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Modern Instruments for Nuclear Reaction Simulations Based on NRV Web Knowledge Base

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Abstract

The NRV web knowledge base on low-energy nuclear physics has been created in the Joint Institute for Nuclear Research. This knowledge base working through the Internet integrates a large amount of digitized experimental data on the properties of nuclei and nuclear reaction cross sections with a wide range of computational programs for modeling of nuclear properties and various processes of nuclear dynamics which run directly in the browser of a remote user. Today, the NRV knowledge base is a powerful instrument for nuclear physics research. The basic principles of the NRV knowledge base are covered, and a brief description of its structure is given. The practical usage of the NRV knowledge base for both scientific and educational applications is demonstrated in detail.

Keywords: Web Knowledge Base, Low-Energy Nuclear Physics, Nuclear Data, Nuclear Reactions

1. INTRODUCTION

Over the last hundred years, progress in nuclear physics has generated a vast amount of the experimental data both on nuclear properties and on reactions induced by nuclear particles. In recent years, advances in the Internet technologies have led to the development of web-based nuclear databases. As a rule, these nuclear databases supply users with ordinary text files with tabular information and are limited to specific information of a specific type. Certainly, cumulative data and its free accessibility assist in the day-to-day work of a modern nuclear physicist. However, variety of data requirements, for example, in the case of planning new experiments, results in the work consisting of the following steps. First, a search for available experimental data. Second, processing of the collected data; in some cases this includes analysis of the data within appropriate theoretical models. Third, a simulation of the experiment and a choice of optimal parameters of the experimental setups. Fourth, when the experiment is completed, the obtained data must be processed and analyzed within modern physical approaches. All these steps require considerable amount of time, resources, and experience.

In order to simplify this work, we suggest using a unique web-based system which we call the NRV web knowledge base on low-energy nuclear physics [1-3]. It has been created in the Joint Institute for Nuclear Research. This knowledge base, working through the Internet, integrates a large amount of digitized experimental data on the properties of nuclei and nuclear reaction cross sections with a wide range of computational programs for modeling of nuclear properties and various processes of nuclear dynamics that run directly in the browser of a remote user.

Today, the NRV knowledge base is both a powerful tool for nuclear physics research and an educational resource. The paper describes the basic principles of the NRV knowledge base and its structure. The practical usage of the NRV knowledge base is demonstrated on the example of the analysis of nuclear elastic scattering reactions within the optical model.

2. NUCLEAR DATA AND MODELING OF NUCLEAR DYNAMICS IN WEB

Intensive research in nuclear physics during the last century resulted in a large amount of experimental data on the properties of nuclei and the cross sections of nuclear reactions. In recent years, online versions of these databases available on the Internet in a digital form via a web browser are the most intensively developed. Among the major resources of nuclear data one can mention, for example, NNDC [4], IAEA-NDS [5], CDFE [6], TUNL [7], NEA [8], etc.

As a rule, the existing nuclear physics resources contain exhaustively detailed information on a specific subject (properties of atomic nuclei or reactions with them) in text or, rarely, in static graphical formats. It is often necessary to collect data of different types visiting many different web sites. In addition, for theoretical analysis and processing of these data, the user must look for and apply specific computational codes.

Over the years of development of nuclear physics and, in particular, study of dynamics of nucleus-nucleus collisions, a number of theoretical approaches has been developed. These include, for example, the software codes providing the possibility of simultaneous modeling of several competing processes occurring in the collisions of nuclei (e.g., FRESCO [9], GRAZING [10], DWUCK [11], etc.). Many of these software packages are freely distributed. The main drawback of many of these codes is an awkward interface. Here, the interface means the way the users interact with the software code, for running of which it is necessary to prepare an input file correctly. Typically, the input file is a text file with a lot of input parameters, for the proper preparation of which it is necessary to study quite complex and not always complete manuals. As a result of running of the program, the user usually obtains another text file, for processing of which some third-party graphical applications should be used. Therefore, the work with these programs for a beginner is challenging.

The NRV provides one of the ways of solution of the indicated problems. It is to organize the work of the computational codes on a remote server available to the users via the Internet providing the access to its resources for a large number of user requests overlapping in time.

3. STRUCTURE AND BASIC COMPONENTS OF NRV

The developed system – the NRV web knowledge base on low energy nuclear physics — is designed to combine nuclear databases together with theoretical approaches to modeling of dynamics of nuclear reactions into a single system with a uniform graphical user interface and easy access. The functioning scheme of the NRV knowledge base is shown in Fig. 1.

The NRV is based on the following principles: (1) constantly updated experimental databases on the properties of nuclei (masses, electromagnetic properties, half-lives, decay modes, level schemes, etc.); (2) constantly updated experimental databases on the cross sections of various nuclear processes; (3) implementation of a large number of quite complex models and algorithms that describe the properties of nuclei and the processes of nuclear dynamics at low and intermediate energies; (4) implementation of a unified, user-friendly, interface.

Within this project, complex computer programs having a visual graphical interface for setting initial parameters as well as for graphical representation and processing of the results are made available via the Internet. This is achieved through the development of the web applications based on the client-server architecture. A special feature of them is that the computer programs are both located and executed on the server and the client receives the results of their work via the Internet. This approach makes the work with the knowledge base independent of the operating system.

The system is accessible using a web browser supporting the Java plugin via the Internet. This allows any user to access the NRV knowledge base from any place with an Internet connection. The interaction between the client and the server is organized using web forms implemented with Java, JavaScript, PHP, and HTML languages.

