

# Theoretical nuclear reaction database based on the microscopic calculations

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#### Introduction

At present, nuclear reaction data measured in all over the world, are accumulated and distributed to public under the international collaborations (NRDC). A nuclear database is one of the most important infrastructure for developments in several fields.

#### **Important items for the database**

- Certainty
  Accuracy
  Completeness ...



Compilation miss, Difficultness of measurements, Evaluation based on empirical ways ...

We construct the nuclear database with **only** theoretical methods.

- ✓ Density distribution (about 3,500 nuclide),
- ✓ Reaction cross section,
- ✓ Differential cross section, for the reaction with 3,500 nuclide + p, n and  $\alpha$  at 20 -1000 A MeV

Collaborators: Y. Hirabayashi, S. Hatakeyama, W. Horiuchi (Hokkaido Univ.)



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- For low-energy reaction
- For high-energy reaction

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#### Methods

For ground state: 3D Skyrme Hartree-Fock+BCS (HF+BCS)

For low-energy reaction: Folding model w/ DDM3Y Int.

For high-energy reaction: Glauber model

### Method (3D Skyrme HF+BCS)

$$\begin{cases} [h, \rho] = 0, \\ 2\tilde{\varepsilon}_k u_k v_k + \Delta_k (v_k^2 - u_k^2) = 0, \quad k > 0, \end{cases}$$

**HF+BCS** Equation

#### Density matrix

$$\rho_{ij} = \langle \Psi | \hat{c}_j^{\dagger} \hat{c}_i | \Psi \rangle \qquad | \Psi_{\rm HF} \rangle = \prod_{i=1}^A \hat{a}_i^{\dagger} | 0 \rangle \qquad | \Psi_{\rm BCS} \rangle = \prod_{k>0} (u_k + v_k \hat{a}_k^{\dagger} \hat{a}_{\bar{k}}) | 0 \rangle,$$

$$|\Psi_{\rm BCS}\rangle = \prod_{k>0} (u_k + v_k \hat{a}_k^{\dagger} \hat{a}_{\bar{k}})|0\rangle,$$

#### Single particle Hamiltonian

$$h = t + \sum_{\beta,\nu} V_{\alpha\beta\mu\nu}$$

$$\tilde{\varepsilon}_k = \frac{1}{2} \{ t_{kk} + t_{\bar{k}\bar{k}} + \sum_{l} (V_{klkl} + V_{\bar{k}l\bar{k}l}) v_l^2 \} - \lambda$$

 $u_{h}^{2} + v_{h}^{2} = 1$ 

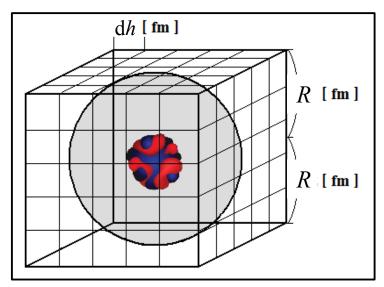
Coordinate space represented s.p. state  $\phi_l(\mathbf{r};\sigma) = \langle \mathbf{r} | \hat{a}_l^{\dagger}(\sigma) | 0 \rangle$ 

In 3D coordinate space representation, Skyrme effective interaction  $V_{\rm sky}$ 



Pauli principal, Nuclear pairing, Nuclear deformation

## Method (3D Skyrme HF+BCS)



$$\begin{aligned}
HF \\
|\Phi_{\mathrm{HF}}\rangle &\equiv \prod_{l=1}^{A} a_{l}^{\dagger} |-\rangle \\
|\phi_{\mathrm{BCS}}\rangle &\equiv \prod_{k>0} (u_{k} + v_{k} a_{k}^{\dagger} a_{k}^{\dagger}) |-\rangle \\
\phi_{l}(\boldsymbol{r};\sigma) &= \langle \boldsymbol{r} | \hat{a}_{l}^{\dagger}(\sigma) | 0 \rangle \\
u_{k}^{2} + v_{k}^{2} &= 1 \\
\phi_{l}(\boldsymbol{r};\sigma) &\to \phi_{l}(x,y,z;\sigma)
\end{aligned}$$

