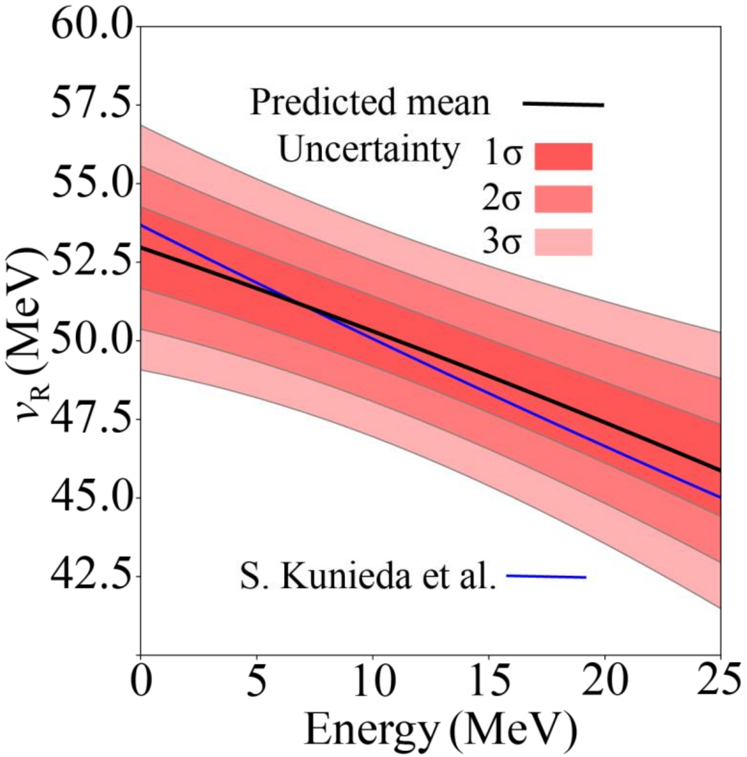
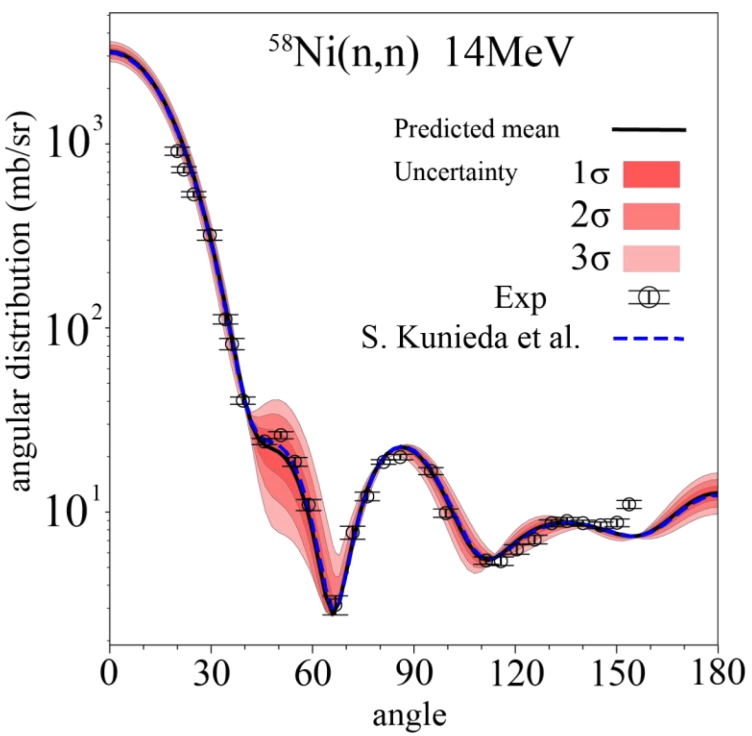
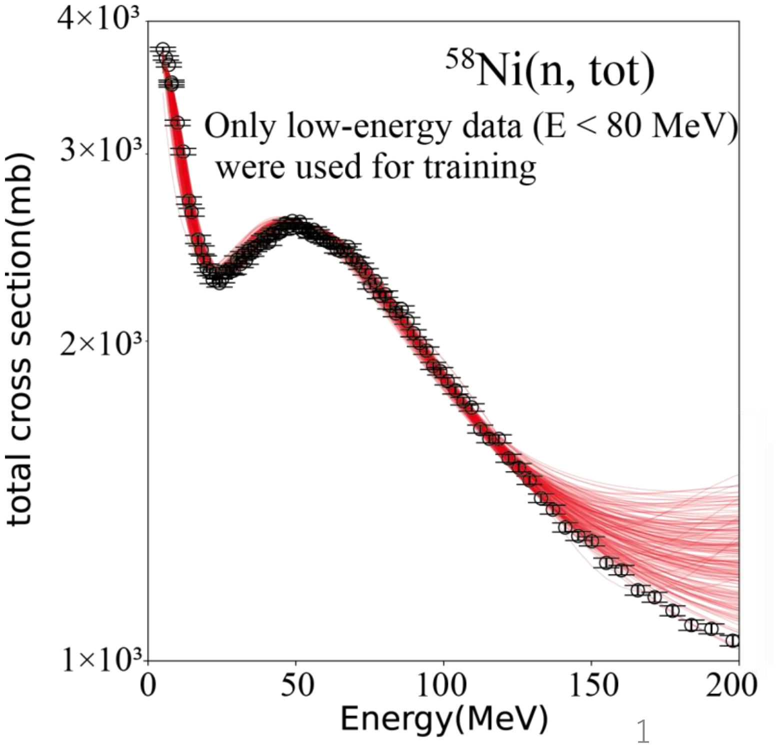
Generating nuclear reaction data by machine learning

Masaaki Kimura (Nishina Center, RIKEN)







Seven Ways AI Will Change Nuclear Science and Technology

As in other fields of science, ML also has strong impact on nuclear science.

IAEA news on Sep. 2022

Nuclear science and fusion research

nuclear science, particularly in areas like data analysis, theoretical modeling, experiment design and fusion research.

Nuclear power

Enhancing the efficiency, safety, and reliability of nuclear power by optimizing procedures and improving reactor design.

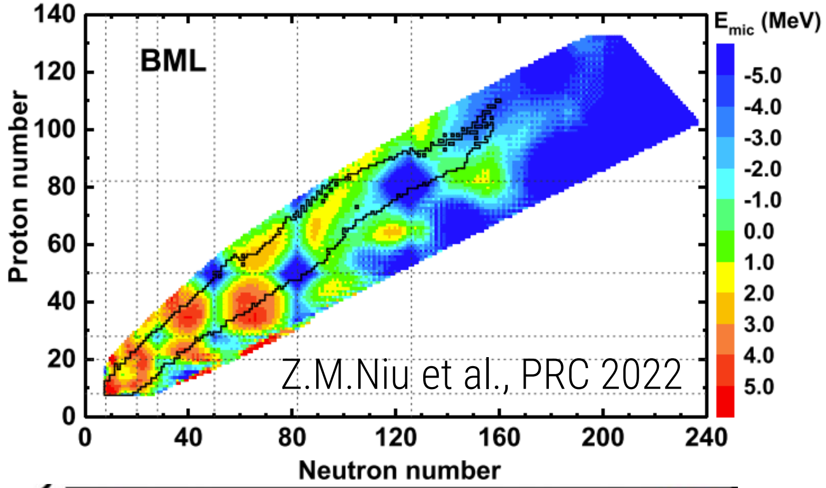
Nuclear security and radiation protection

Improving radiation detection, enhancing physical protection systems, and identifying cyber-attacks on nuclear facilities.