The communication between the server and the client as well as creation of dynamic content is organized and implemented by means of the PHP language and the AJAX technology. Substantial computer resources required for modeling of complex processes of nuclear dynamics (for example, the duration of the calculation may range from a few seconds to a few days), require special organization of the interaction of the remote user with the server. For this purpose, the server has a resident service that starts the execution of computational programs, monitors the calculation progress, and sends intermediate information to the client. After calculation, all the results are sent to the user as an HTML document for further processing and analysis. This approach allows one to run complex computational programs and obtain final results in a web browser, even in the case of a very long calculation.

The databases are a valuable component of the NRV knowledge base. For storing experimental data we use the open-source relational database management system MySQL.

All the NRV sections have detailed descriptions and/or references (including hyperlinks) to relevant publications.

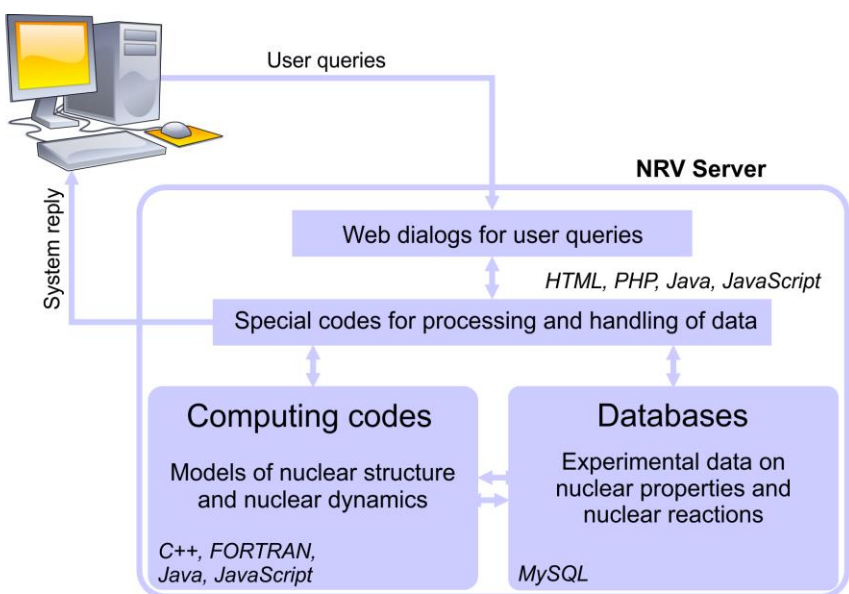

Figure 1. The functioning scheme of the NRV knowledge base

3.1 Databases on nuclear properties and nuclear reactions

Our databases on the experimental properties of nuclei contain the data obtained mainly using some of the most reputable existing databases: NNDC [6] and AMDC [12]. Some of the information (e.g., nuclear radii) is found and entered into our databases independently, using the original publications in journals. We also independently create and fill databases of digitized experimental cross sections of nuclear reactions (angular distributions of elastic scattering, fusion excitation functions, evaporation residue cross sections, etc.) based on original publications. For brevity, in the following we will refer to all of these databases as NRV databases.

The presently available NRV databases on experimental properties of nuclei and experimental cross sections of nuclear reactions include information on

- Ground states: spins, parities, half-lives;
- Excited states: energies, spins, parities, half-lives (widths);
- Decays: modes, intensities;
- Abundances of nuclides;
- Nuclear charge radii;
- Nuclear Masses;
- Electric quadrupole moments;
- Magnetic dipole moments;
- B(E2) transitions: energies of the first excited 2^+ states, adopted (recommended) values, reduced electric quadrupole transition rates, quadrupole deformation parameters;
- B(E3) transitions: energies of the first excited 3^- states, reduced electric octupole transition rates, octupole deformation parameters.

In addition to the experimental data on the properties of nuclei, we have a database on theoretical properties of ground-states (deformations, shell corrections, and mass excesses) based on Ref. [13]. The NRV databases are constantly updated.

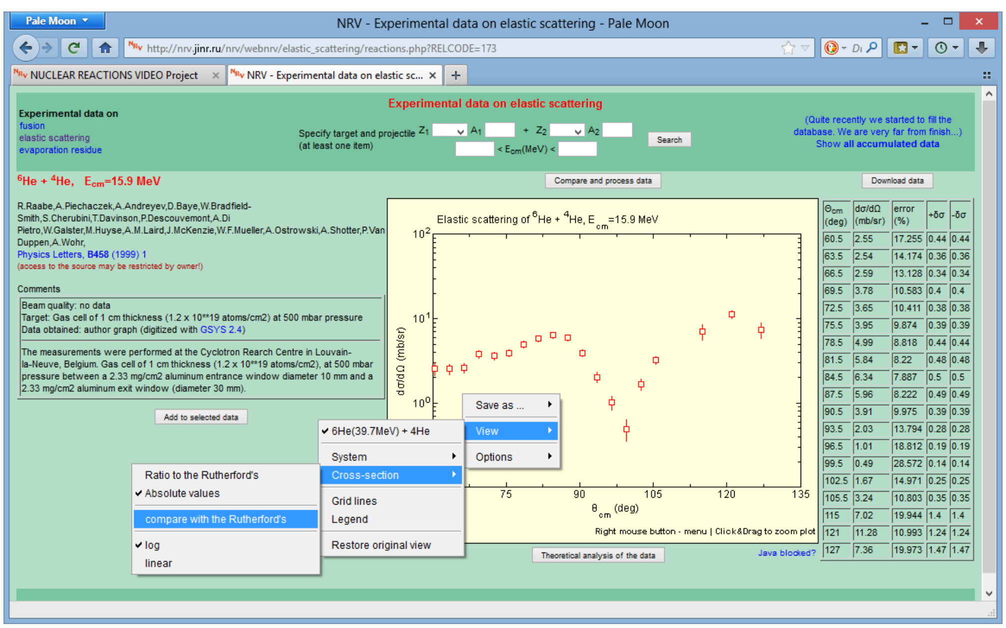

Figure 2. Example of presentation of information on the experimental elastic scattering cross section for the reaction $^6He + ^4He$

