理論から見たRIBF取得すべきデータ2

九州大学
湊　太志

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ARTICLE

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Nuclear data generation by machine learning (I) application to angular distributions for nucleon-nucleus scattering

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ABSTRACT
In order to increase the efficiency of nuclear data evaluation, we have tested a combination of a nuclear reaction model and machine learning algorithm. We calculated nucleon-nucleus elastic scattering angular distributions by using the nuclear reaction model code, and optimized the potential parameters of an optical model to reproduce experimental data by means of the Bayesian optimization. We present optimization cases with the single parameter and two or more parameters, and show that our framework gives the angular distributions that are in good agreement with the observed ones.

ARTICLE HISTORY
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KEYWORDS
Optical potential parameter; parameter optimization; gaussian process regression; angular distribution

Background

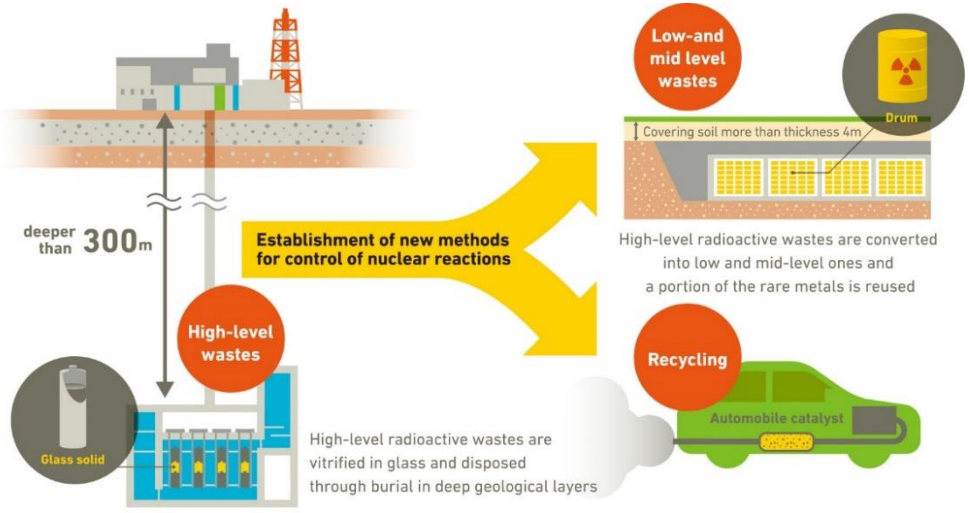
① Development of next generation reactors

日本型タンク型ナトリウム冷却高速炉の概念図

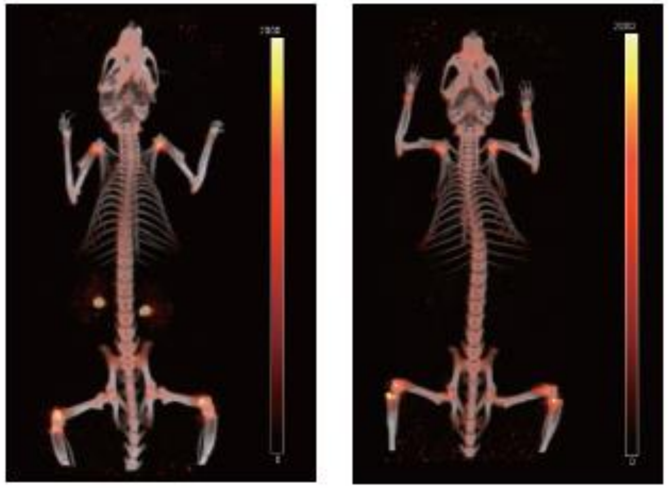
JAEAプレスリリース"日仏ASTRID協力の成果を
反映したナトリウム冷却高速炉の検討"より

② Development for Techniques to reuse radioactive nuclides

革新的研究開発推進プログラム ImPACT



③ RI Productions



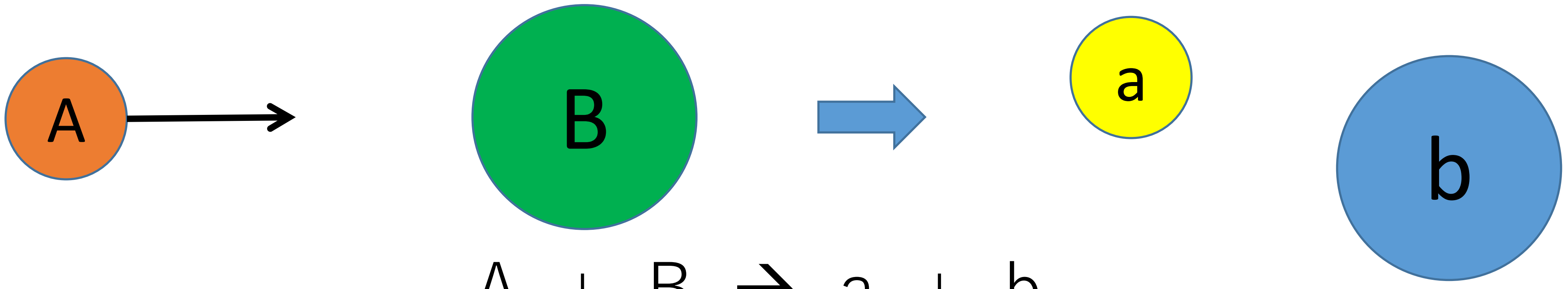
(a) (b)

Fig. 3. (Color) CT-SPECT images of healthy mice obtained 2 h after the intravenous administration of 14 MBq of MDP labeled with ^{99m}Tc obtained from the (a) ^{100}Mo(n, 2n) reaction product ^{99}Mo and (b) fission-^{99}Mo. Most radioactivity is concentrated in the spine, knees, shoulders, and skull; some radioactivity is also seen in the kidneys in (a).