For light nuclei  $6 \le Z \le 20$  R = 12 fm, dh = 0.8 fm

For middle &  $20 \le Z \le 82$   $\it R=15$  fm,  $d\it h=1.0$  fm heavy nuclei

For heavy nuclei  $82 \le Z \le 92$  R = 20 fm,  $\mathrm{d}h = 1.0$  fm

# of lattice point 15,000 ~ 34,000 (half of cubic)

$$R_{\rm A=300} \sim 8 {\rm \ fm}$$
  $\bar{R} \sim 1.2 A^{1/3}$ 



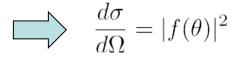
Potential scattering theory: How to prepare the potential?

Schrodinger Eq.

$$\left\{-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + U(\boldsymbol{R})\right\}\Psi(\boldsymbol{R}) = E\Psi(\boldsymbol{R})$$

w/ the boundary condition:

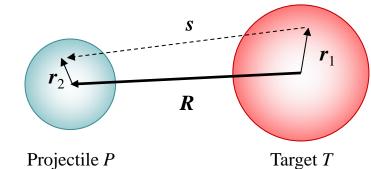
$$\Psi(\mathbf{R}) \to e^{ikz} + f(\theta) \frac{e^{ikR}}{R} \quad (\mathbf{R} \to \infty)$$



Single Folding:  $U_{SF}(\mathbf{R}) = \int d\mathbf{r}_1 \; \rho_T(\mathbf{r}_1) v_{NN}(E, \mathbf{R} - \mathbf{r}_1)$  When projectile

$$U_{SF}(\boldsymbol{R}) = \int d\boldsymbol{r}_1 \; \rho_T(\boldsymbol{r}_1) v$$

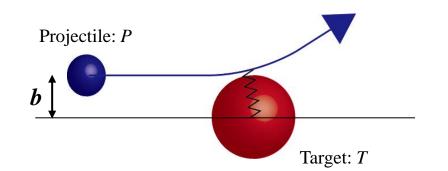
Double Folding:  $U_{DF}(\mathbf{R}) = \int\!\int d\mathbf{r}_1 d\mathbf{r}_2 \; \rho_T(\mathbf{r}_1) \rho_P(\mathbf{r}_2) v_{NN}(E, \mathbf{s})$ 



nucleon-nucleon Int. (DDM3Y)

In the eikonal and adiabatic approximation, ...

$$\sigma_{R}(E) = \int d\boldsymbol{b} \left( 1 - |e^{i\chi(\boldsymbol{b}, E)}|^{2} \right)$$
$$\sigma_{R} = \sigma_{T} - \sigma_{el}.$$



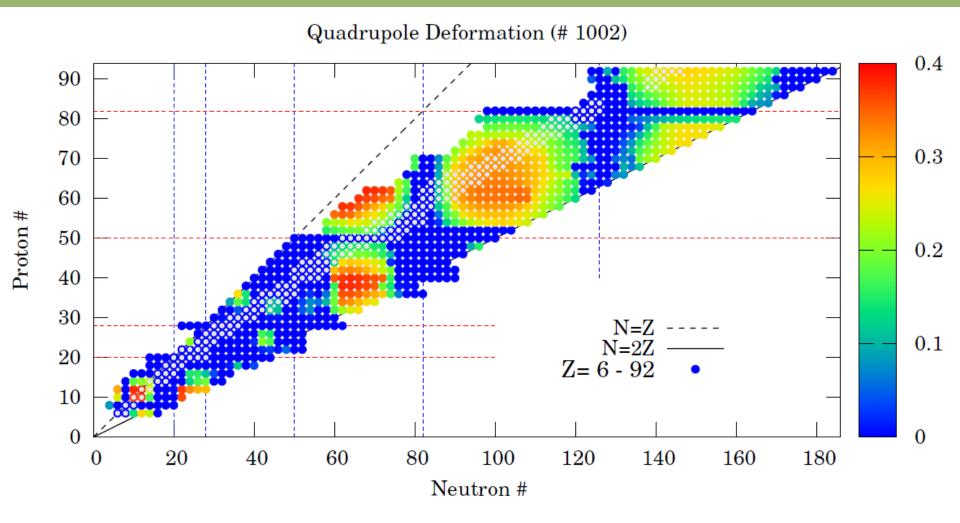
Glauber model + OLA + NTG (Optical Limit Approximation, Nucleon-Target formalism in the Glauber)