At present, the following possibilities of work with the experimental data are implemented:

- Access to the data on nuclear properties via the Nuclear Map section. The data can be retrieved both for a single nucleus and for a group of nuclei (*Systematics* section).
- Access to the data on the reaction cross sections. An example of presentation of information on the experimental elastic scattering cross section for the reaction ^{6}He + ^{4}He at 15.9 MeV is shown in Fig. 2. The data is displayed both in the text and in the graphical formats. In addition, information on the data source (reference and hyperlink to the publication) and a brief description of the experiment are given. The selected data may be saved in the text (tabular) or in the graphical formats on the user's computer (*Download data* button). There is also a possibility of processing the cross sections for the current reaction on order to plot it in appropriate for user form. *Compare and process data* button allows one to plot the data for different reactions available in the NRV database in the same frame. *Theoretical analysis of the data* button redirects the user to the section of the theoretical analysis of fusion cross sections for the selected reaction.
- Use of the experimental data on nuclear properties to determine the model parameters. This option significantly simplifies the use of many theoretical models.

3.2 Models of nuclear properties

Shell model and two-center shell model. The NRV knowledge base includes the programs for calculating single-particle levels (energies and wave functions) for spherical and deformed nuclei in the framework of the shell model with the mean field in the form of the Woods-Saxon potential as well as the two-center shell model [14,15] which provides the possibility of the calculation of single-particle levels from the configuration of two separate nuclei to the compact shapes of the compound nucleus. An example of the calculation of single-particle levels using the Woods-Saxon potential for the spherical nucleus ^{208}Pb is shown in Fig. 3.

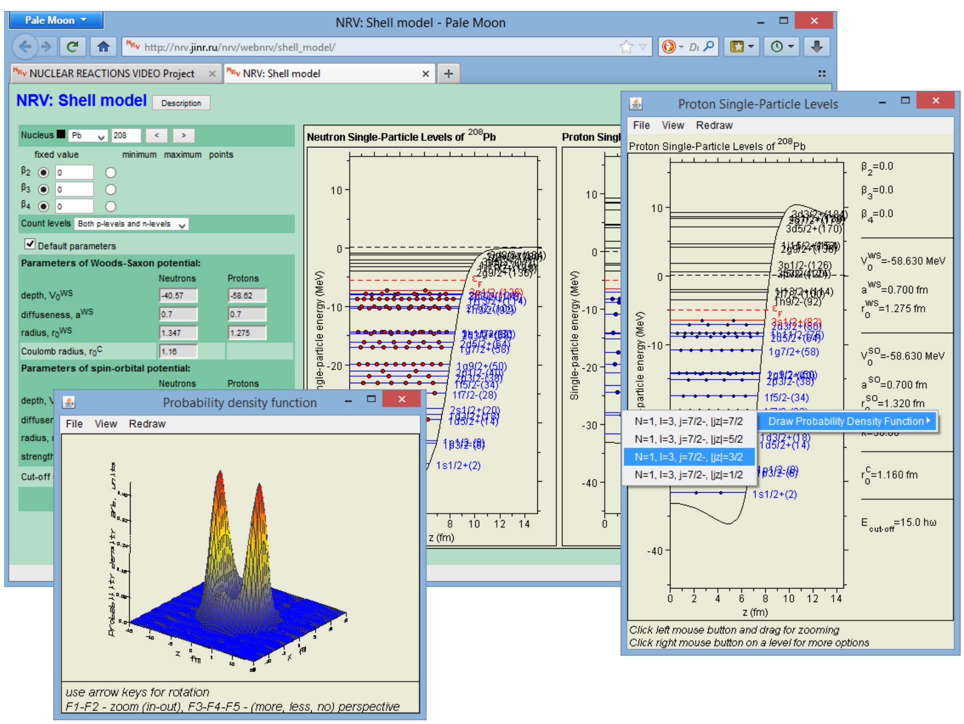

Figure 3. Example of calculation of single-particle levels and probability density function for one of the proton states of the ^{208}Pb nucleus.

Alpha decay. This part of the project allows one to study the properties of the alpha decay process: half-life, experimental decay chain, decay scheme as well as the alpha-particle wave function calculated for a particular potential, the parameters of which can be varied using the web interface. The code is based on Refs. [16-20]. For calculation of the decay energy, the experimental masses of the ground states are used if they are available in the NRV database; otherwise, a theoretical estimation [13] is provided. The spins and the parities of the ground states are also taken from our database, if available; otherwise, the minimum possible spins and positive parities are assumed. For estimation of the half-life, we use the WKB approximation, the empirical Viola-Seaborg relation [16] with the parameters [17], the Viola-Seaborg relation [16] with the parameters [18], as well as the relation of Sobiczewski et al. [19].