K. Hashimoto et al., J. Phys. Soc. Japan 84, 043202 (2015)

④ Others

Nuclear Reactions



A + B → a + b

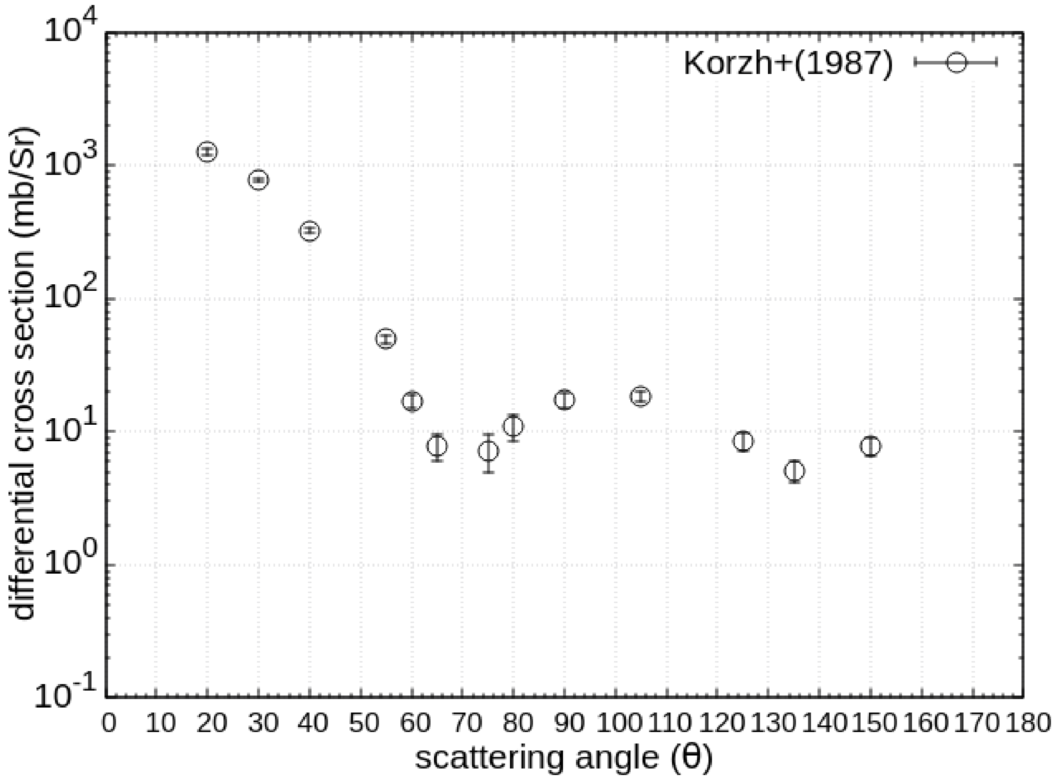
ex.) n+^{99}Mo → ^{100}Mo + γ → Medical RI prod.

ex.) n+^{235}U → X + Y + x + y → Energy production

What nuclei (a & b) are produced through A + B reaction?
→ Experiments

elastic
n+^{54}Fe → n + ^{54}Fe

$$\frac{d\sigma}{d\theta}$$



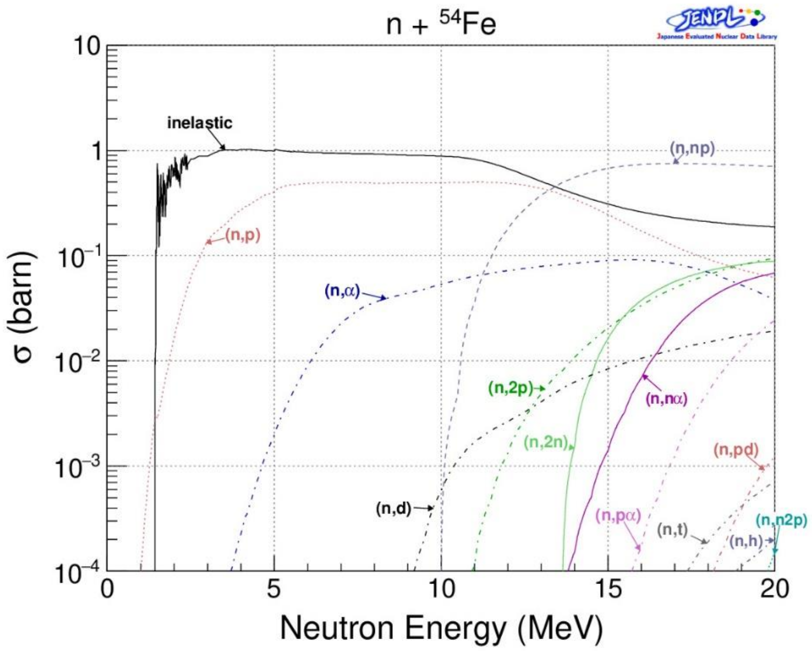
Experimental information is limited
Need to complement with theoretical models

Nuclear Data

≒ Experimental Data + Nuclear Theoretical Models

https://wwwndc.jaea.go.jp/index_J.html

Japanese Evaluated Nuclear Data Library

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0.000000+0 5.941921+1          0          2          0          02643 4  2    2
0.000000+0 0.000000+0          0          0          1        1182643 4  2    3
       118          2                                           2643 4  2    4
0.000000+0 1.000000-5          0          0          2          02643 4  2    5
0.000000+0 0.000000+0                                           2643 4  2    6
0.000000+0 1.000000+0          0          0          2          02643 4  2    7
0.000000+0 0.000000+0                                           2643 4  2    8
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0.000000+0 1.000000+2          0          0          2          02643 4  2   11
7.816011-7 1.832432-8                                           2643 4  2   12
0.000000+0 1.000000+3          0          0          2          02643 4  2   13
2.229795-5 4.241528-6                                           2643 4  2   14
0.000000+0 2.000000+3          0          0          2          02643 4  2   15
1.476442-4 9.179985-5                                           2643 4  2   16
0.000000+0 4.000000+3          0          0          4          02643 4  2   17
3.952600-4 2.218300-4-9.30852-10 2.350879-8                     2643 4  2   18
0.000000+0 6.000000+3          0          0          4          02643 4  2   19
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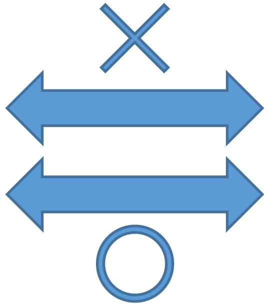
Nuclear Models

・Calculated cross sections

with default input parameters

with adjusted input parameters



Experimental cross sections

There are “technicians” who find model parameters reproducing experimental data.