Phase shift function: 
$$i\chi(\boldsymbol{b},E) \simeq -\int \int d\boldsymbol{r}_P d\boldsymbol{r}_T \; \rho_P(\boldsymbol{s}_P) \rho_T(\boldsymbol{s}_T) \Gamma(\boldsymbol{s}_P-\boldsymbol{s}_T+\boldsymbol{b},E)$$

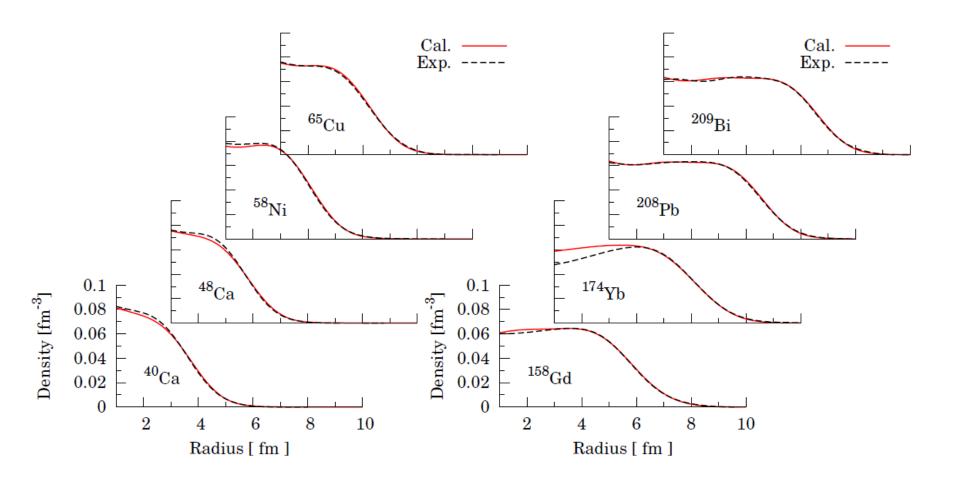
Profile function: 
$$\Gamma(\boldsymbol{b}, E) = \frac{1 - i\alpha_{NN}(E)}{4\pi\beta_{NN}(E)} \sigma_{NN}^{\text{tot}}(E) \exp\left[-\frac{1}{2\beta_{NN}(E)}\beta^2\right]$$

