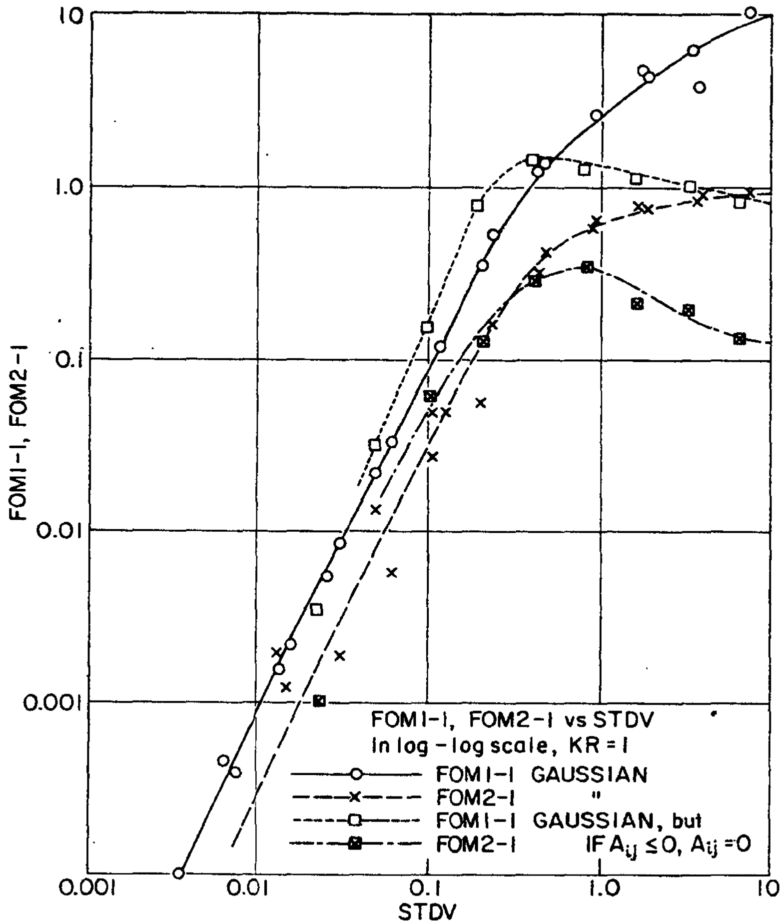

FOMI-I, FOM2-I vs STDV
In log - log scale, KR = I
FOMI-I GAUSSIAN
FOM2-I "
FOMI-I GAUSSIAN, but
FOM2-I IF $A_{ij} \leq 0$, $A_{ij} = 0$
FOMI-I, FOM2-I
STDV
10
1.0
0.1
0.01
0.001
0.001
0.01
0.1
1.0
10

Fig 13

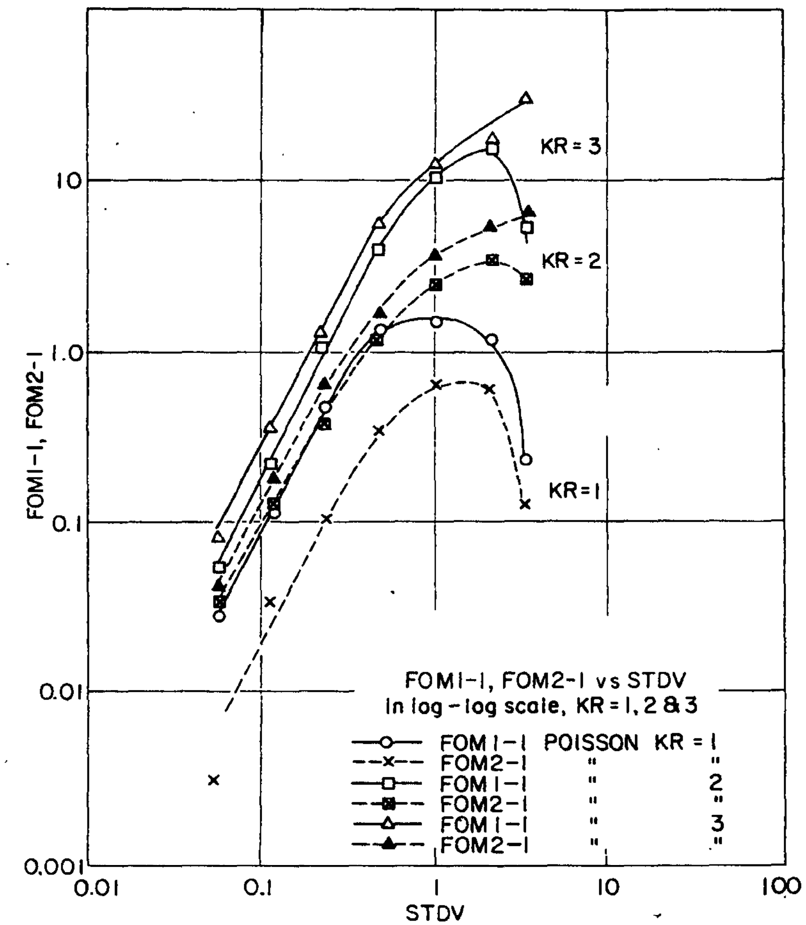

KR = 3
KR = 2
KR = I
FOMI-I, FOM2-I vs STDV
In log - log scale, KR = I, 2 & 3
FOM I-I POISSON KR = I
FOM2-I " "
FOM I-I " 2
FOM2-I " "
FOM I-I " 3
FOM2-I " "
FOMI-I, FOM2-I
STDV
10
1.0
0.1
0.01
0.001
0.01
0.1
1
10
100

Fig 14

This procedure is somewhat similiar to religious liturgy, certifying you that you are now closer to the truth or to God.

References

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Shashi data means the Monte-Carlo results by Mrs Shashikara Das

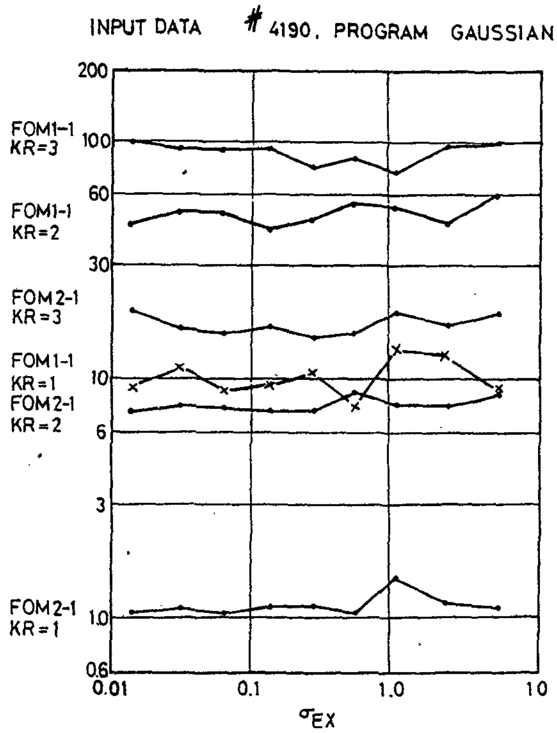

Fig 15