Generalized Least Squares（GLS)

Time consuming when # of parameter is huge

(My experience: 2 years for ^{23}Na [hundreds parameters])

Optical Potential Model

ELSEVIER

Available online at www.sciencedirect.com

SCIENCE DIRECT

Nuclear Physics A 713 (2003) 231–310

NUCLEAR PHYSICS A

www.elsevier.com/locate/npe

Local and global nucleon optical models from 1 keV to 200 MeV

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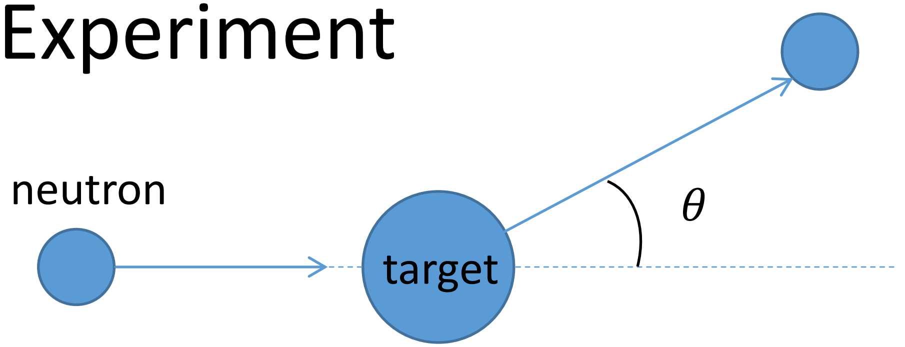
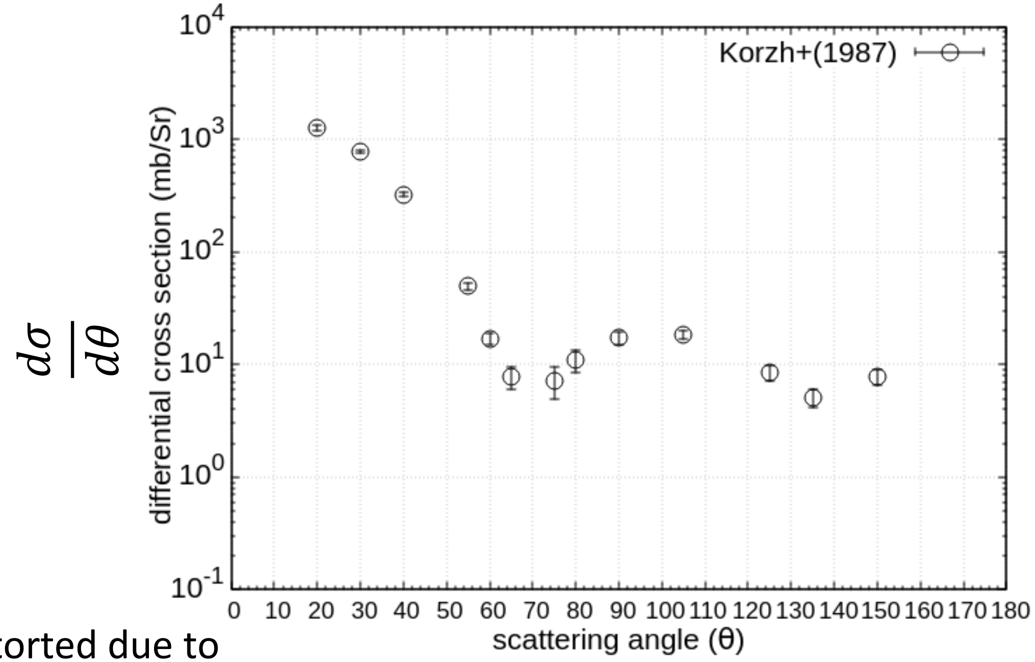
たぶん、一番使われている光学ポテンシャル (Optical Potential)

Neutron-Nucleus Reactions

Experiment





Theory（Evaluation）

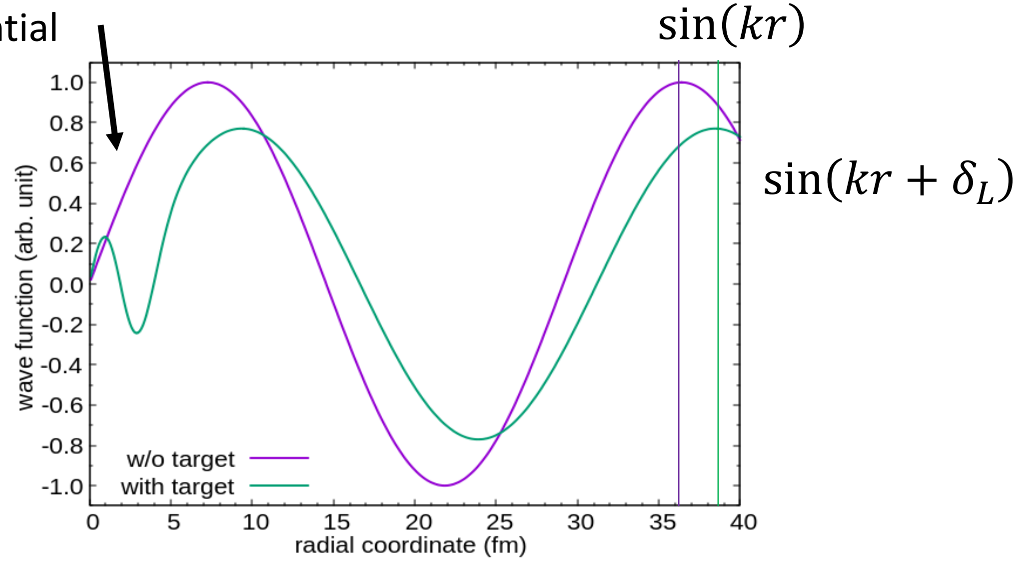
$$\frac{d\sigma}{d\theta} = |F(\theta)|^2$$

$$F(\theta) = \frac{1}{2iK}\sum_L (2L+1)(S_L - 1)P_L(\cos\theta)$$

S matrix $S_L = e^{2i\delta_L}$

Phase shift δ_L is calculated from
Schrodinger-like Eq. with a boundary condition

Distorted due to nucl. potential



Neutron-Nucleus Optical Potential (Kuenida-type)

$$V(E;r) = K\left[-V_R(E)U(r) + i\left\{4W_D(E)a_D\frac{d}{dr}U(r) - \cdots\right\} + \cdots\right]$$

$$\begin{cases} U(r) = \dfrac{1}{1+\exp((r-r_0)/a)} \\ V_R(E) = \left(V_R^0 + V_R^1 E + V_R^2 E^2 + V_R^3 E^3 + V_R^{DISP} e^{-\lambda_R E}\right)\left(1 + \dfrac{1}{V_R^0 + V_R^{DISP}}(-1)^{Z'+1} C_{viso}\dfrac{N-Z}{A}\right) \\ W_D(E) = \left(W_D^{DISP} + (-1)^{Z'+1} C_{wiso}\dfrac{N-Z}{A}\right) e^{-\lambda_D E}\dfrac{E^2}{E^2 + WID_D^2} \end{cases}$$