Beta decay. This part of the project allows one to study the properties of the beta decay process: allowed decay types, half-life, and decay scheme. The code is based on Refs. [21–23]. The total half-life is calculated taking into account all energetically allowed transitions. Energies, spins, and parities of the states are taken from the NRV database, but the possibility of varying them manually is also provided. In the case of absence of reliable spectroscopic data, only transitions to the ground state of the daughter nuclei may be chosen (this is done by setting the appropriate checkboxes).

Fission. This part of the project allows one to study the processes of induced fission and spontaneous fission. For the induced fission $Z - N$ or $Z - A$ distribution of fragments, mass distribution, and charge distribution are displayed. The calculation of these distributions is performed using the GEF code [24] specially adapted for operating within the NRV knowledge base. The multiplicities of pre- and postfission neutrons are calculated according to Ref. [25]. The total kinetic energy of the fragments is calculated according to Refs. [25,26]. The web interface allows one to vary the excitation energy and the angular momentum of the nucleus as well as the range of Z, N, A taken into account. For the spontaneous fission, the experimental half-life taken from the NRV database (if any) as well as theoretical estimates calculated according to Refs. [23,27,28] are displayed.

Decay of excited nuclei. This part of the project allows one to calculate level densities, decay widths, and survival probabilities of excited nuclei. The code is based on the statistical model of decay of excited rotating nucleus by fission and evaporation of neutrons, protons, alpha particles, and dipole gamma quanta [29–31]. The properties of the nuclei are taken from the NRV database (if any), but the possibility of varying them manually is also provided. In addition, the interface allows one to vary the range of excitation energies, the level density parameters, moments of inertia, the type and the parameters of the collective enhancement of the level density.

3.3 Models of nuclear reactions

The sophisticated computer programs implementing physical models of nuclear properties and nuclear reactions are located and executed on the side of the computing server (these programs are usually created in C++ or FORTRAN). The users can keep track of starting the programs and the progress of their execution using HTML forms in the browser. Almost all dialogs for preparing model parameters have the option of setting these parameters to default values chosen based on the experimental properties of nuclei, available systematics, or our own experience in using the corresponding codes.

Elastic scattering. The system includes the optical and the classical models of elastic scattering of nuclei. These models allow the user to calculate the differential cross section of elastic scattering, S-matrix, field of trajectories, the deflection function, partial wave functions, phase shifts, etc. The possibility of choosing the optical model parameters according to the global parametrizations as well as the possibility of their automatic fitting to the experimental data (available in the NRV database or entered by the user manually) significantly simplifies the analysis.

Inelastic scattering. The cross sections of the processes of inelastic excitation of collective states can be analyzed within the DWBA approach (DWUCK4 code [11]) and the coupled channel approach (FRESCO code [9]).

Transfer reactions. The system provides the possibility of studying few-nucleon transfer cross sections in the framework of the DWBA approach and the semiclassical GRAZING code [10]. The GRAZING code of the NRV allows one to calculate mass, charge, total kinetic energy, and angular distributions of the transfer reaction products.

Fusion. The fusion cross sections and the fusion barrier distribution functions can be calculated in the NRV system within the quantum [32] and the empirical [33] coupled channel approaches. Both approaches allow one to take into account the coupling of relative motion of colliding nuclei with their collective degrees of freedom (surface vibrations and/or rotations). In addition, within the empirical model there is a possibility of taking into account the influence of neutron transfer channels on the fusion cross section [34, 35].

Evaporation residues. The combination of the codes for calculation of fusion cross sections with the code of the statistical model of decay of excited rotating nucleus allows one to simulate the processes of fusion with subsequent fission or survival with respect to neutron, proton, alpha-particle, and gamma-quantum emission. The system has an additional possibility of taking into account the probability of formation of the compound nucleus from the configuration of two touching nuclei, which is extremely important for the reactions leading to the formation of superheavy nuclei. The option Calculate *Z-N* yield allows one to analyze the mass and the charge distributions of fission fragments based on the GEF code [24]. The partially implemented option Decay of fragments presently provides a possibility of calculation of pre-scission, post-scission, and total neutron, proton, alpha-particle, and gamma-quantum multiplicities.

Radiative capture. This part of the project allows one to study the radiative capture reactions of the type $a\ (b, \gamma)\ c$ within the potential model [36]. It is assumed that the nuclei a and b are structureless. The state of the nucleus c is obtained by the solution of the Schrödinger equation for the relative motion of the clusters a and b in their effective interaction potential. The spectroscopic factor of this state can be included into the calculations. The code allows one to calculate the radiative capture cross sections and the astrophysical S-factors taking into account $E1$, $E2$, and $M1$ electromagnetic transitions. At the moment we do not have our own database of experimental radiative capture cross sections and S-factors. However, this data may be found in the databases NACRE [38] and NACRE-II [39]. The hyperlinks to these databases are provided on the NRV web site.

Fragmentation. This part of the project allows one to study fragmentation reactions. The yields of different products are calculated using the phenomenological code EPAX3 [37].

Kinematics. This section provides the possibility of kinematic analysis of nuclear reactions with two and three particles in the exit channels as well as Q-value calculations for different processes.

Driving potentials. The potential energy of a heavy nuclear system is a key quantity determining its evolution in the processes of nucleus-nucleus collisions. The NRV provides the possibility of calculation and visualization of the multidimensional adiabatic (within the two-center shell model) and diabatic (within the double-folding and the proximity models) driving potentials [29].