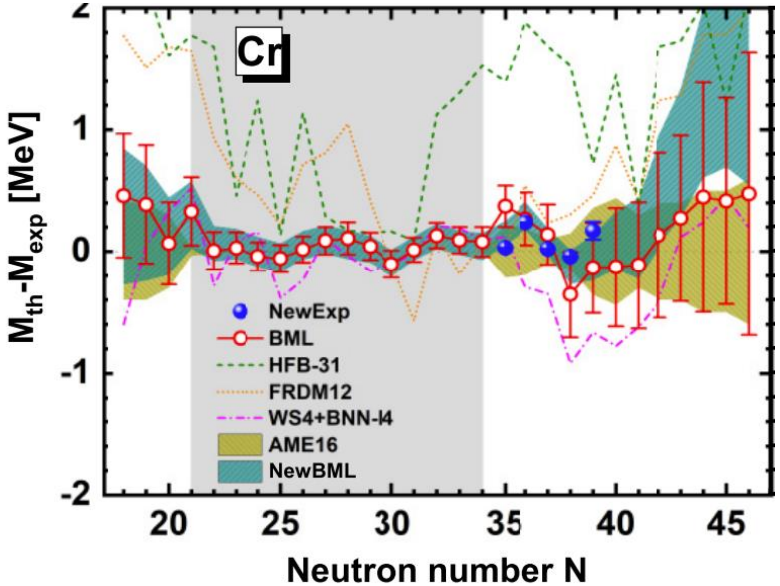
ML in fundamental nuclear physics

Nuclear mass & decay lifetime prediction

ML improves nuclear model predictions



Z.M.Niu et al., PRC 2022

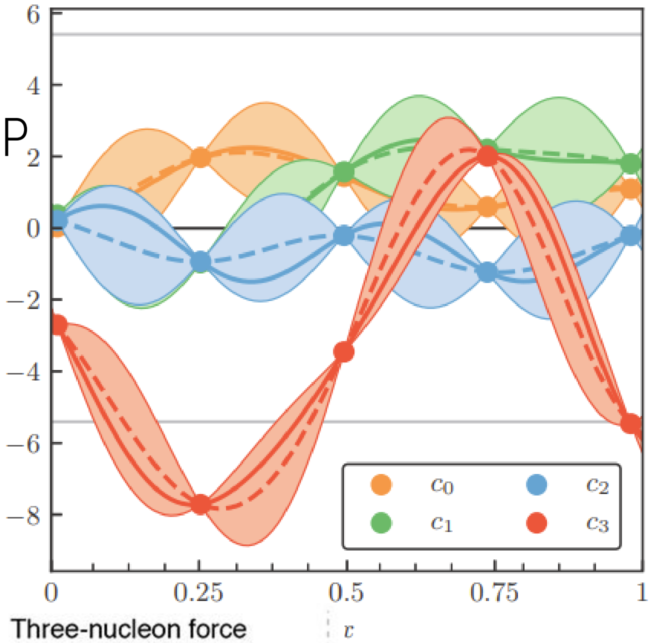


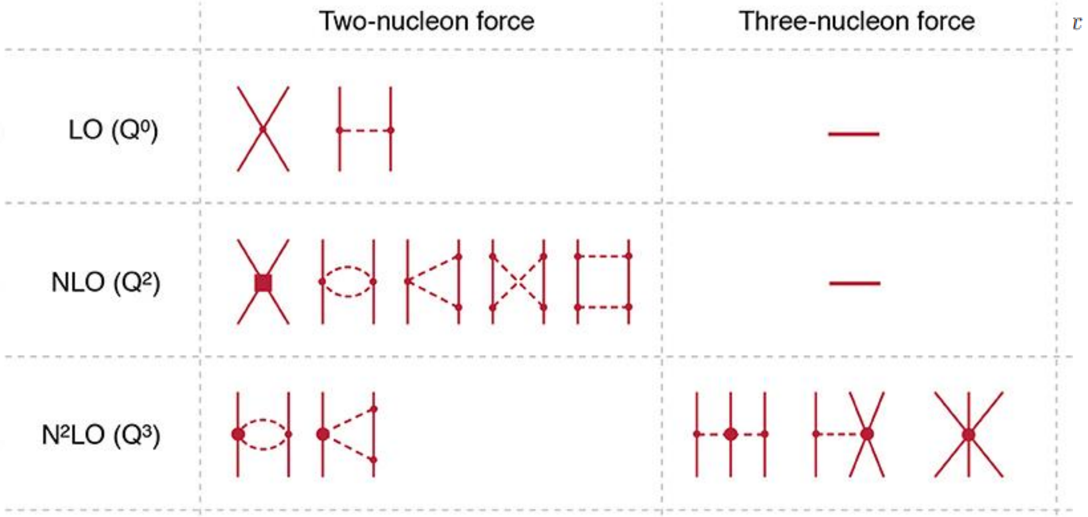
Determining parameters of nuclear interaction

Low-energy coupling constants of chiral EFT are determined by GP

J. A. Melendez, PRC 2019

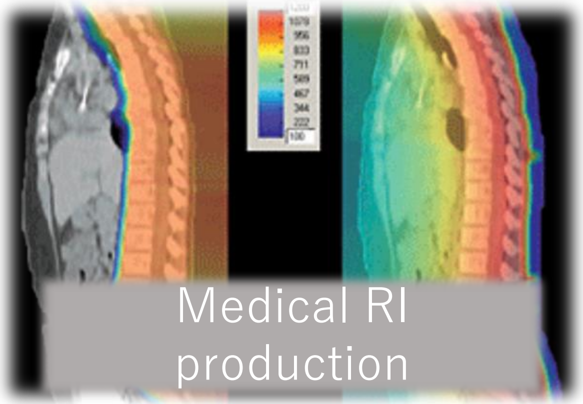
E. Epelbaum et al., Front. Phys. 2020

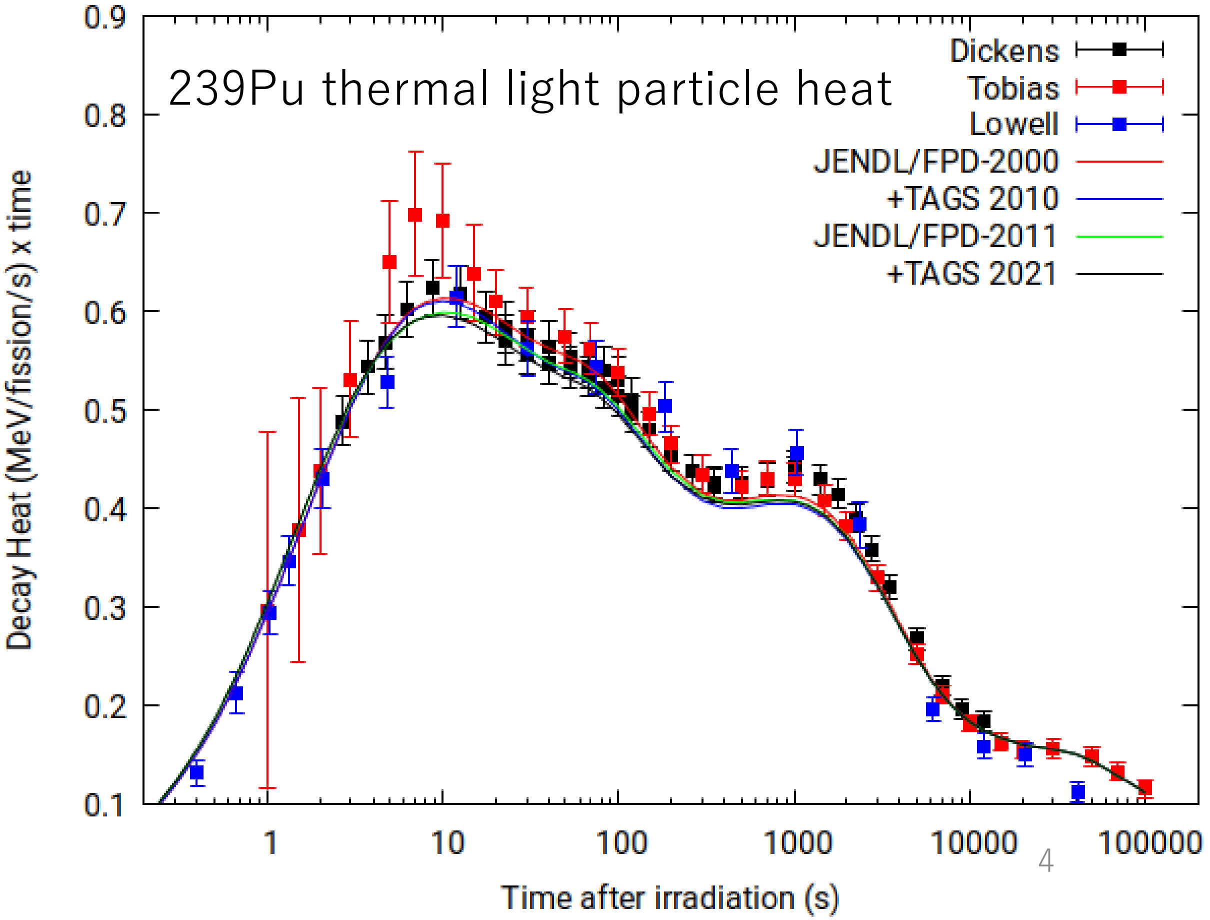




ML in applied nuclear science

For the practical use of nuclear reactions, nuclear database is indispensable which requires statistical data analysis and model predictions
⇨ ML has stronger impact on applied nuclear science.