4 parameter search $\qquad \boldsymbol{x} = \{V_R^0, r_0, a, W_D^{DISP}\}$

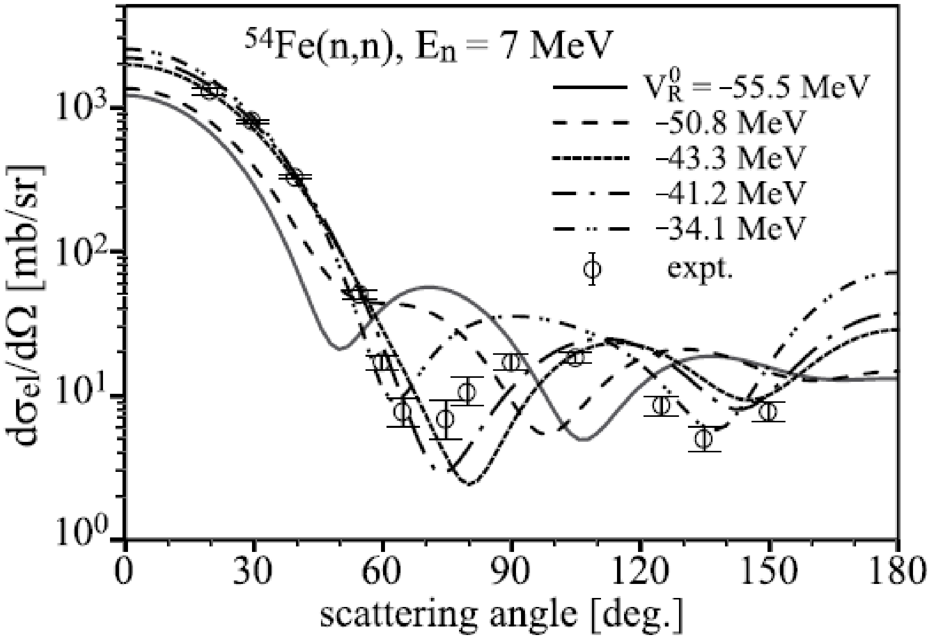
Objective Function

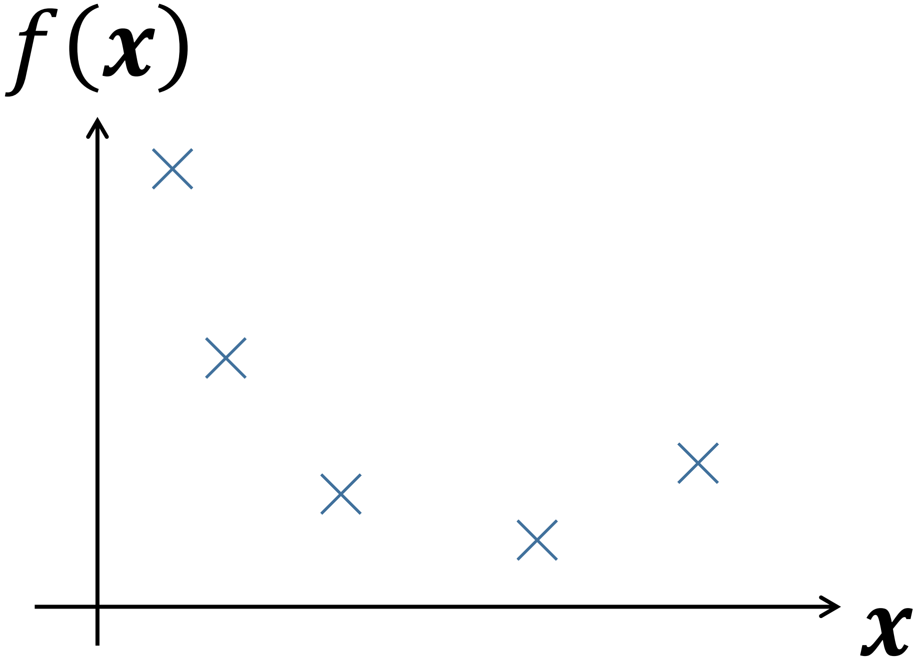
$$f(\boldsymbol{x}) = \sum_i \left(\frac{\sigma_{exp}^{(i)}}{\Delta\sigma_{exp}^{(i)}} \left[\log_{10} \sigma_{th}^{(i)}(\boldsymbol{x}) - \log_{10} \sigma_{exp}^{(i)} \right] \right)^2$$