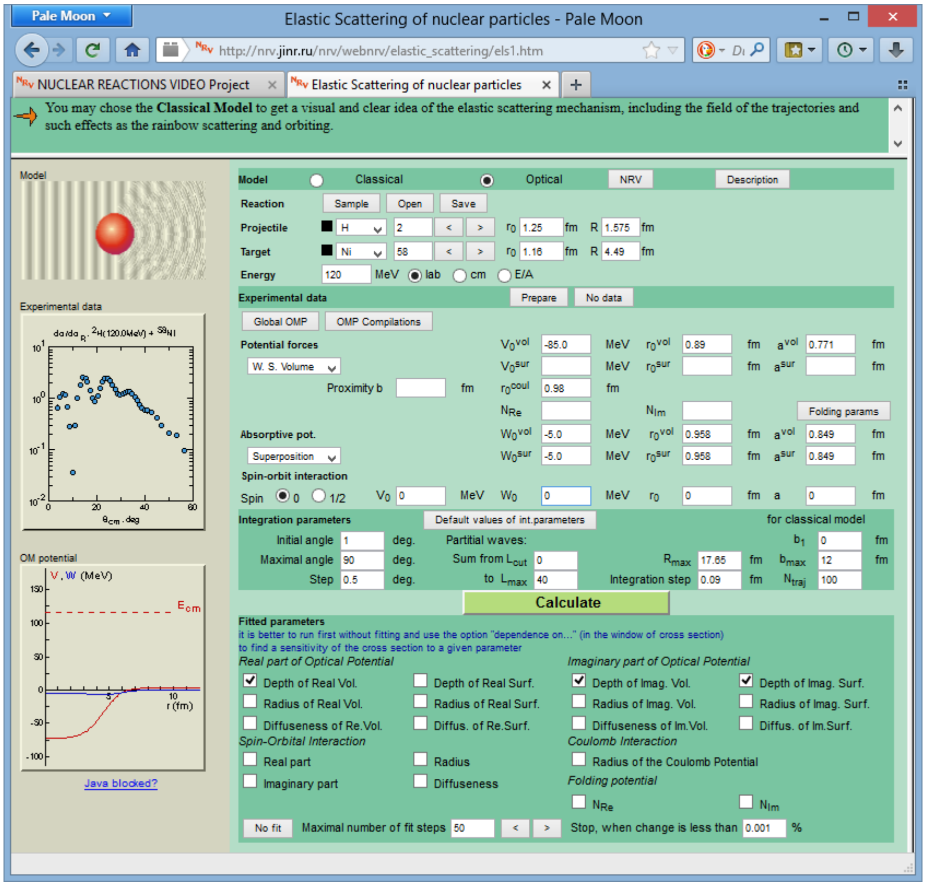

Figure 4. Screenshot of the NRV web dialog for preparation and starting of the optical model calculations

4. ANALYSIS OF NUCLEAR ELASTIC SCATTERING WITHIN NRV KNOWLEDGE BASE

The most important goal of creating the NRV knowledge base is to provide the user with the opportunity of modeling of many channels of nuclear reactions at low and intermediate energies: elastic and inelastic scattering, transfer reactions, fusion, etc. This section demonstrates the capabilities of the NRV knowledge base in the analysis of elastic scattering reactions on the example of the d(120 MeV) + ^{58}Ni reaction studied experimentally in [40].

The *Elastic scattering* section of the NRV is based on the computer code calculating the corresponding cross sections within the well-known phenomenological optical model. The model details may be found in numerous textbooks on nuclear physics, e.g. in Ref. [41]. Here we just remind the reader that the main ingredient of the optical model is the complex optical potential modeling the scattering dynamics and coupling with inelastic channels.

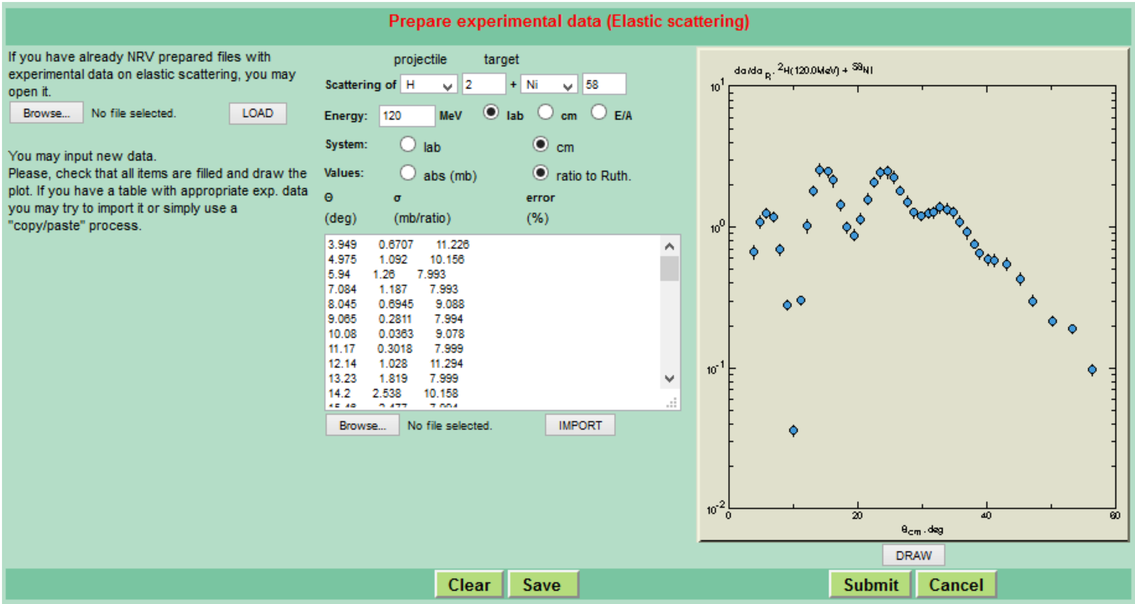

Figure 5. Screenshot of the NRV web dialog for preparation of the experimental data on elastic scattering