to reproduce the nucleon-nucleon collision

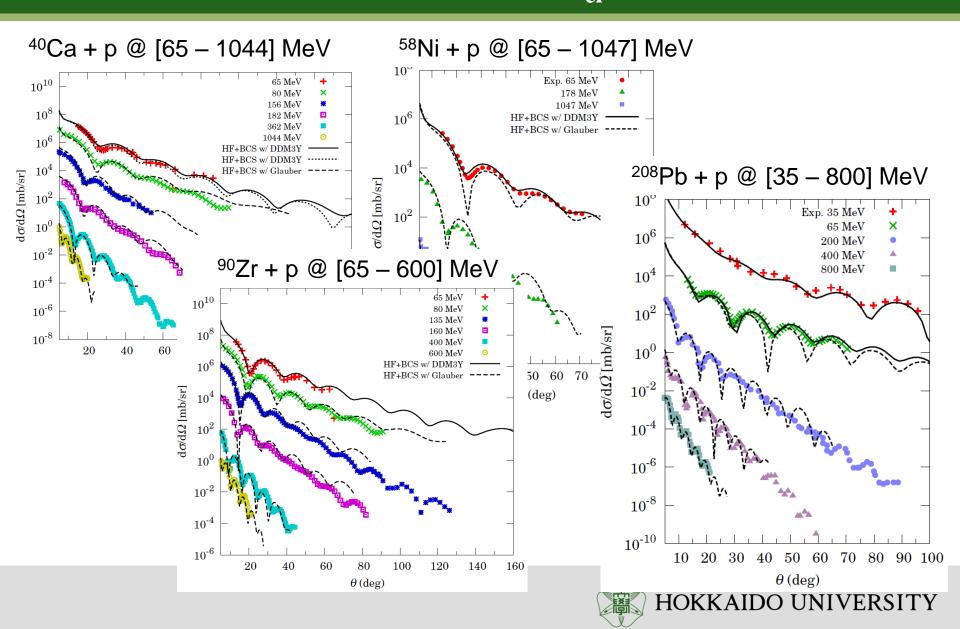
## **Results (ground state)**



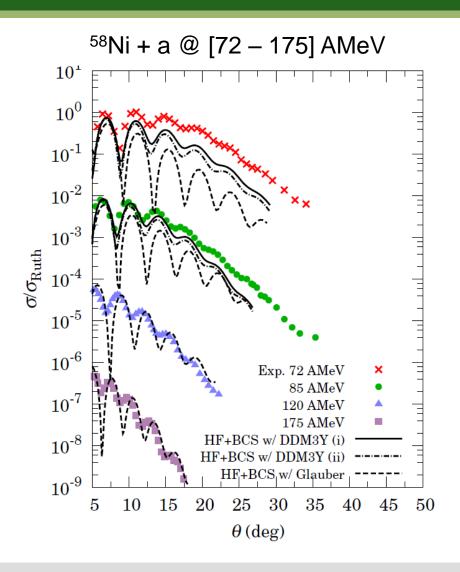
# **Results (charge density)**

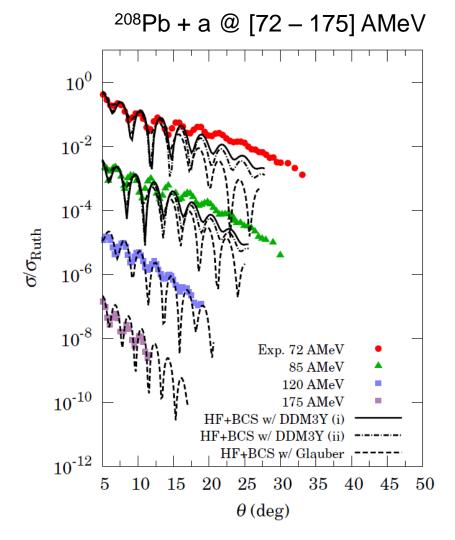


## Results (Differential cross section $\sigma_{\rm el}$ )



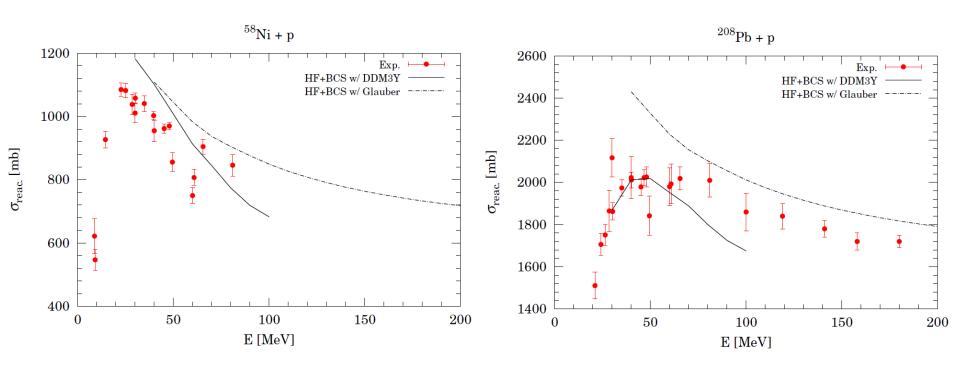
### Results (Differential cross section $\sigma_{\rm el}$ )