ML in applied nuclear science

For the practical use of nuclear reactions, nuclear database is indispensable which requires statistical data analysis and model predictions
⇨ ML has stronger impact on applied nuclear science.

Plan of this talk

- What is the nuclear reaction data and its evaluation?
- An example for ML assisted/generated nuclear data
- Overview of TRIP project at RIKEN
- Summary

What is the nuclear reaction data?

The nuclear reaction database is a compilation of reaction conditions and reaction observables such as reaction energy, cross-sections, reaction products, errors etc.
There are two kinds of database

(1) Experimental Nuclear Reaction data (EXFOR)

Extensive compilation of experimental nuclear reaction data managed by IAEA

It contains 22,000+ experiments since 1934 (Discovery of neutron was in 1932!), including the Nihonium experiments

Not suitable for practical use
- Scattered and missing data
- Inconsistent data

Entry for Nihonium experiment in 2004

```
ENTRY          E1920    20180123   20180124   20180123      E110
SUBENT      E1920001    20180123   20180124   20180123      E110
BIB               14          53
TITLE      Experiment on the synthesis of element 113 in the
           reaction 209Bi(70Zn,n)278-113
AUTHOR     (K.Morita, K.Morimoto, D.Kaji, T.Akiyama, S.Goto,
            H.Haba, E.Ideguchi, R.Kanungo, K.Katori, H.Koura,
            H.Kudo, T.Ohnishi, A.Ozawa, T.Suda, K.Sueki, H.S.Xu,
            T.Yamaguchi, A.Yoneda, A.Yoshida, Y.L.Zhao)

                       (partially omitted)

DECAY-DATA (113-NH-278,,A,11680.)
           Alpha decay (11.68+-0.04 MeV, 344 micro-sec) measured
           (111-RG-274,,A,11150.)
           Alpha decay (11.15+-0.07 MeV, 9.26 msec) measured
           (109-MT-270,,A,10030.)
           Alpha decay (10.03+-0.07 MeV, 7.16 msec) measured
           (107-BH-266,,A,9080.)
           Alpha decay (9.08+-0.04 MeV, 2.47 sec) measured
```

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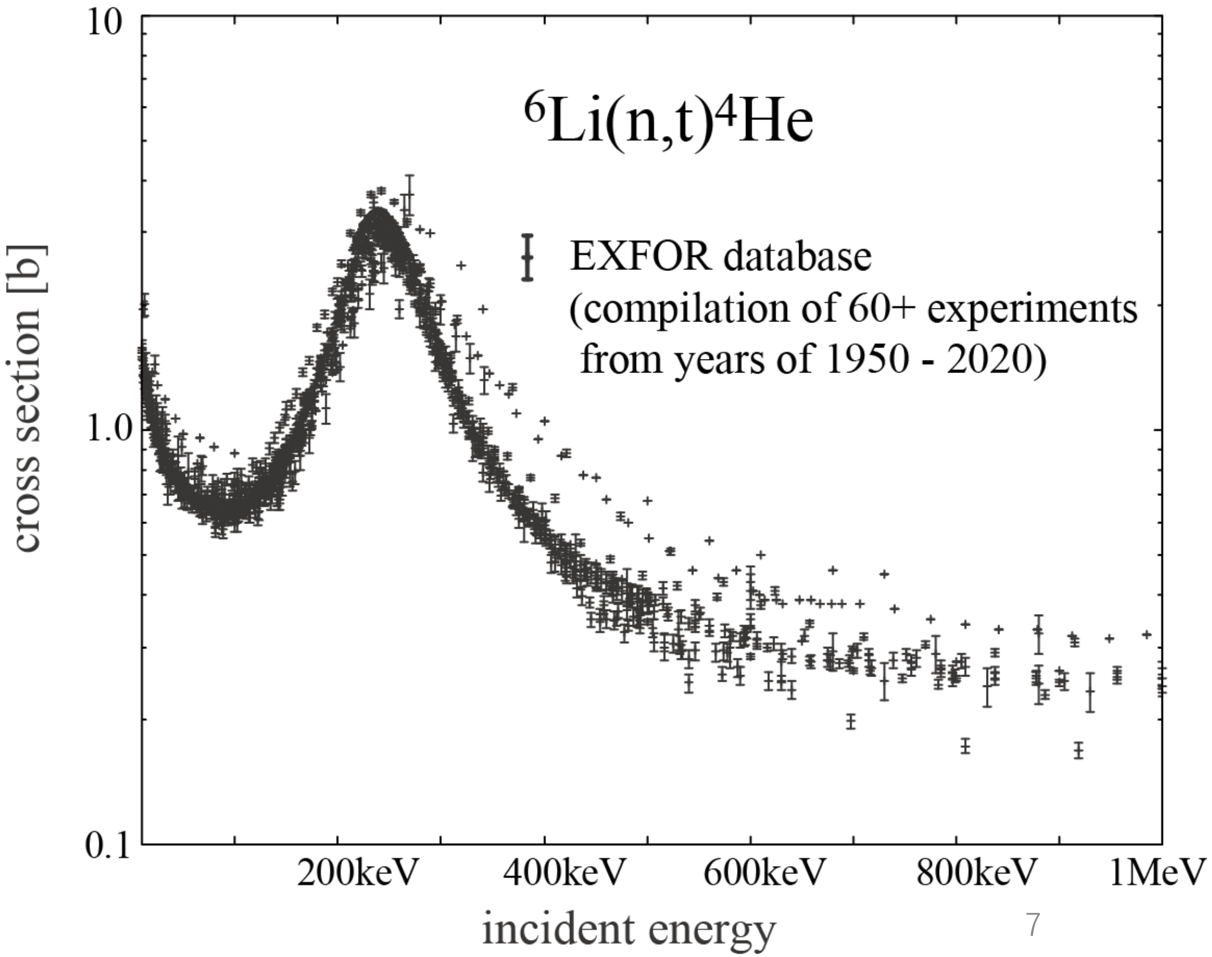


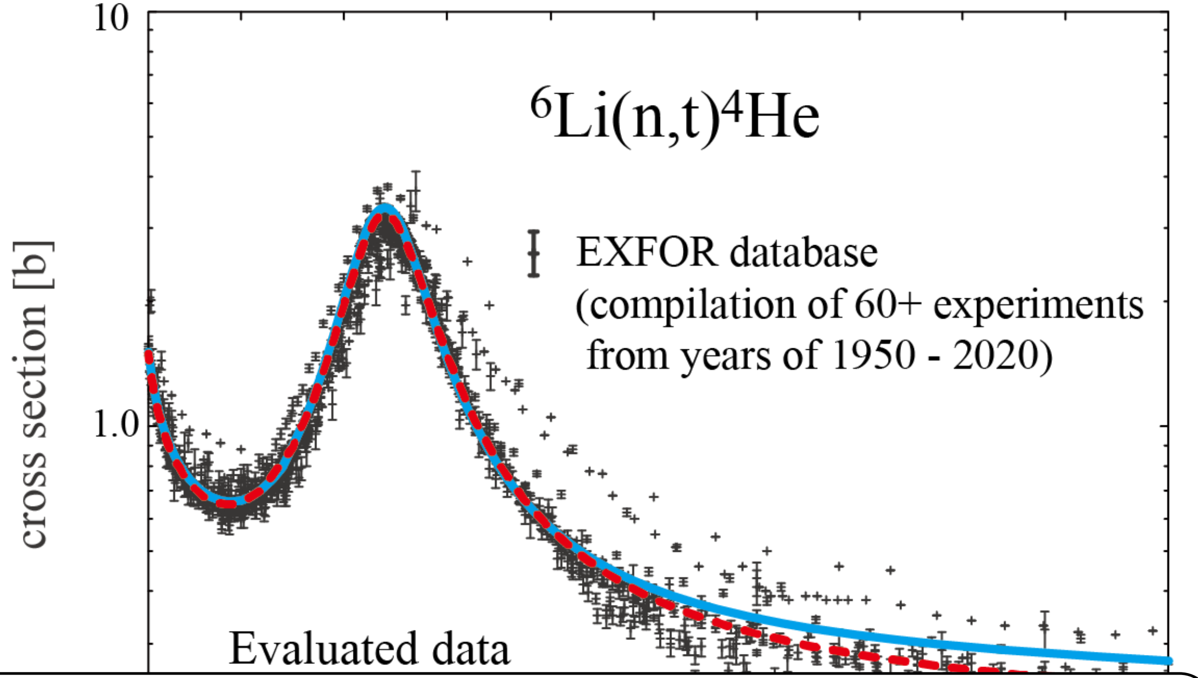
What is the nuclear reaction data?

