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Interactive Information System for Preparation and Verification of Nuclear Data in the High-energy Range

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The report describes integrated systems software packages designed to increase the efficiency of research in the field of nuclear data preparation for calculation studies of advanced nuclear system projects. The report also describes an algorithm for obtaining evaluated nuclear data using the software developed based on state-of-art multicriterial decision making methods.

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I. INTRODUCTION

In the last decade there has been a certain increase of interest in nuclear reactions at high energies. This is due both to scientific problems, and numerous applications. These include the development of high-energy neutron sources, the production of medical radioisotopes, radiation protection of spacecraft and accelerators [1].

Meeting these goals requires a large amount of nuclear data for a wide range of nuclides and energies that could reach up to several tens of GeV. It is impossible to get all the data experimentally. Thus, it is needed to develop analytical methods and their accuracy should be checked by measurements made in certain conditions. This includes the development of models and theories, assessment technologies, their implementation in computer programs and, finally, the formation of recommended evaluated nuclear data. In addition to obtaining the data themselves, there are problems of processing, evaluation, validation, verification and visualization of the data [1].

1. Integrated Software Systems

To improve the efficiency of research in the area of nuclear data preparation for calculation studies of advanced nuclear system projects, two groups of program systems were developed on the basis of state-of-art models of nuclear reactions at high energies. Their aim is to develop a tool that provides an opportunity for more accurate and complete models in this domain on the basis of quantitative comparison to experiments, reducing the complexity of scientific research. Application of such systems in this field seems appropriate in connection with the diversity of models and the need to work with large volumes of information.

The first category of the software systems under development is Interactive Visual Systems (IViS). The expediency of elaborating such systems is dictated by the fact that the high-energy nuclear reaction models are multiparameter ones, and this brings up the task of choosing the best internal model parameters. To solve this problem, it is advisable to use programs that implement modern methods of multicriteria decision making. Currently, the present system has been designed for the Russian model of high energy nuclear reactions CASCADeX [2] (IViS CASCADeX) and work on a number of other models (DISCA, ISABEL/EVA [3]) is underway.

The second category under development is Information Interactive Systems (InIS). The necessity of designing this kind of software systems is dictated by the need to integrate the existing models of nuclear reactions in order to create a visual environment for cross verification and validation of various models and ultimately building evaluated libraries of nuclear data based on the results of this work. Currently, Information Interactive System for high energy activation nuclear-physical data preparation (InIS HAND (Information Interactive System - High Energy Activation Nuclear Data)) has been developed.

The software systems developed are complementary. Thus, the optimum parameter values of different models of high-energy nuclear reactions, found with the help

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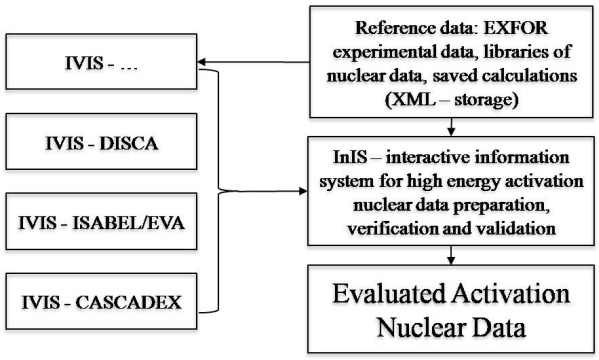

Fig. 1. Connection between IViS and InIS.

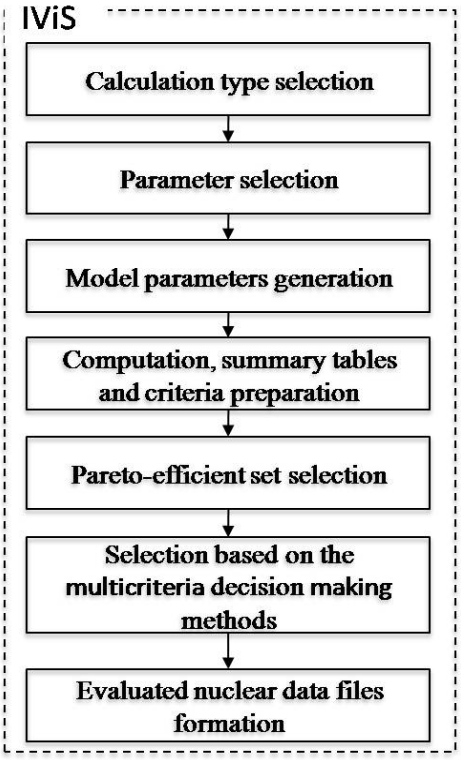

Fig. 2. Follow chart of IViS-software functioning.

of IViS-systems may be transferred to the InIS-system for cross-verification of different models, with certain parameters selected on the basis of the IViS-system results (see Fig. 1).

