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PROTOTYPING OF AN EXPERT SYSTEM FOR NUCLEAR DATA EVALUATION

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ABSTRACT: A prototype guidance system for the nuclear cross section calculation has been developed in a 16-bit personal computer. The system was consisted of two main parts: the first part is for selection of the code system, and the second one is for selection of the best input parameters for the selected codes. Priciples of guidance were taken from several literatures and recomendations.

(Nuclear Data Evaluation, Selection of parameter, Guidance System, personal computer)

Introduction

An expert system in the field of the nuclear data evaluation is considered to be one of the solutions to the rapidly increasing requests on the nuclear data for various applied fields in Japan in spite of deficiency of the mon-power for the evaluation.

There are many kinds of nuclear codes for various cross section calculation, and only limited experienced researchers know which code is good for their purposes , how to use the selected codes correctly, and how to choose the input parameters to the codes.

If the collection of various kinds of knowledge about the nuclear codes and proper way of usage are systematized and implemented in a computer system (knowledge base system) so as to be accessed easily, it would be very convenient for beginners, unskilled persons in the nuclear calculation, and even for the experts themselves. The knowledge base system will be very flexible to revision and modification according to the progress of the theories, techniqeus and development of codes for the nuclear calculation.

In the present paper, an atempt of making a proto-type guidance system for nuclear cross section calculation by some nuclear codes is described. In the system we have assumed that the objective area of the nueleus is limited to the structural material near iron and the range of the incidnent neutron energy is fast neutron region above 1MeV, because there have been many calculational studies on the nulcei of this area. The guidance principles were taken from proceedings of several recent meetings /1/, /2/, /3/, /4/, /5/ and papers /6/,7/,/8/,/9/,/10/,11/, and was implemented in the system for the methods of code selection and detemination of the input parameters. Outline of the principles are described in sections 2 and 3.

Outline of the Guidance Principles

Selection of Code

Proper codes should be selected according to the several conditions: region of target nuclei in the periodic table, and region of the incident neutron energy (resonance, unresolved, or fast neutron region).

If they hope to calculate the neutron cross sections in the energy range less than several MeV, they should use the statistical model (Hauser-Feshbach model) code with width fluctuation effect such as CASTHY /12/ or equivalent. Above this energy region, the number of open channels increases and the width fluctuation effect becomes small. Multistep Hauser-Feschbach (MSHF) model code, such as GNASH/13/, TNG/14/ and STAPRE/15/ are suitable for the calculations in the energy range. For example, the GANSH code has a capability of tracing the all open channels upto the 10 CN's (parent nuclei) /16/ and 7 decay modes/17/ of the CN's. Therefore they can use this code up to the incident energies of about 50 MeV. Of cource, it is necessary to prepare all transmission coefficients of all outgoing particles for every CN by mean of other optical model codes prior to use. Another MSHF code, TNG /14/ is also available and has different features /15/ from GNASH.

Above 10 MeV, the contributions of the precompound (PC) reaction mechanism become important for (n,xn'ycp) reactions, where x=1,2 or 3 or y=0,1,2 and cp=charged particles. The nuclear theory of this mechanism are now under development and there has been no definite model. In all available MSHF codes, a sort of the PC model is built in. For this reason we had better use the PC model which is included in the existent code exept for minor modification, if necessary. If someone want to use a recently developed model, he has to implement the model into the code by himself, and this process is usually not recomended except for the experts.

In this energy region, the direct reaction (DR) mechanism may also dominate in the elastic and inelastic scatterings. If it is necessary to evaluate properly both scatterings in magnitude and angular distributions, use of the DWBA or coupled channel(CC) model calculation is essential. Especially the CC model is recomended if apparently the ground state of the target nucleus couples strongly to the collectively excitated states.

In Fig.1, a diagram of typical code systems and relationship between them for the nuclear data calculation given by Yamamuro et al./16/. is shown.

Selection of various input parameters

In this section, outline of the priciples of input parameter determination mainly for the optical model potential, level density formula

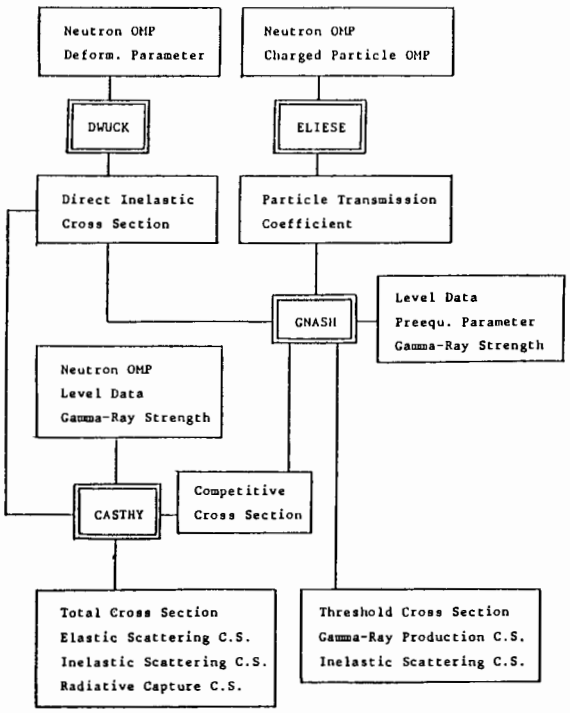

Fig.1 Example of code system for the nuclear cross section calculations, given by Yamamuro et al/16/.

and gamma-strength functions.