$\sigma_{exp}^{(i)}$: angular differential cross sections of ^{54}Fe

Collect initial samples at 5points of V_R^0

$$V_R^0 = -55.5, -50.8, -43.3, -41.2, -34.1 \text{ MeV}$$

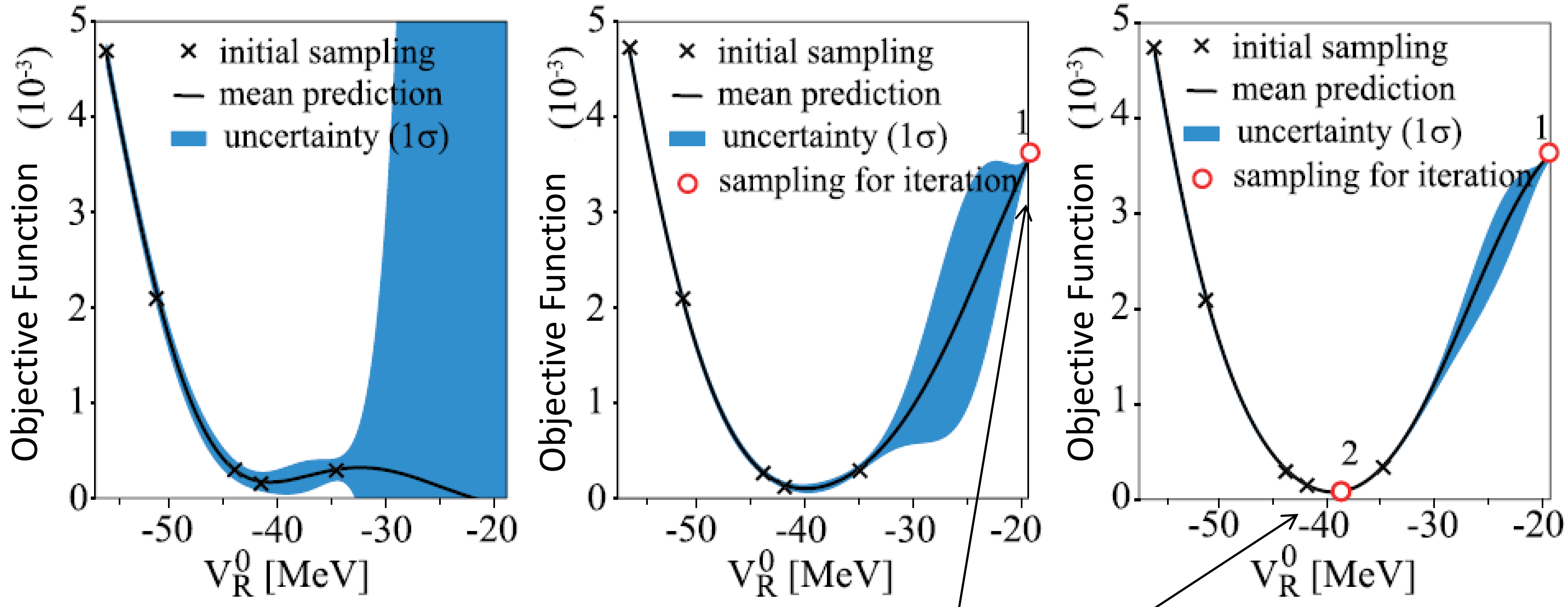




→ Search next V_R^0 by Gaussian Process (GP)

Gaussian Process (GP) and Objective Function

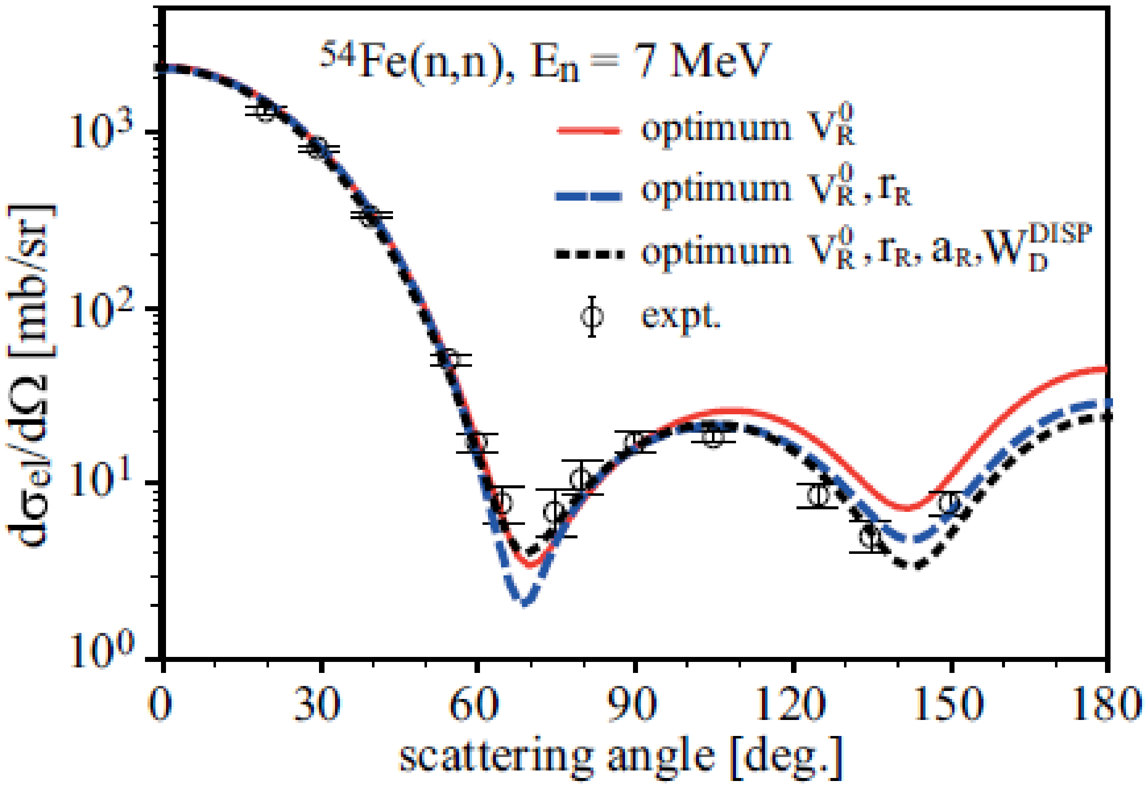
1st Step | 2nd Step | 3rd Step



Kernel: RBF(radial basis function)

Lower Confidence Bound (LCB): $x_{new} = argmin(M(x) - 2\sigma)$

mean



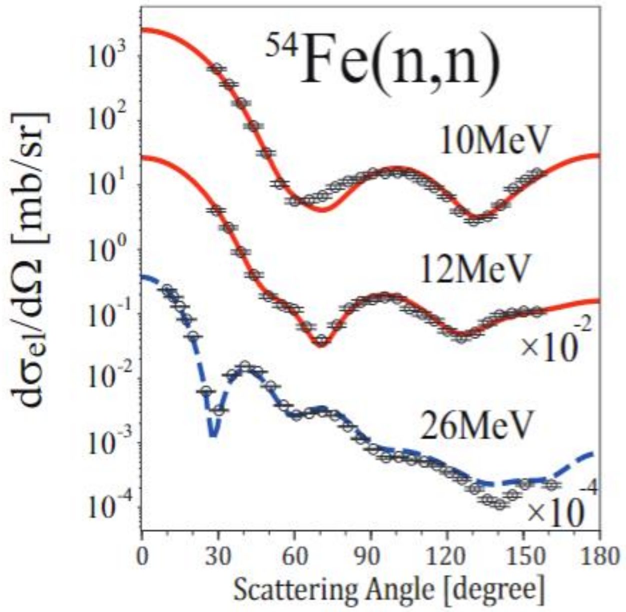
4 parameter search

$$\boldsymbol{x} = \{V_R^0 = -43.5, r_0 = 1.282, a, = 0.525, W_D^{DISP} = 11.2\}$$