The optical nucleus-nucleus potential (OP) is treated as a combination of the Coulomb, nuclear and spin-orbit terms, where the last two ones have the radial dependence of the Woods-Saxon form. One may define the OP in the following form

$$U_{OM}(r) = U_C(r) + V_0 f_V(r) + iW_0 f_W(r) + 4a_{VD}V_D \frac{d}{dr} f_{VD}(r) + i4a_{WD}W_D \frac{d}{dr} f_{WD}(r)$$
$$+4a_{SO}(V_{SO} + iW_{SO})(\vec{l}\cdot\vec{s})\frac{1}{r}\frac{d}{dr} f_{SO}(r), \quad (1)$$

where the function $f_i(r) = 1/\left(1 + exp\frac{r - R_i}{a_i}\right)$, parameters R_i and a_i are the radius and the diffuseness of the corresponding term, V_i and W_i are the depth parameters. The spin-orbit potential includes the scalar product of the relative angular momentum vector $\vec{l}$ and the projectile spin vector $\vec{s}$. Thus, the optical potential has 17 parameters including the Coulomb radius R_C since the Coulomb term is defined as

$$U_C(r) = Z_1 Z_2 e^2 \begin{cases} \frac{1}{r}, r > R_C, \\ \frac{1}{2R_C}\left(1 - \frac{r^2}{R_C^2}\right), r \le R_C, \end{cases} \quad (2)$$

where $Z_1 e$ and $Z_2 e$ are the electric charges of the colliding nuclei.

Solution of the Schrödinger equation with the optical potential allows one to extract the scattering amplitude and calculate the elastic scattering cross section.

The main advantage of the optical model is the possibility of finding OP parameters by fitting the calculated cross section to the corresponding experimental data. The fitting procedure may be performed in the automatic regime using the computing codes for minimization of the function

$$\chi^2(\theta) = \frac{1}{N}\sum_{i=1}^{N}\frac{\left(\sigma_{exp}(\theta_i) - \sigma_{th}(\theta_i)\right)^2}{\Delta\sigma_{exp}^2(\theta_i)} \tag{3}$$

where θ_i is the scattering angle in the center-of-mass system, N is the number of experimental points, $\sigma_{exp}(\theta_i)$ and $\Delta\sigma_{exp}^2(\theta_i)$ are the measured cross section and the corresponding error, $\sigma_{th}(\theta_i)$ is the cross section calculated within the optical model.