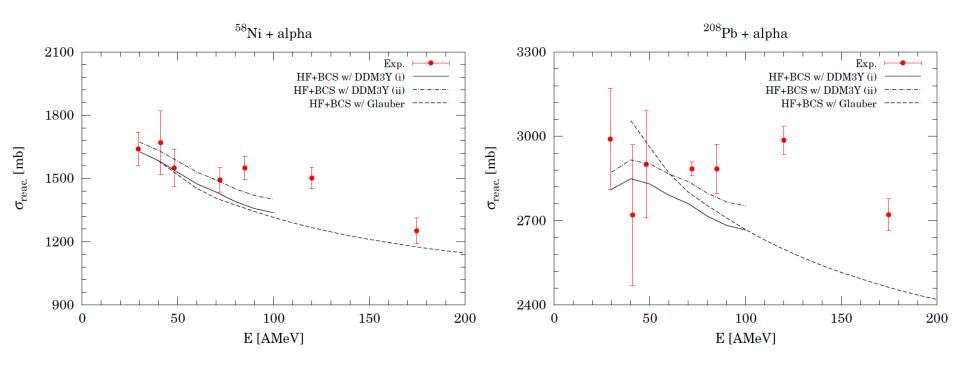




# **Results (Reaction cross section)**



## **Results (Reaction cross section)**



#### **Interface to use the Database**

#### **MFG Theoretical Nuclear Reaction Database**

MFG: Mean-field model, Folding model and Glauber model

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#### What is the MFG Theoretical Nuclear Reaction Reaction Database?

This database is constructed by using the results of theoretical calculation only, which can provide the reaction data without depending on empirical way.

The ground states of nuclei are calculated by self-consistent Skyrme Hartree-Fock+BCS method, and for the reaction calculation Folding and Glauber model are employed. The details of theoretical methods are explained in the paper. When you use the data listed in the MFG database, please refer to it.

Subject nuclide: about 3,500 isotopes with Z=6-92 including odd-nuclide, as following periodic table.

#### Subject nuclide for MFG database

1 H																2 He	
3	4												6	7	8	9	10
Li	Be												C	N	O	F	Ne
11	12												14	15	16	17	18
Na	Mg												Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
55	56	57-71	72	73	74	75	72	72	72	72	80	81	82	83	84	85	86
Cs	Ba	Lanthnide	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
87	88	89-103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Fr	Ra	Actinide	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	MC	LV	Ts	Og

57-71 Lanthnide	57 La	58 Ce	59 Pr		62 Sm					
89-103 Actinide	89 Ac				94 Pu					

## **Summary & Future works**

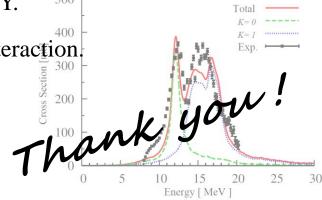
- We construct the theoretical reaction database included the ground state nucleon densities, reaction and differential elastic reaction cross sections for the whole nuclear mass region (A=12-276, with Z=6-92) and in the whole energy region (E<sub>in</sub>=20 1000 AMeV).
  - ✓ For the ground state: 3D Skyrme HF+BCS model.
     For the low- and high-energy reaction: Folding and Glauber models
     Collaborators: Y. Hirabayashi, S. Hatakeyama, W. Horiuchi (Hokkaido Univ.)

✓ We will complete the database construction, in this FY.

We will extent the database to those with other interaction

✓ New projectile will be added (deuteron, photon)

Comparison with TALYS results



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