RIBFで生産される実験データを、機械学習の学習データとして用い、
核反応理論に含まれている多くのパラメータを最適化・推定する。
それにより核反応を使用するシミュレーションの精度を大幅に向上する。

核反応模型＋機械学習

RIBFで生産される
実験データ



弾性散乱角度微分断面積が一番最適なデータ

Nishina Optical Potential 2023
(NOP2023)

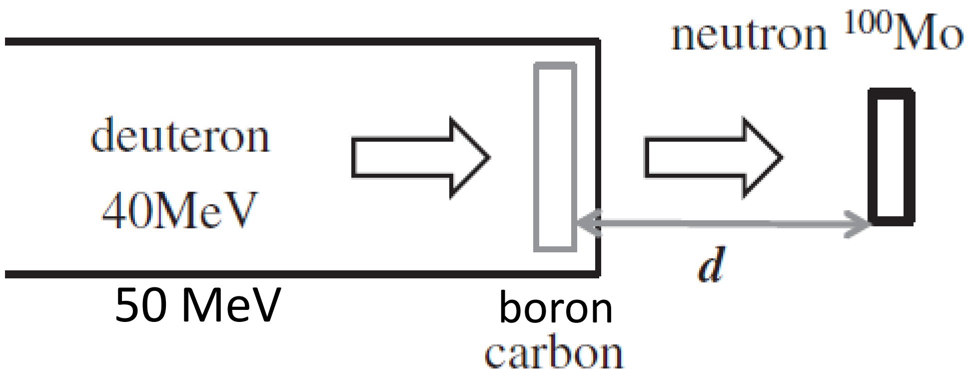
新しいデータが取得できたら、
機械学習で自動更新！

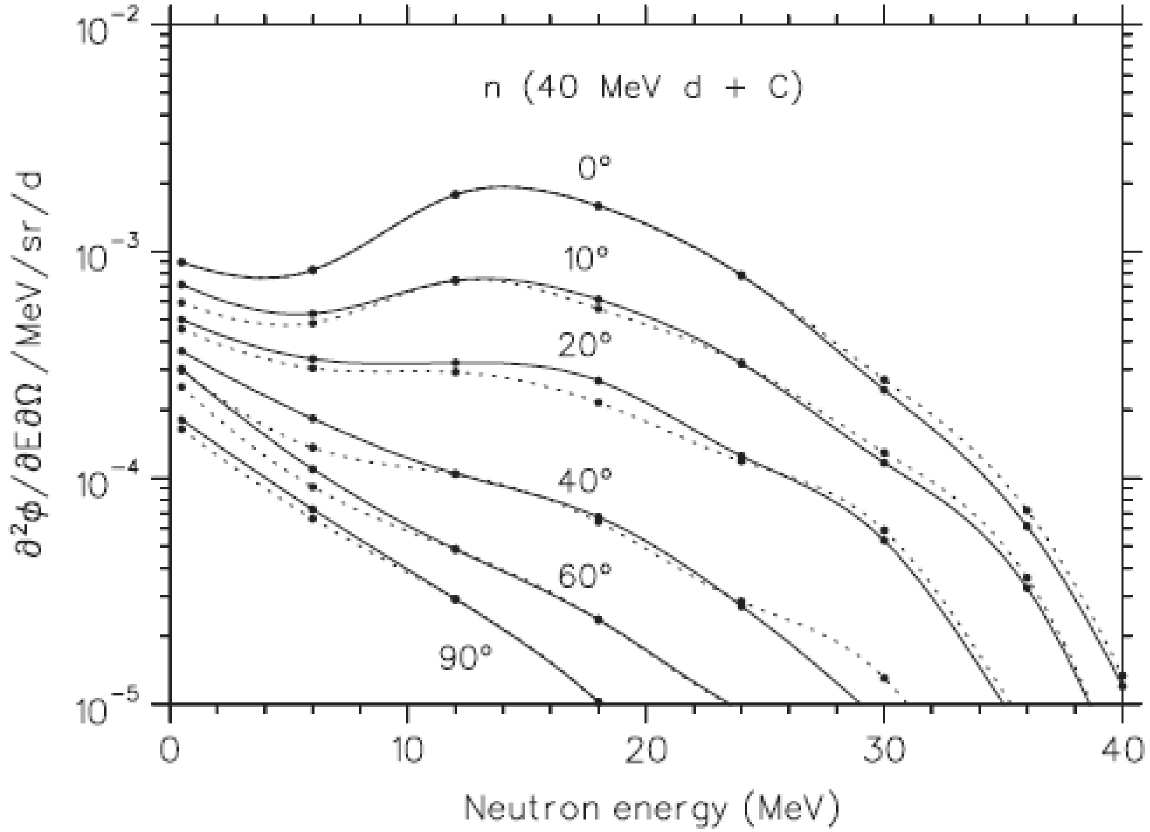
NOP2024
↓
NOP2025
↓
NOP2026
↓
NOP2027
↓
…