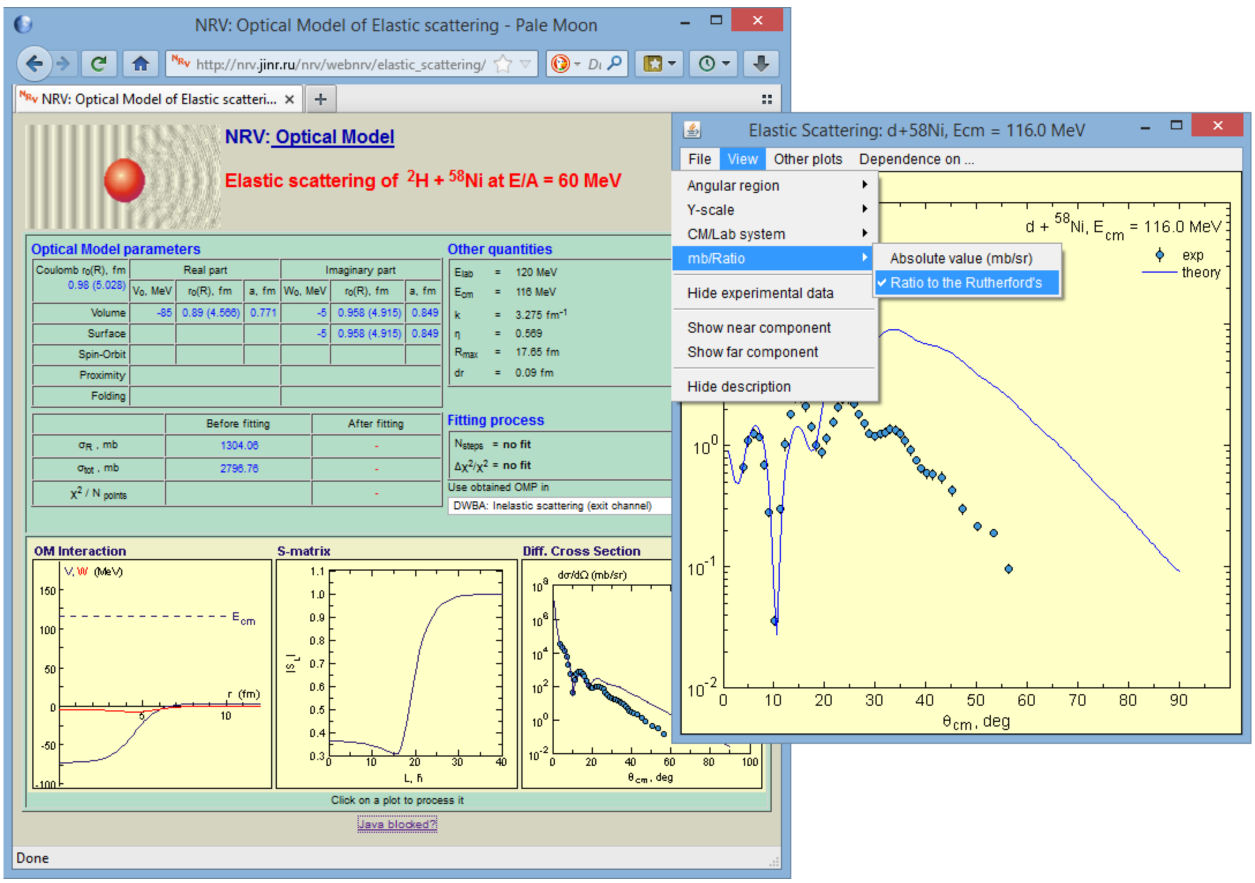

Figure 6. Screenshot of the NRV web page with the results of the optical model calculation

The NRV knowledge base provides the users with an instrument for preparation of all the ingredients necessary for starting the optical model calculation and processing of the obtained results. Fig. 4 demonstrates the screenshot of the corresponding web dialog. The dialog consists of the two main parts. The first includes numerous web controls for setting values of different reaction parameters. The user may start with choosing projectile and target nuclei, collision energy, experimental data (see below), optical potential, and then start the calculation by pressing the *Calculate* button. The second part is the panel on the left-hand side with the model logotype, experimental data, and optical potential corresponding to the user-defined parameters.

Preparation of the experimental data is organized via the web dialog shown in Fig. 5 and available by pressing the *Prepare* button on the optical model web dialog (see Fig. 4). The user may also choose the no-data regime (press the *No data* button), then the optical model provides the theoretical cross section only, without possibility of fitting OP parameters.

In the dialog show in Fig. 5, the user must define all the reaction parameters, e.g. the projectile and the target, collision energy, laboratory or center-of-mass system, the cross section units, and the data itself including the scattering angle, the cross section, and the errors in percent. The plot on the right-hand side represents the current set of data (press the *DRAW* button to update it).

In order to simplify data preparation, the NRV provides a possibility of downloading the data to the user's local drive for the fast upload later (use the *LOAD* button on the left-hand side).

It is recommended set the integration parameters controlling the accuracy of the numerical calculation. The button *Default values of int. parameters* sets them up in an automatic regime. When all the parameters are defined, the user may start the calculation of the elastic scattering cross section by pressing the *Calculate* button.

The screenshot of the resulting web page is shown in Fig. 6. The page contains tabular information on the optical model parameters together the with plots of the optical potential, the scattering S-matrix and the calculated elastic scattering differential cross section (curve) in comparison with the corresponding experimental data (dots). All these plots are interactive and may be shown in a separate Java window by single click on the web page. An example of the Java window with the elastic scattering cross section is shown on the right-hand side of Fig. 6. The window has its own menu implementing many additional functions for processing of the data, e.g. representing the cross section in the laboratory or in the center-of-mass system, in mb/sr units or as a ratio to the Rutherford cross section. It also contains the *Dependence* on menu item that provides the user with the opportunity of studying the influence of each OP parameter on the theoretical cross section. All the obtained results are available for download to the user's local drive in text or graphical formats JPG, GIF, PNG, or EPS (via the *File* menu of the Java window).

Fig. 6 shows that the calculated cross section overestimates the experimental data considerably, i.e., the applied optical potential is not appropriate for the studied reaction. In order to improve the results, one may try to fit OP parameters minimizing the χ^2 value. The choice of the parameters for the fit may be done in the *Fitted parameters* section of the main dialog (see Fig. 4). In Fig. 4, three checkboxes in the *checked* state correspond to the selection of the real and the imaginary potential depths as the fitted parameters. Start of the calculation in this case results in the web page shown in Fig. 7, where, together with the initial values of the OP parameters (blue curve), the values after the fitting procedure are given in the table (red curve). It can be seen that the χ^2 value decreases more than 2000 times, from 7526.7 before fitting to 3.3 after fitting.