Optical model potential parameters

The most important input parameters are those for the neutron optical model (OPM) potential. These parameters should be determined very carefully because almost the result of the calculation would be determined by them /11/. According to several recent model calculation studies /6/,/7/,/8/,/9/,/10/,/11/, there are three methods to choose the parameters.

The first one is to adopt a global opticlal model parameter set. Modern global parameter sets are more superior than old ones in general /5/. However the most global parameters were determined by fitting the data of the representative nuclei in the periodic table, and not the best parameters in the specific nuclei. Therefore the global parameters are suitalble to the purpose of the primary calculation or the initial parameter set of the detailed and iterative calculations. Yamamuro showed that that Walter-Guss potential are implemented in his system (SINCROS-I), and calculate the various type of cross section rather wide range of nulei from aluminum to lantanum/11/. The second way is to choose the parameter set which had been determined in a previous evaluation/calculation which reprocduced the cross sections well. Those parameters, however, are not always the best ones when the new experimental data come out after the evaluation. The third way is to determine the parameters independently on the previous works, but this process is tedious and not prefereable in general.

In any cases described above, the parameter values must be reevaluated by comparing the results with the recent reliable experimental data set. First, the parameter set should be checked by the Lagrange's criterion, so called "SPRT" method /1/. The optical model parameters should reproduce the important optical model quantities, such as S- and P- wave strength functions and scattering radius R' for the slow neutrons. The optical model calculation should reproduce the total (T) cross section behavior in the entire energy range, except for the resonance structure. In order to get best results, the iteration porocess is necessary. Volume integrals of both real and imaginary well depth show sometime good index of the parameter systematics /5/.

Charged Particle Optical Potential

The proton and alpha-particle optical potentials are also important because the recent nuclear development needs the accurate cross sections of the charged particle emission reactions in the high energy regions, especilly for the damage evaluation of the irradiated materials. the cross section of the particle emission is very sensitive to the parameters. The charged particle optical potentials, however, have not been studied extensively as the neutrons. Usually, these charged particle parameters are selected among the global parameter sets. Among many paramere sets, the Huizenga and Igo's set /18/ for alpha is considered not to be suitable, because that parameter set results in the abnormally large cross sections /18/.

Level Density Parameters

Level density (LD) formula and its parameters are also important for determining not only the cross sections itself but also the energy distribution of the emmitted particles /4/,/11/.

Usually as the LD model in the cross section calculations, the phenomenological Fermi-gas formula have commonly been used, because the formula has rather simple expression and have been studied comprehensively and improved. In spite of recent remarkable impovement of the microscopic model of the density, these trend will continue for comming several years.

First, the Gilbert-Cameron formula /19/ is recommeded, because this formula have been used in almost every calculation code available in Japan. The parameters of the formula are also studied for almost every nucleus. However, the back-shifted Fermi-gas formula /20/ should be tested if the former one failed the fitting because It is very easy to replace by the latter.

For any formula and paramerers, the result should be checked by comparing the results to the recent experimental data. Average resonance level spacing /21/ is one of the important experimental data. Particle (neutrons and charged particles) emission spectra are very sensitive to the desity parameters /11/. There have been many high quality emission data for neutrons at 14.1MeV which are suitable to search the best parameter set by fitting the spectra. As for the charged particles, the Grimes' data /22/ should be refered. Reasonable parameter set must be searched by iteration process.

Gammma-ray transmission coefficient (GTC)

These parameters are influential not only to the gamma-ray production cross sections and spectra but also to the particle cross sections through the competition processes.

The profile of the GTC are usually so called giant-dipole resonance type whose parameters are taken from the systematics by Gardner et al /23/. Specific nuclei's parameters are determined by interpolation.

Absolute value of the GTC should be normalized to the ratio of the experimental data of the gamma width < > and average level spacing <D>. However the experimental data sometime have large systematic errors. In the important nuclei, the coefficient should be renormalized so that the reliable capture cross sections at low energy region are reproduced.

Other parameters

Other important parameters in the cross section calculations are the following ones,

.Precompound (PC) model parameters
.Direct reaction (DR) calculation
and others which are unique to the code.

In the PC model parameters, the Kalbach's constant /24/ or its related parameter and level spacing parameter g are important. We had better consider that this parameter is an adjustable one /11/, especially for alpha.