Nuclear Data for Medical RI Productions

加速器中性子を使ったRI製造

Y. NAGAI et al., J. Phys. Soc. Jpn. 82 (2013) 064201





G. Lhersonneau et al. NIMA 603 (2009) 228–235

100Mo(n,2n)99Mo -- > 99mTc

Y. NAGAI et al., J. Phys. Soc. Jpn. 82 (2013) 064201

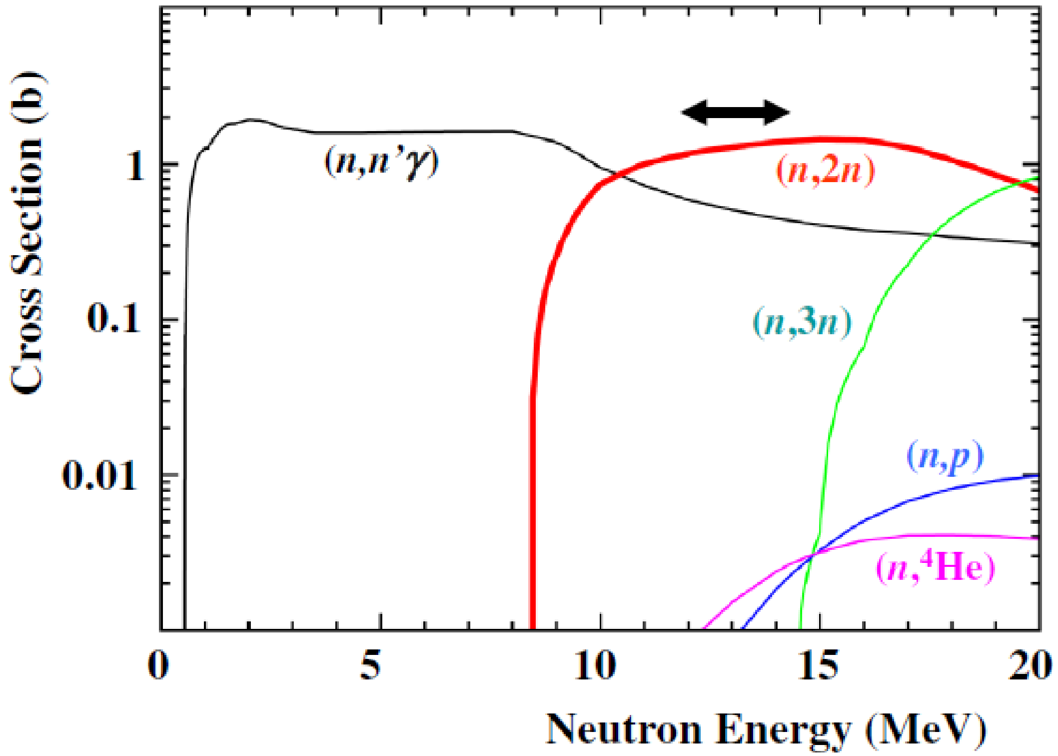
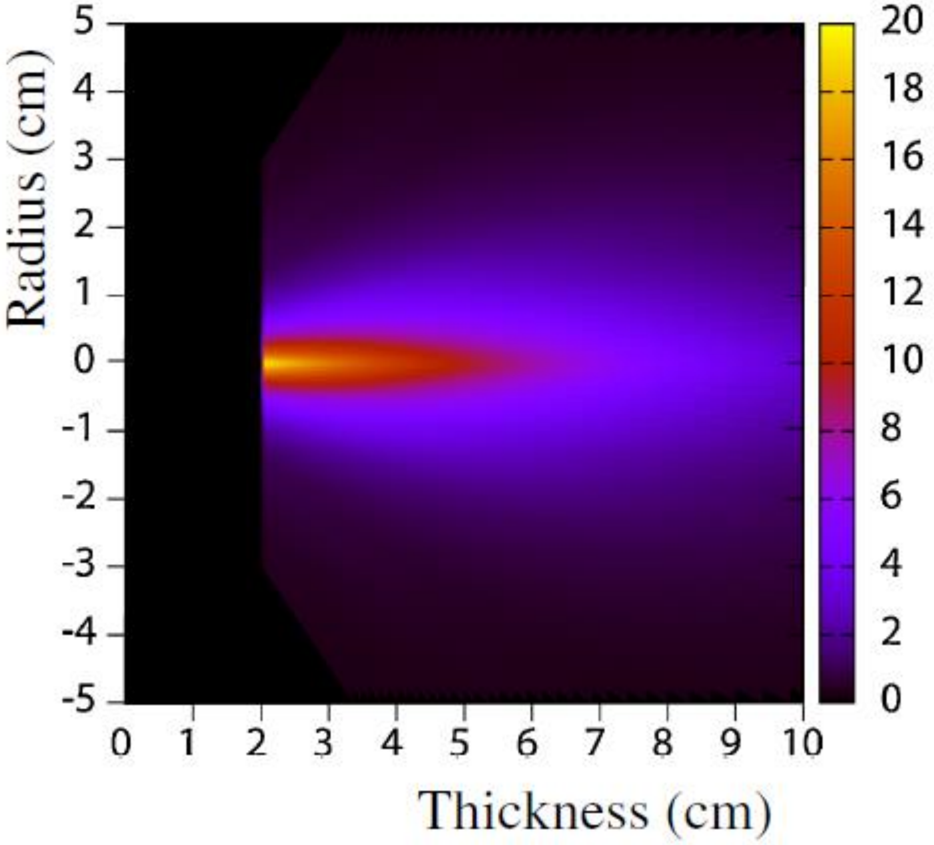
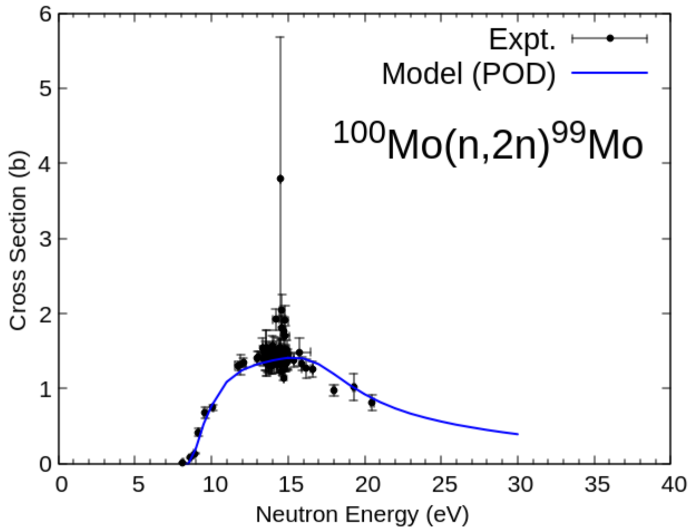
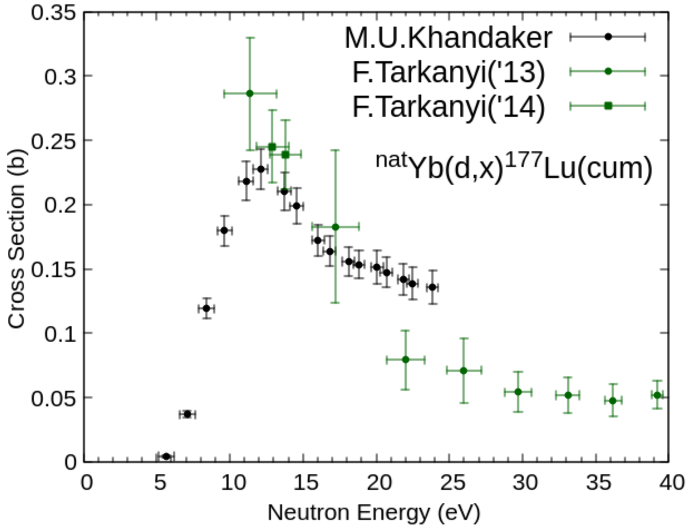