The nuclear reaction database is a compilation of reaction conditions and reaction observables such as reaction energy, cross-sections, reaction products, errors etc. There are two kinds of database

(2) Evaluated nuclear data
(ENDF, JEFF, JENDL, TENDL,…)

Compilation of recommended value and its error

Building evaluated nuclear data requires
- Examination of precision and reliability of data
- Nuclear model calculations to determine the recommended value



You can imagine that this procedure is man-power/time/money demanding process

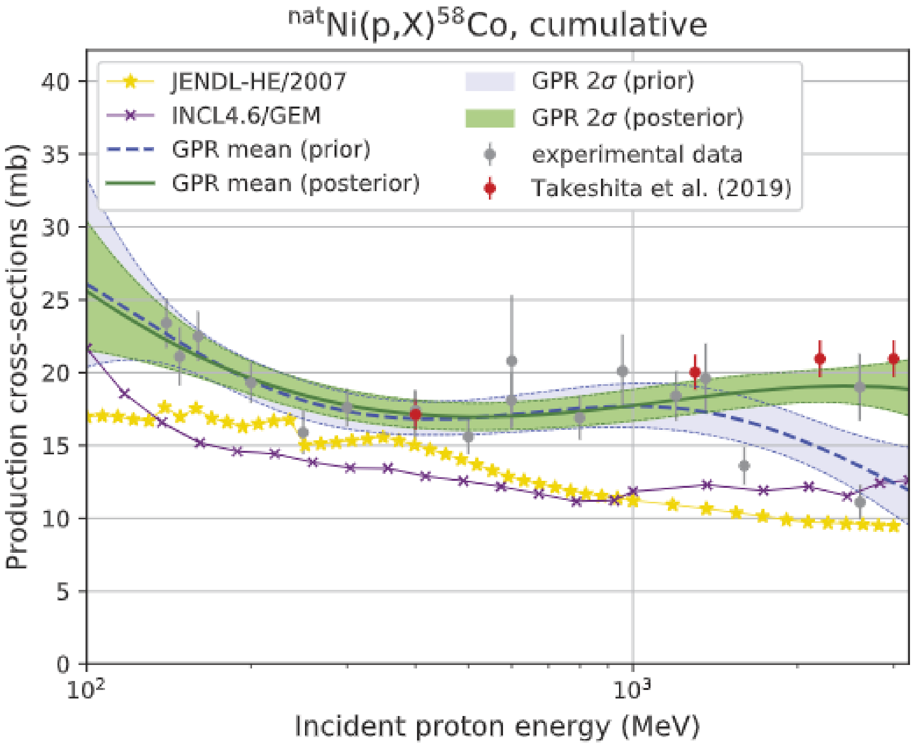
And ML is a game changer…

Nuclear data assisted/generated by ML

Actually, many institutions, companies and organizations have been applying ML tech. for the evaluation of nuclear database

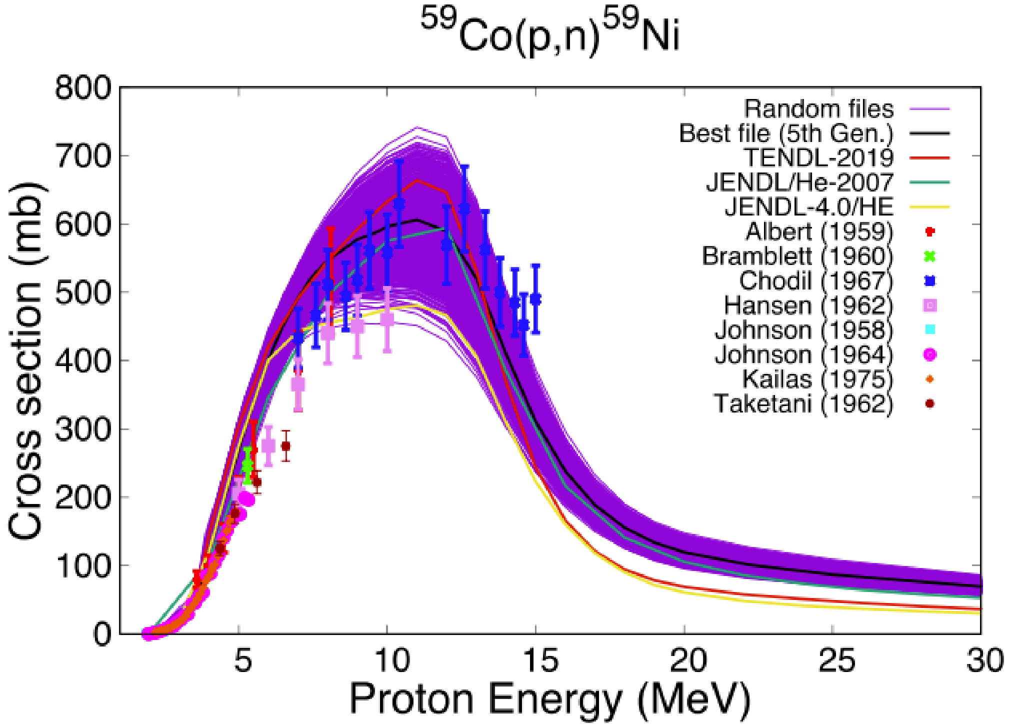
H. Iwamoto, J. Nucl. Sci. and Tech. (2020)

Gaussian Process Regression



E. Alhassan et al, Nucl. Sci. Tech (2022)

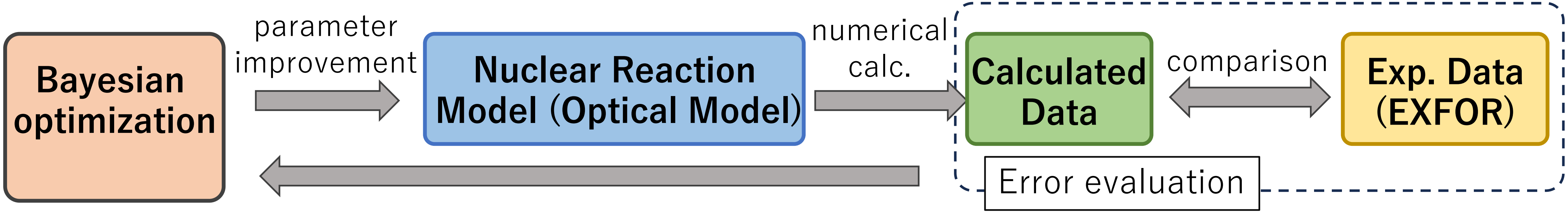
Iterative Bayesian Monte Carlo



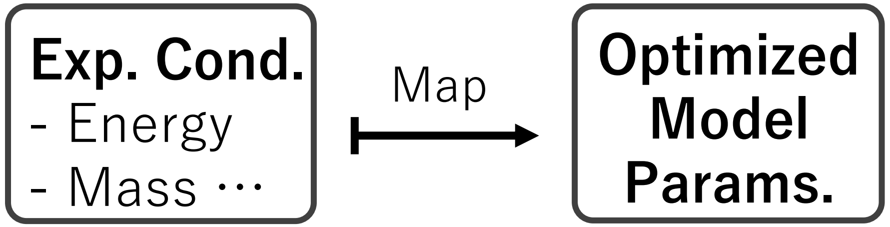
In this presentation, I introduce our prototype system to generate database

An overview of our prototype system

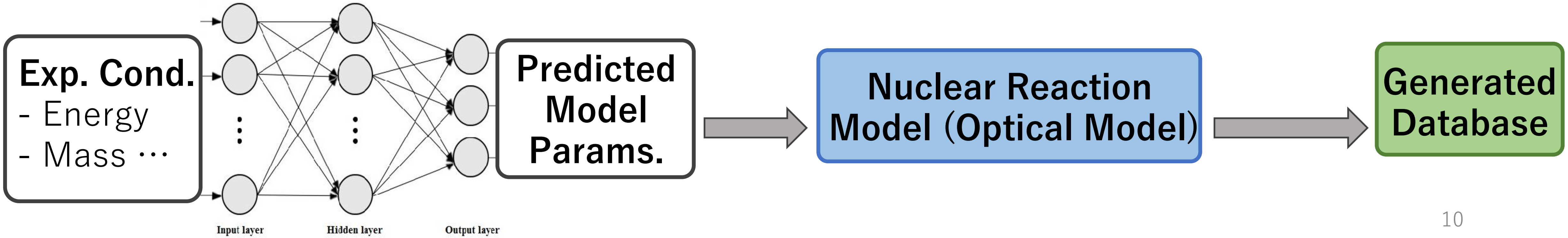
① Optimization of Model Parameters



This creates a dataset which maps between optimized model params and experimental conditions (energy of reaction, mass of target nucleus,…)