In the direct reaction calculation, the coupling scheme and the deformation parameters are important. These parameters are also selected in similar manners discussed above.

Guidance System

Expert shell

The knowledge and recomended processes for the calculations should be implemented in the knowledge base. Considering the prototype one, we chose the small expert construction system, TELL /25/ (expert shell) which ran in a 16-bit microcomputor with 2-Mbyte extended RAM.

TELL is based on the PROLOG language (PROLOG-KABA /26/) with its extension tool, WING /27/. TELL supports three kinds of knowledge expression, such as 'production rules' for backward and foreward inference, 'frame expression' and 'table inference'. The last one is a fuzzy like inference with a values table and unique to the TELL. Table header of the table will be fired when the sum of weight(-99 - 99) of fired items in the table excede the predetermined threshold value (0 - 999). Thus the table inference is effective for reduction of the redundant production rules. TELL also supports Japanese input and output, multi-window system, mouse interface and graphics, and is accessible to the data base file made by dBASE-II /28/.

Basic structure of the system

The system is consisted of two main parts. The first one corresponds to the code selection, and the second one to the parameter determination.

In the first part, the system asks two basic questions to the user on the nuclei to be calculated and the region of energy. The system checks the whether the answered regions are covered by the system: structural material elements near iron and the energy less than 50MeV.

The system asks additional questions to the user on kinds of reactions (assumled to be neutron, proton and alpha-particle emission) and a kind of calculation purpose, detailes or rough calculation (estimation), etc. Some time in the rough calculations the systematical model or simple model such as PEGASUS /29/ are preferable

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[Start rule block for the neutron optical
     potential selection]
   › assumed answer for basic question : Fe-54
                                          and 56
   ›for additional questions: detailed calcu-
                                  lation
   ›                                      etc.
Q1: is there any recent (after 1980)
    calculation/evaluation for the nuclei?
A1: YES [then go to ...] (not shown)
  : NO [then G1]
G1:It is recomended to adopt a global optical
     potential
Q2: do you have definite GOPM candidate to be
     selected?
A2: YES [then go to ...] (not shown)
  : NO
     [start rule block for GOP selection]
     [read the frame block of the NEUTRON GOPM]
     [select the best GOPM from its slot values]
G2: use Walter and Gass GOP as a starting value
     [start rule block for best OPM determination]
Q3: do you want to revise the OPM parameter
     once(1), or twice or more(2)?
A3: 1 then go to ...(not shown)
  : 2 [start SPRT checking rule]
G3:calculate s-wave (S0) and p-wave (P0)
     strength functions and potential scattering
     radius, and compare with the recent exp.
     data.
Q4: good agreement?
A4: YES [then go to ..] (not shown)
    NO
G4:vary V,aR,rR and WI,aI,rI and get best fitting
Q5: good agreement?
A5: NO [then go to...] (not shown)
     YES
G5: calculate total (T) cross section curve
    in the entire energy range, and compare with
    the best experimental data.
Q6: good agreement?
A6: NO [then go to ...] (not shown)
  : YES
G6: calculate elastic( ang. dist.), inelastic1 and
    noelastic cross section in the entire energy
    range, compare with the best experiment.
Q7: good agreement?
A7: YES [then go to ...] (not shown)
   NO
G7: include the deformation parameters in the OPM.

          ..... (continued)
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Fig. 3 Example of a part of dialogue between user and the present expert system, where,
Q: questions asked from the system
A: answers by user
G: guidances given by the system
[inference processes of the system]

rather than the MSHF model codes because of the simpleness of parameter input and fast calculation. The reasoning of the code selections are the table one.

In the socond part of the system, the part is devided into 5 independent rule blocks, such as the block for the OPM and parameters, for the LD formula and parameters, for the GTC's, for the PC part, and for the DR. The first OPM part is devided into subblocks, for the neutron, proton and alpha-particle, etc.

Almost rules implemented in the second part are the production rules. Example of the questions, answers and guidance dialogue for the case of the neutron OPM parameter selection is shown in Fig. 3 (original dialogue is witen in Japanese). For the present, no experimental data base is included in the system, the user should consult the other data bases or some references in order to answer the questions given from the system.

Summary

A prototype guidance system for the nuclear cross section calculation has been developed in the 16-bit personal computer. Test run of the system showed that it presented proper guide. However, the system is far from the application use, because the system is limited in the small region of the nuclei, adopted rules are limited and the experimental data base has not been included. It is also necessary to develop new technique of the determination of the best parameter set from a lot of and various types of the experimental data, and criteria for fitting the cross sections.

We are now planning to develope a guidance system in a 32-bit work station witch will linked with a main frame computer as the socond step.

In future, it would not be impossible to develope a semi-automated nuclear data evaluation system which would be consisted of a high level workstation with multi-window, multi-task and multi-langeuage, high level graphics, linked with other codes and data base systems in large scale, and be accessible from remote areas in the country by computor network.

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