II. CALCULATION STUDIES BY USING INIS AND IVIS SOFTWARE

Let us look at how to conduct computational research in this area by using the tools developed.

1. Interactive Visual Systems

IViS-systems include the physical model calculation code, forms of input and output data to be filled, an

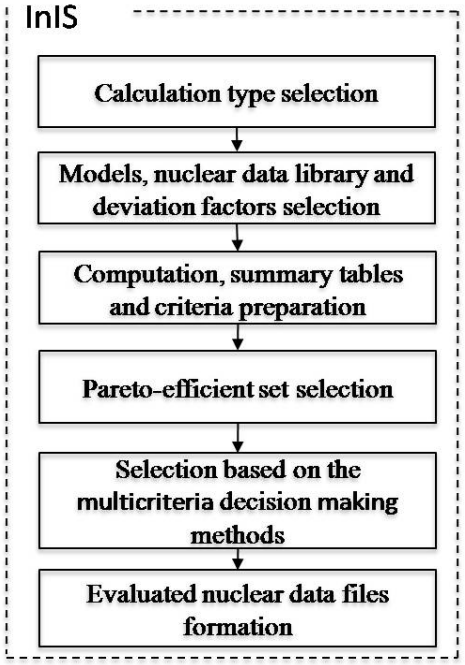

Fig. 3. Follow chart of InIS-software functioning.

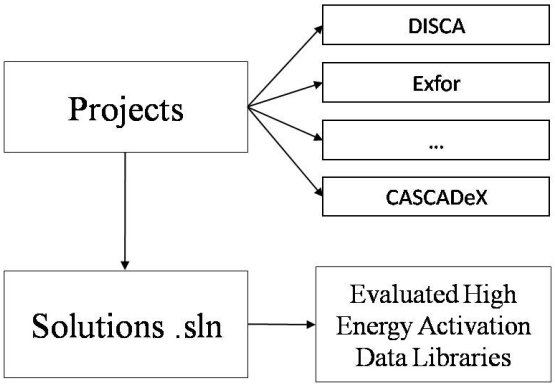

Fig. 4. The data structure in InIS.

optimization module and the module processing the results of calculations. Also IViS-systems have access to ready-made libraries of nuclear data, to the experimental data and calculations for other models that are stored in XML-format.

The main function of IViS systems is the choice of model parameters providing the best accordance with experiment. The Fig. 2 shows the algorithm of working with this software system to select the best model parameters. The first step is to select the type of calculation in accordance with the available experimental data: mass distribution, excitation functions, double-differential cross-section. Then one must specify the range of variable parameters, a set of criteria and parameters of random search. For the assessment procedure it is necessary to specify the reference data on which deviation factors will be evaluated. Reference data can be the results of previous calculations, the experimental data or

Table 1. Existing deviation factors.

F	Evaluation of integrated proximity to the experiment, provided that the data can be very different $\langle F\rangle = \frac{\sum_{i=1}^{N} F_i}{N} = 10^{\sqrt{\frac{\sum_{i=1}^{N} (\lg(\sigma_i^{\exp}))-\lg(\sigma_i^{calc}))^2}{N}}}$,
H, D	Evaluation of integrated proximity to the experiment. The exponent reflects the acceptable compensation degree for small values of some terms by large values of others. The higher the index, the greater the possible compensation degree $H = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[\frac{\sigma_i^{\exp}-\sigma_i^{calc}}{\Delta\sigma_i^{\exp}}\right]^2}$, $D = \frac{1}{N}\sum_{i=1}^{N}\left\lvert\frac{\sigma_i^{\exp}-\sigma_i^{calc}}{\Delta\sigma_i^{\exp}}\right\rvert$,
L	Evaluation of integrated proximity to the experiment, provided that the contribution of various areas is roughly equal $L = \sqrt{\frac{\sum_{i=1}^{N}\left[\frac{\sigma_i^{calc}}{\Delta\sigma_i^{\exp}}\right]^2\cdot\left[\frac{\sigma_i^{\exp}-\sigma_i^{calc}}{\sigma_i^{calc}}\right]^2}{\sum_{i=1}^{N}\left[\frac{\sigma_i^{calc}}{\Delta\sigma_i^{\exp}}\right]^2}}$,
R	Evaluation of relative integral proximity to the experiment $R = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{calc}}{\sigma_i^{\exp}}$,

data retrieved from a library of nuclear-physical data.