② Train Deep Neural Network and predict parameters



Coupled channel optical model

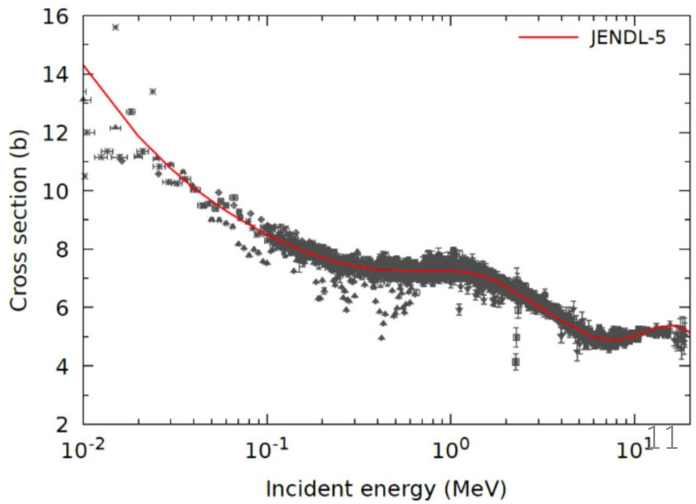
To calculate (generate) nuclear reaction cross-sections,
we employ coupled channel optical model

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2 L(L+1)}{2mr^2}+V_{opt}-E_c\right]\chi_{c'c}(r)=\sum_{c''}V_{c'c''}(r,r')\chi_{c''c}(r')$$

- It is a set of Schrödinger equations for the several important reaction channel wave functions, $\chi_{c''c}(r')$
- The radial wave functions are solved with OpenMPI communications between channels and trivial parallelization for reaction parameters (incident energy, target nuclei,…)

Optical potential V_{opt} describes the interaction between incident particle and target nucleus

- Total cross section, total reaction cross section
- Angular distributions of elastic/inelastic cross section
- Neutron transport coefficient, Strength function



Optical potential and its parameters

A standard functional form of the optical potential

$$V_{opt}(r) = -V_R f_R(r) + i\left\{4W_D a_D \frac{d}{dr} f_D(r) - W_V f_V(r)\right\}$$

$$+ V_{\mathrm{Coul}}(r) + (V_{SO} + iW_{SO}) \frac{d}{rdr} f_{SO}(r) \boldsymbol{L} \cdot \boldsymbol{S}$$

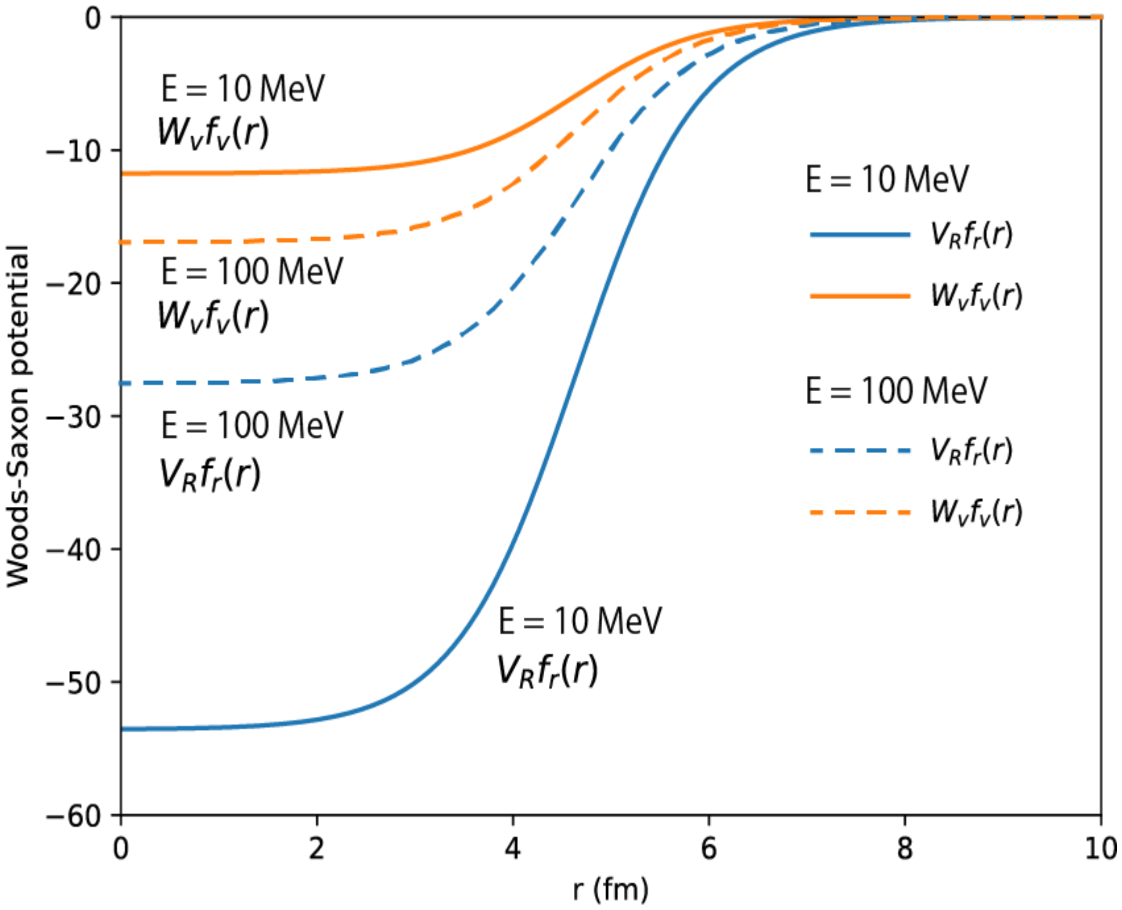
Parameters:

V_R , W_V , …

Dependent on proton and neutron numbers (atomic and mass numbers) Z, N, A

Dependent on incident energy and Fermi energy of the target nucleus, $E^{\dagger} = E - E_{Fermi}$

n-^{58}Ni potential



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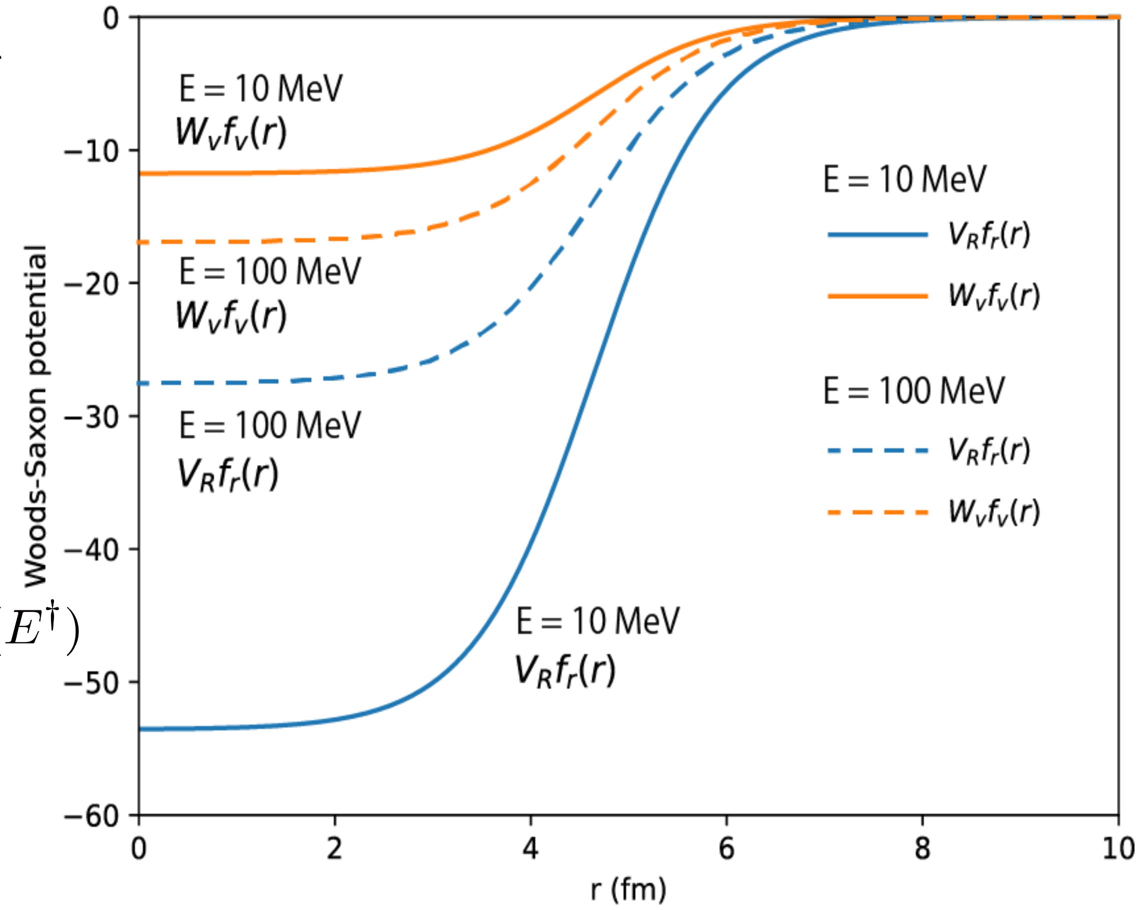
Parameters:

$$V_R = (V_R^0 + V_R^1 E^\dagger + V_R^2 E^{\dagger 2} + V_R^1 E^{\dagger 3} + V_R^{DISP} e^{-\lambda_R E^\dagger})$$
$$\times\left[1 + (-)^{Z'+1}\frac{C_{viso}}{V_0^R + V_R^{DISP}}\frac{N-Z}{A}\right] + C_{Coul}\frac{ZZ'}{A}\phi_{Coul}(E^\dagger)$$

n-^{58}Ni potential



Complicated and phenomenological function
is assumed. Computational/Human resources demanding

Optical potential and its parameters

A standard functional form of the optical potential

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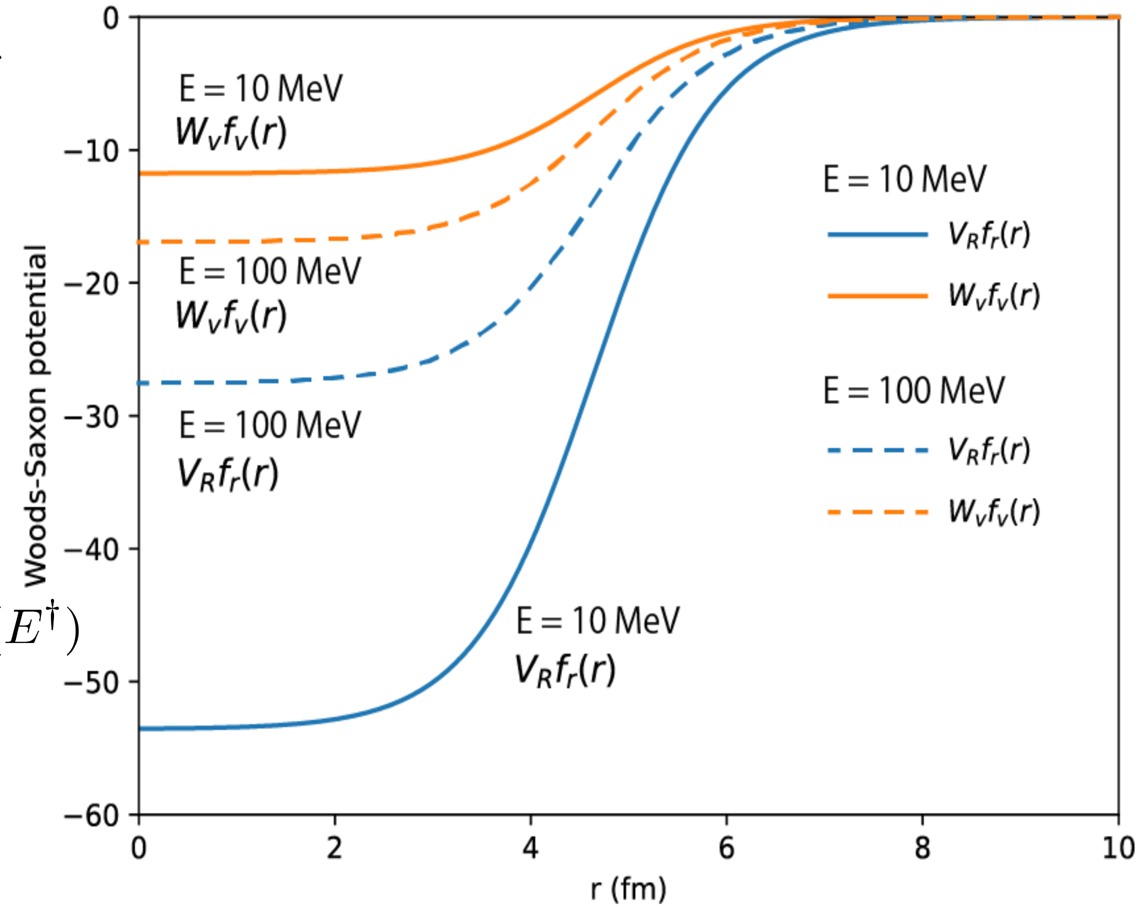
$$\Rightarrow \quad V_R = V_R(E, E_{Fermi}, N, Z)$$

n-^{58}Ni potential

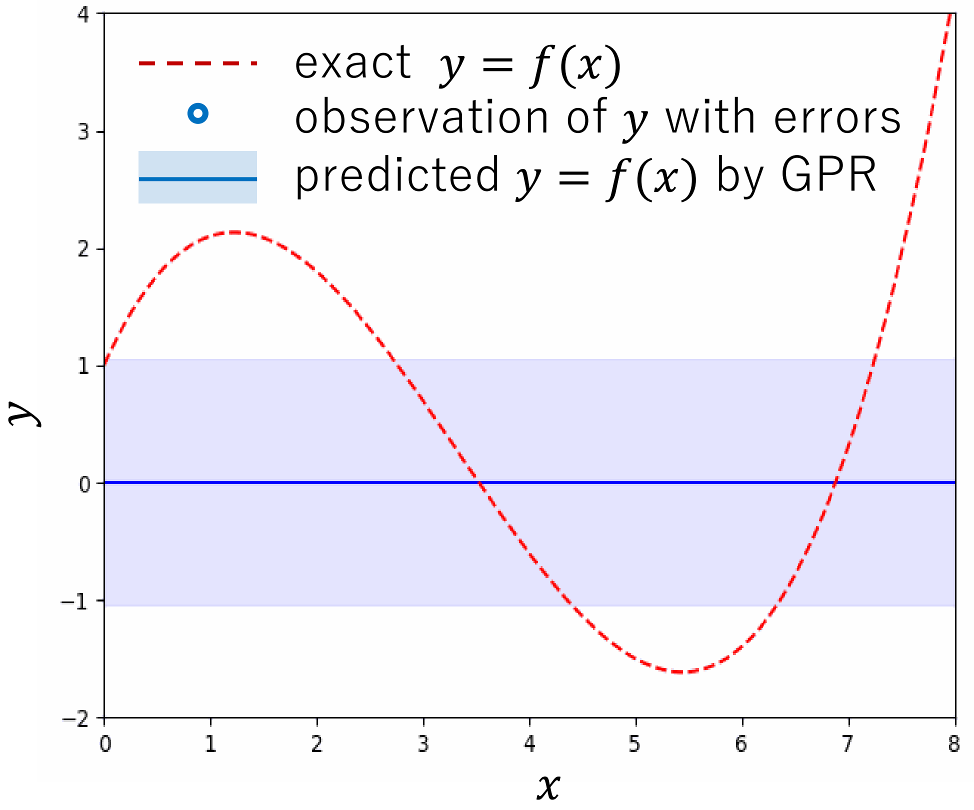


We do not introduce ad-hoc functional form, but use Gaussian Process Regression and Neural Network to optimize and guess the potential parameters

Optimization of the potential parameters

From known experimental data, we optimize the optical potential by the Bayesian optimization with Gaussian Process Regression (GPR)