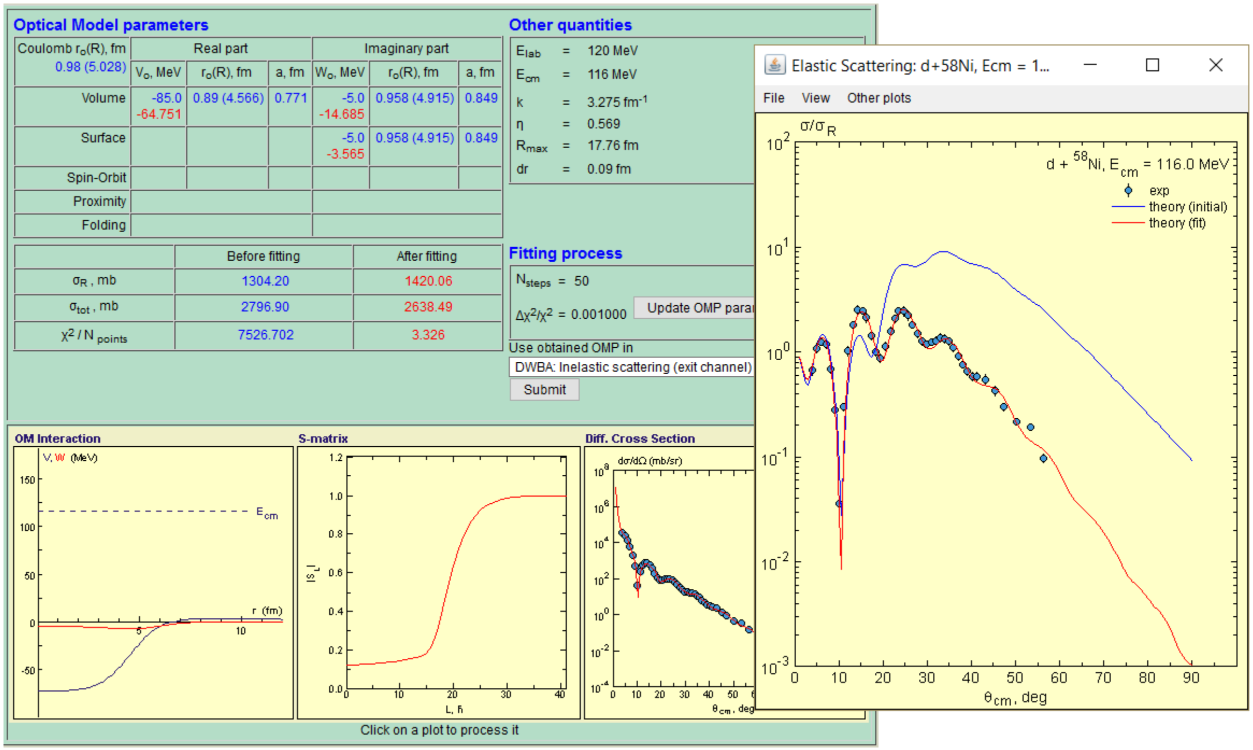

Figure 7. Screenshot of the NRV web page with the results of the optical parameters fitting

After fitting, the cross section agrees with the experimental data very well. The Java window allows one to compare the cross sections before and after fitting (see the right-hand panel in Fig. 7).

The optical model calculation in the fitting regime is very sensitive to the initial OP parameters since unrealistic (non-physical) values may result in inappropriate optical potential. In order to avoid such a scenario, the NRV provides the possibility of choosing the initial set of parameters based on the global optical model parametrizations (via the *Global OMP* button in Fig. 4). A number of global OP parametrizations for the elastic scattering reactions induced by light ions (with projectile mass $A_P \leq 7$) have been published during the last 40 years.

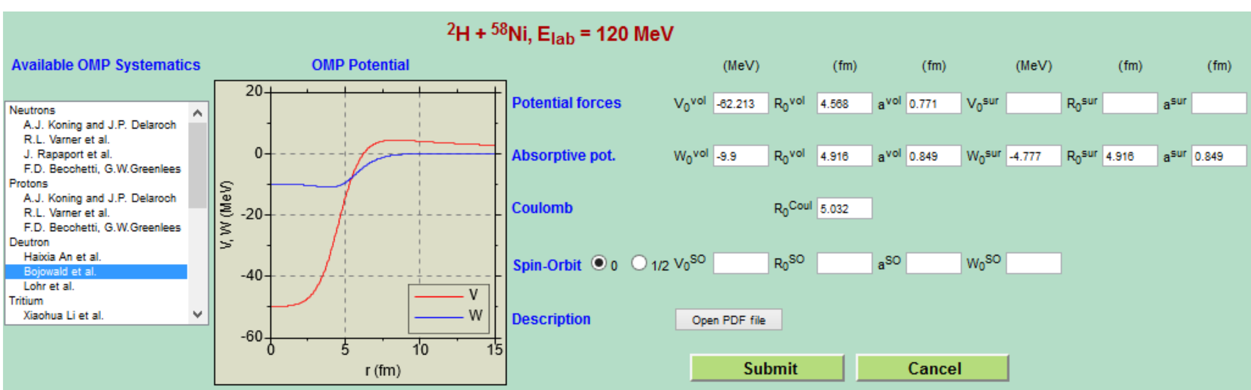

Figure 8. Screenshot of the NRV web dialog with the compilation of global optical model parametrizations

The NRV web dialog providing access to the choice of the OP parameters based on the global optical model parametrizations is shown in Fig. 8. It helps the user define the initial OP set yielding quite good description of the corresponding data. Usually, very little modification of this OP is necessary, if the reaction corresponds to the conditions (such as the collision energy and the target mass range) under which the parametrization was constructed. More information on the particular parametrization may be obtained by pressing the *Open PDF file* button in Fig. 8.

5. CONCLUSIONS

In this work practical usage of the NRV knowledge base was demonstrated in detail on the example of the analysis of nucleus-nucleus elastic scattering. The further development of the NRV knowledge base is planned in the following directions: (1) filling and updating of the existing nuclear databases as well as adding new ones; (2) implementation of new physical models as well as extending the possibilities of the existing ones; (3) modernization of the user interface, in particular, transition from the use of Java applets to the use of new technologies, such as HTML5 and JavaScript.

The NRV is an efficient tool for acquisition and development of skills of work with modern theoretical approaches to the description of properties of individual nuclides, modeling of dynamics of nuclear collisions, as well as the skills of work with experimental data and their systematization. The development of manuals and guidelines for the implementation of practical work may effectively introduce the NRV knowledge base in the educational process of any university preparing students in the field of nuclear physics.

6. ACKNOWLEDGEMENTS

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