If the number of criteria is more than two, automatic selection of the effective set of model parameters is done after the calculation. The final choice of the optimal set of parameters is carried out by using methods of the multicriterial decision making.

At the moment, the Analytic Hierarchy Process [4] is implemented for the final selection of the best set of model parameters from the nondominated totality. To use this method the user has to carry out a paired comparison of the selection criteria. The end result of the program will be the most suitable model parameters in terms of the selected reference data and the user's preferences.

To select model parameters, a method of global optimization based on the usage of so-called low discrepancy sequences of points was proposed and implemented.

2. Information Interactive System for High Energy Activation Nuclear Data preparation

InIS-systems are designed to automate the preparation, verification and validation of nuclear data in the high energy range and allow a user with no special skills to prepare activation nuclear data, to evaluate it statistically using the existing experiments, to verify the models and present the results graphically.

The algorithm of the best model selection in InIS

Table 2. Additional proposed deviation factors.

Cov	Cross-section behavior trend evaluation $cor = \frac{\frac{1}{N}\cdot\sum_{i=0}^{N-1}(\sigma_i^{\exp}-\langle\sigma^{\exp}\rangle)\cdot(\sigma_i^{calc}-\langle\sigma^{calc}\rangle)}{\frac{1}{N}\cdot\sum_{i=0}^{N-1}(\sigma_i^{\exp}-\langle\sigma^{\exp}\rangle)\cdot\frac{1}{N}\cdot\sum_{i=0}^{N-1}(\sigma_i^{calc}-\langle\sigma^{calc}\rangle)}$,
Rm	Cross-section maximum deviation evaluation $Rm = \max\left(\frac{\sigma_i^{calc}}{\sigma_i^{\exp}}\right)$.

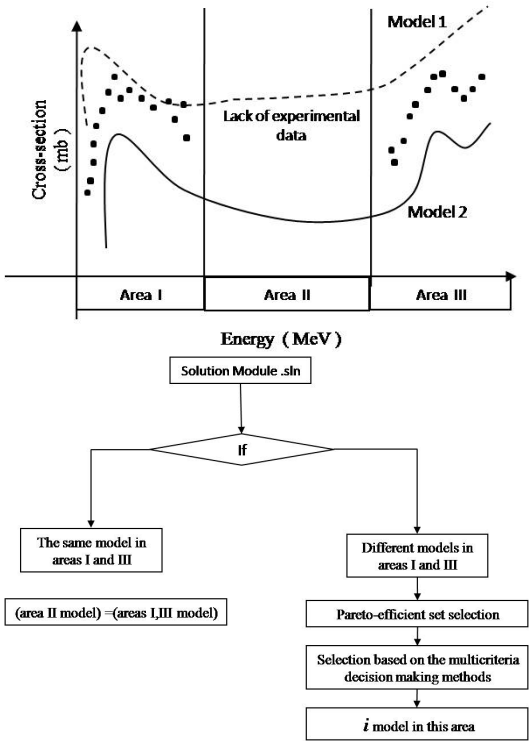

Fig. 5. The selection of models in InIS.

HAND system is similar to that of the best parameters selection in IViS-systems (see Fig. 3). The main difference is in comparison of different model calculations, which in particular can have optimal parameters set for each model, based on IViS-systems work results.

In InIS HAND there is no unit designed for finding the optimal model parameters. However, a wide range of service functions which make different models user-friendly (visualization, ENDF format recording, evaluated and experimental nuclear data libraries handler, calculations sewing together, *etc.*) is implemented in the system.

This software system consists of two structural elements - projects and solutions. The projects represent the basic element of the system. They contain the calculated and experimental information necessary for the analysis (see Fig. 5). Several projects are integrated into solutions that provide a full range of service functions needed for the evaluated activation nuclear data files generation.

One of the problems in this area is the lack of experimental data, both in a certain energy range and in the mass number range. To compensate for these deficiencies, the following algorithm was proposed for model selection in the area with no experimental information (see Fig. 5).

III. DEVIATION FACTORS IN INTEGRATED SOFTWARE SYSTEM

To evaluate the calculation correlation to the reference data in the software systems described, the deviation factors are now widely used in this field [5]. Also, a number of factors suggested by some authors and reflecting their conception of possible calculation estimation methods is being used. The whole totality of different factors is presented in the table. Simultaneous consideration of such a broad set of factors is dictated by the fact that currently there is no common and consistent methodology for comparison to experiments in this domain.

The software developed has been used for the calculations in the framework of the IAEA project on "Benchmark of Spallation Models", as well as for updating activation data libraries [6].

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