GP predicts the output $y = f(x)$ for given input x by assuming that the probability distribution of the outputs $f(x_1), f(x_2), \ldots, f(x_N)$ for a set of inputs $x_1, x_2, \ldots, x_N$ follows a multivariate Gaussian distribution.



$$p(\boldsymbol{y}, \boldsymbol{y}^* | \boldsymbol{\theta}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}^* \end{bmatrix} \middle| \boldsymbol{\Sigma}(\boldsymbol{\theta}) = \begin{bmatrix} \boldsymbol{K} & \boldsymbol{K}_* \\ \boldsymbol{K}_*^T & \boldsymbol{K}_{**} \end{bmatrix}\right),$$

$$(\boldsymbol{K})_{ij} \equiv k(x_i, x_j), \quad (\boldsymbol{K}_*)_{ij} \equiv k(x_i, x_j^*), \quad (\boldsymbol{K}_{**})_{ij} \equiv k(x_i^*, x_j^*),$$

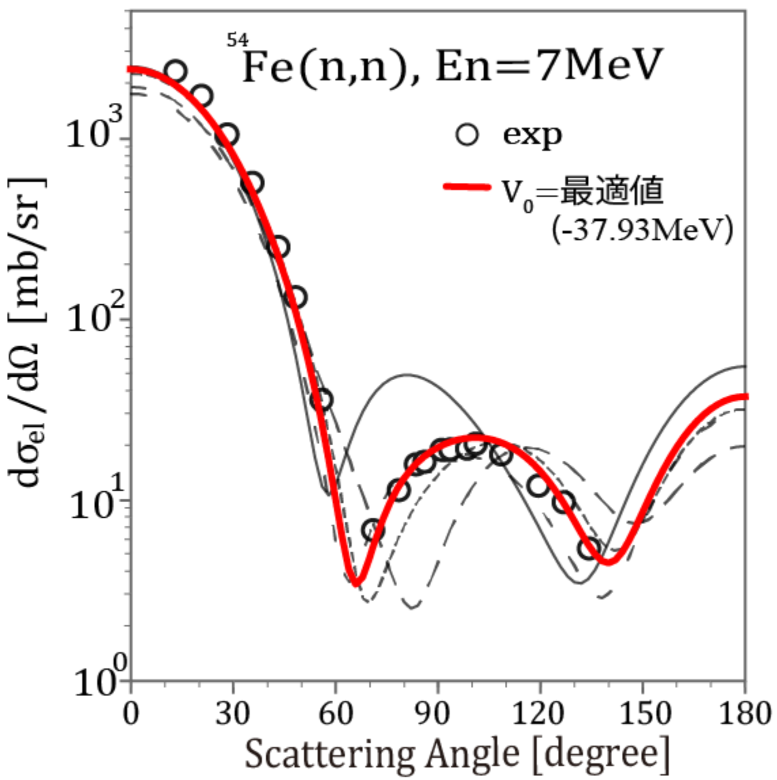
$$p(\boldsymbol{y}^* | \boldsymbol{y}) = \mathcal{N}(\boldsymbol{\mu}^* + \boldsymbol{K}_*^T \boldsymbol{K}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}), \boldsymbol{K}_{**} - \boldsymbol{K}_*^T \boldsymbol{K}^{-1} \boldsymbol{K}_*) \equiv \mathcal{N}(\boldsymbol{M}(\boldsymbol{x}^*), \boldsymbol{\Sigma}^*),$$

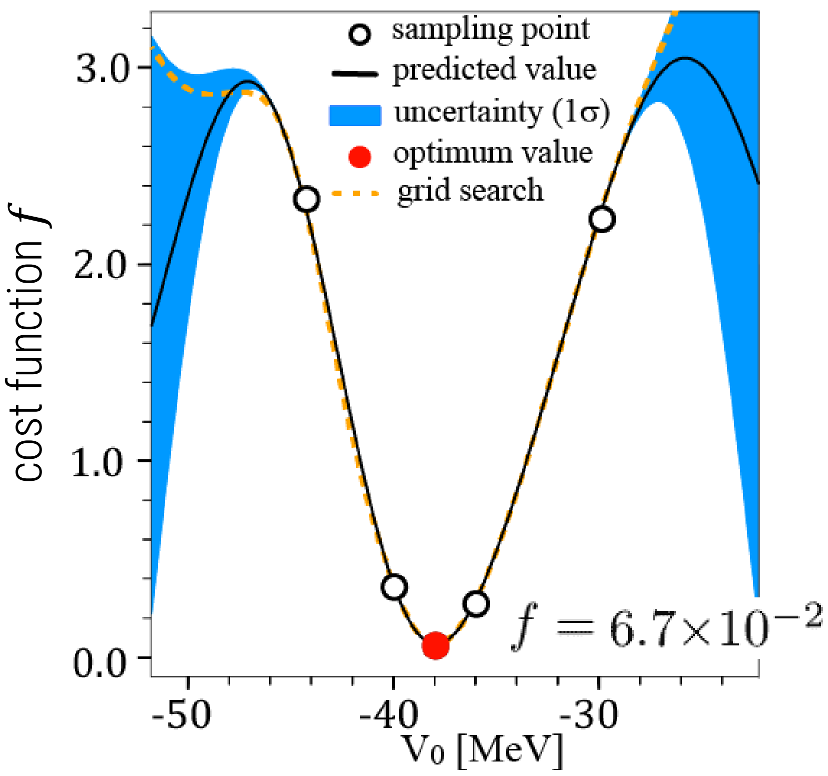
① Optimization of Model Parameter by Bayesian Opt.

From known experimental data, we optimize the optical potential

We minimize the cost function (prediction error)

$$f(V) = \sum_{i \in \mathrm{sample}} \left\{ \log \sigma_i^{\mathrm{obs}} - \log \sigma_i^{\mathrm{calc}}(V_R) \right\}^2 / N_{\mathrm{sample}}$$





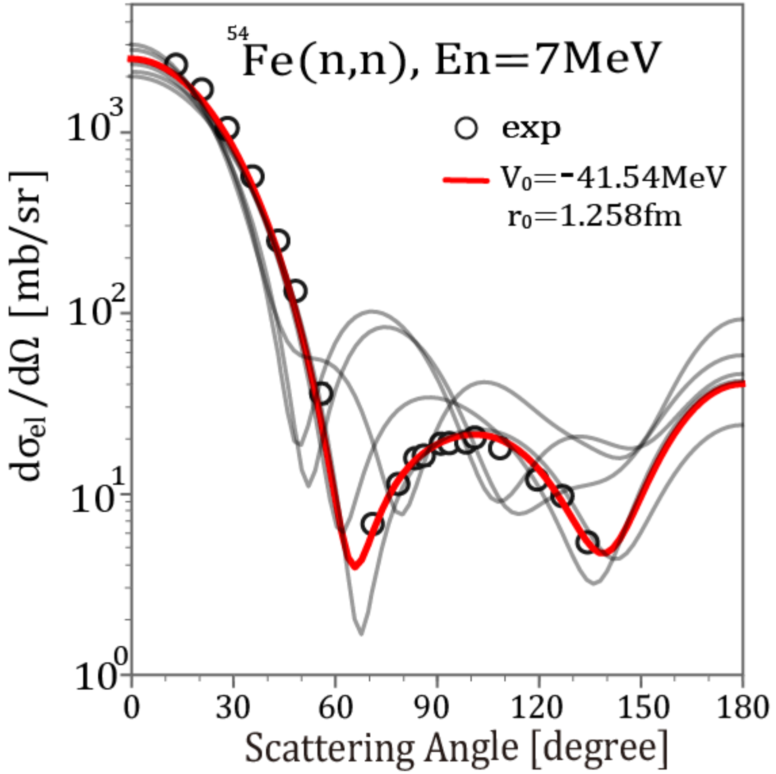
① Optimization of Model Parameter by Bayesian Opt.