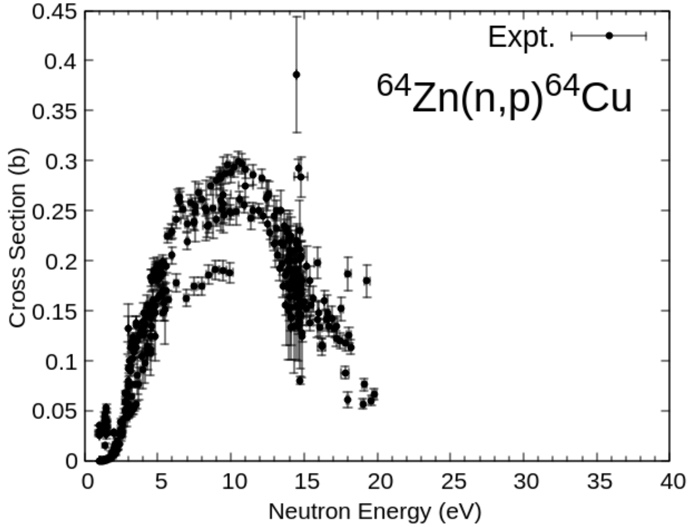
Fig. 2. (Color online) Neutron induced reaction cross sections on ^{100}Mo.

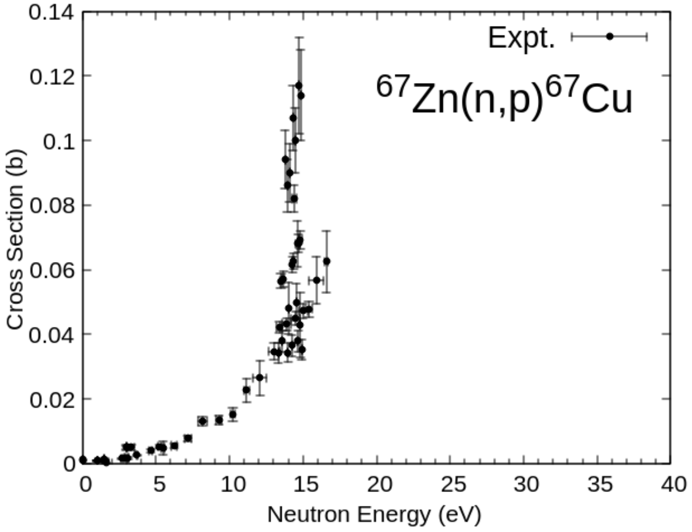


F. MINATO and Y. NAGAI, J. Phys. Soc. Jpn., Vol. 79, No. 9 LETTERS


Expt.
Model (POD)
$^{100}Mo(n,2n)^{99}Mo$
Cross Section (b)
Neutron Energy (eV)


M.U.Khandaker
F.Tarkanyi('13)
F.Tarkanyi('14)
$^{nat}Yb(d,x)^{177}Lu(cum)$
Cross Section (b)
Neutron Energy (eV)


Expt.
$^{64}Zn(n,p)^{64}Cu$
Cross Section (b)
Neutron Energy (eV)


Expt.
$^{67}Zn(n,p)^{67}Cu$
Cross Section (b)
Neutron Energy (eV)

$^{nat}C(d,xn)$の二重微分断面積データ

8) 6-C-0(D,X)0-NN-1,,PY/DA/DE,,TT C4: MF=? MT=? Op=0

Quantity: [TTD] Double-diff.product yield for thick target

g	12	+	i	X4	X4+	X4±	T4	2009 G.Lhersonneau+	4.00e7		34	+ J,NIM/A,603,228,2009	O1746002 [1]	2009LH01 An[6]=0:90 E2[27]=3.2e5:4e7
g	13	+	i	X4	X4+	X4±	T4	1984 K.Shin+	3.30e7		31	+ J,PR/C,29,1307,1984	E2343002 [1]	1984SH04 An=0 E2[31]=2.4e6:3.2e7
g	14	+	i	X4	X4+	X4±	T4		3.30e7		29		E2343003 [1]	1984SH04 An=15 E2[29]=3.4e6:3.2e7
g	15	+	i	X4	X4+	X4±	T4		3.30e7		30		E2343004 [1]	1984SH04 An=45 E2[30]=3.6e6:3.3e7
g	16	+	i	X4	X4+	X4±	T4		3.30e7		26		E2343005 [1]	1984SH04 An=75 E2[26]=2.4e6:2.8e7
g	17	+	i	X4	X4+	X4±	T4		3.30e7		20		E2343006 [1]	1984SH04 An=135 E2[20]=3.6e6:2.6e7

9) 6-C-0(D,X)0-NN-1,,PY/DA/DE,,TT/CH C4: MF=? MT=? Op=0

Quantity: [TTD] Thick targ.prod.yld. d/dA/dE per electric charge

18	+	i	X4	X4+	X4±	T4	2021 M.K.A.Patwary+	1.20e7	3.00e7	1401	+ J,NST,58,252,2021	E2706002 [1]	An[5]=0:45
19	+	i	X4	X4+	X4±	T4	2020 H.Takeshita+	1.34e7		31	+ J,NIM/A,983,164582,2020	E2681002 [1]	2020TA17 An=3:4
20	+	i	X4	X4+	X4±	T4		1.34e7		29		E2681013 [1]	2020TA17 An=0
21	+	i	X4	X4+	X4±	T4		1.34e7		32		E2681014 [1]	2020TA17 An=15
22	+	i	X4	X4+	X4±	T4		1.34e7		32		E2681015 [1]	2020TA17 An=30
23	+	i	X4	X4+	X4±	T4	2014 Y.Tajiri+	5.00e6		104	+ J,NSTP,4,582,2014	E2591002 [1]	An[6]=0:140 E2[19]=1.3e6:1e7
24	+	i	X4	X4+	X4±	T4		9.00e6		183		E2591003 [1]	An[8]=15:140 E2[26]=1.5e6:1.4e7
25	+	i	X4	X4+	X4±	T4	2004 M.Hagiwara+	4.00e7		727	+ J,JNM,329-333,218,2004	E1985002 [2]	An[10]=0:110 E2[77]=1e6:4.1e7

必ずしもデータ数は充実していない（d@13MeV, 33MeV, 40MeV）

理研で中性子源としての使える可能性のある原子核を考慮するため、
様々な標的核に対するの情報が取りだせられれば･･･