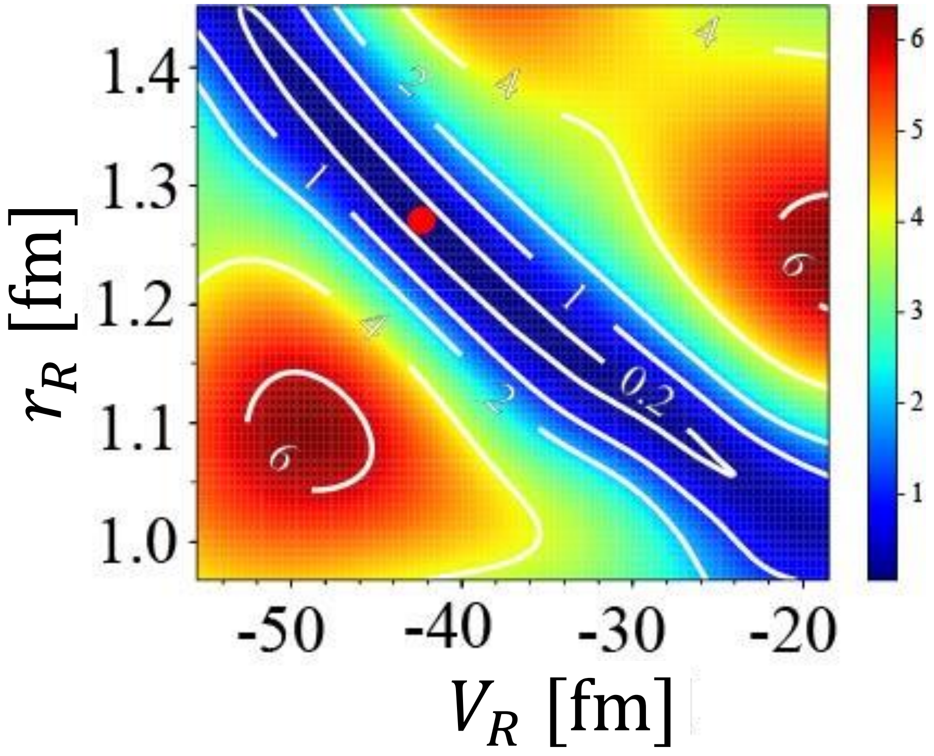
From known experimental data, we optimize the optical potential

GPR works reasonably even for the multidimensional parameter search
(Number of parameters are 4 to 10)

We repeat this procedure for known experimental data to obtain the mapping data collection

$$E, E_{\mathrm{Fermi}}, Z, N \;\rightarrow\; V_R(E, E_{\mathrm{Fermi}}, Z, N),\; W_V(E, E_{\mathrm{Fermi}}, Z, N), \ldots$$





Overview of TRIP: interdisciplinary platforms

TRIP1 : High-quality data acquisition

TRIP3 : Expansion of computable domain

DX Platform

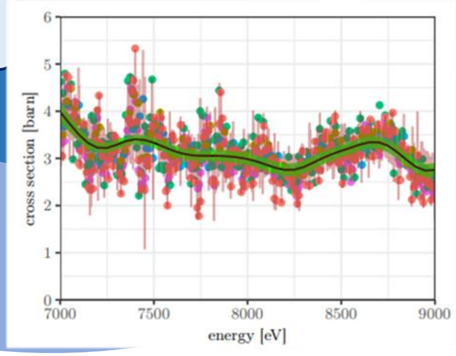
- Accumulating high-quality data
- Open access to data

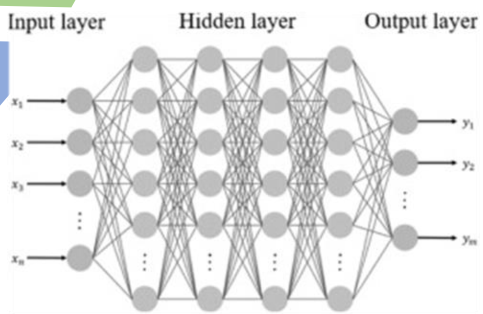
Quantum Computing Platform

- Quantum computing
- Hybrid computing

Data Acquisition **Quantum Computing** **AI x Math.**

TRIP2 : Predictive science with AI x Math.





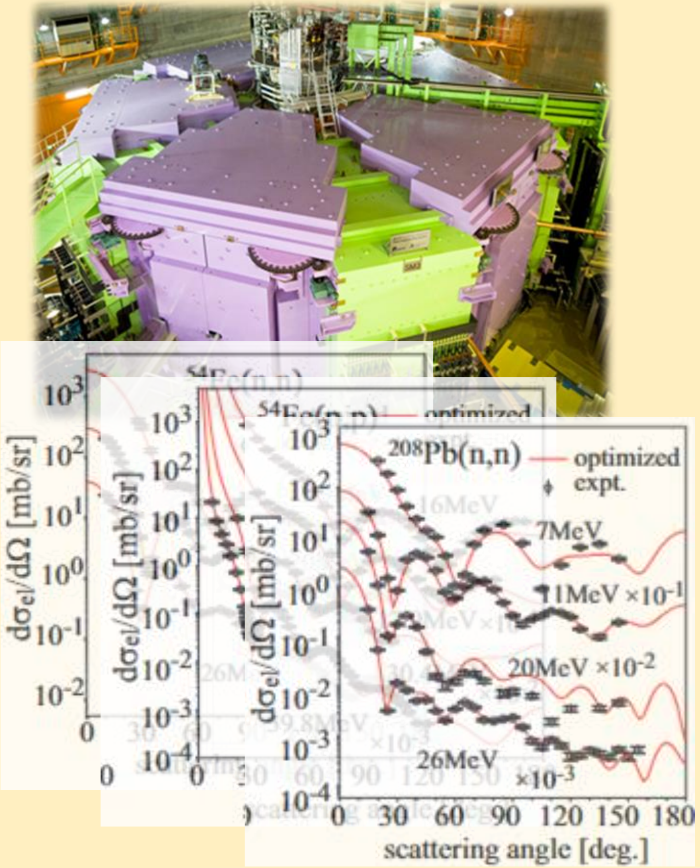
AI x Math Platform

Developing predictive analysis methods using math and AI for diverse research

TRIP Use Case : "Predictive Control of Nuclear Transmutation"

Experiment

- High-quality data measurement at RIKEN
- A pilot experiment in this Autumn

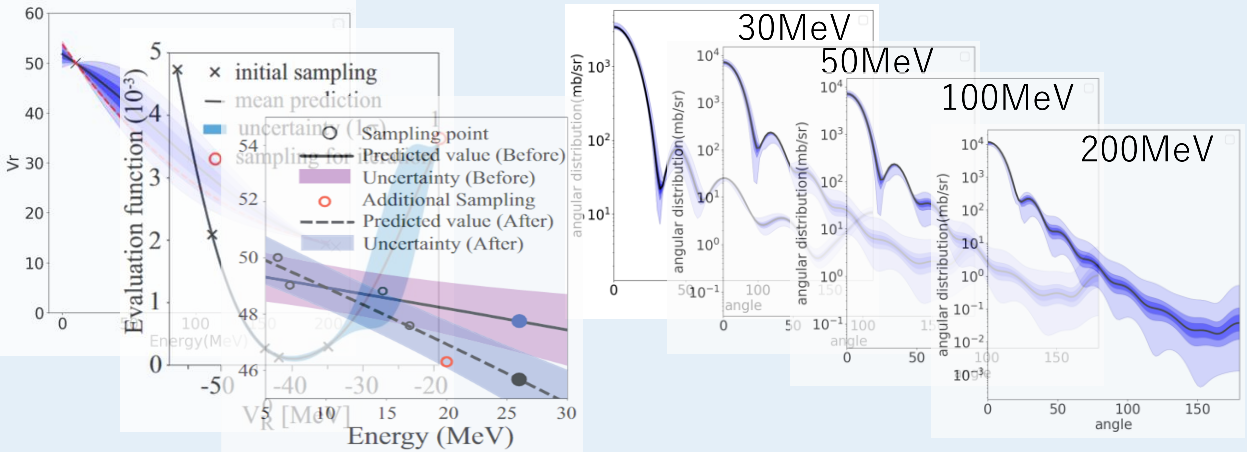


Data input

Feedback

AI x Nuclear reaction model

AI learns and estimates the optical potentials to generate high-precision scattering data for neighboring nuclei at arbitrary energy.



Similar system will also be implemented for

- R-process nuclei
- Nuclear Fission
- Nuclear Fragmentation Reactions

Summary

○ Nuclear reaction database is essential for the application of nuclear reactions.
In particular, evaluation of nuclear data is indispensable

○ ML will innovate the nuclear data science
- It evolves nuclear data science from a fitting process into predictive science.
- It can propose experiments required for database construction/improvements.
- It can dramatically reduce the costs associated with evaluation.

○ A prototype system for nuclear data generation was introduced
- BO with GPR was used to optimize the optical potential parameters
- Optimized parameters were used to train DNN
- If sufficiently large dataset is given, DNN can generate reasonable data, but otherwise not.