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R-Matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region (1)

Summary Report of an IAEA Consultants' Meeting
IAEA Headquarters, Vienna, Austria
7-9 December 2015

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ABSTRACT

A Consultant's Meeting was held at the IAEA Headquarters, from 7 to 9 December 2015, to discuss the status of R-matrix codes currently used in calculations of charged-particle induced reaction cross sections at low energies. The ultimate goal was to initiate an international effort, coordinated by the IAEA, to evaluate charged-particle induced reactions in the resolved-resonance region. Participants reviewed the capabilities of the codes, the different implementations of R-matrix theory and translatability of the R-matrix parameters, the evaluation methods and suitable data formats for broader dissemination. The details of the presentations and technical discussions, as well as the actions that were proposed to achieve the goal of the meeting are summarized in this report

March 2016

Contents

1. Introduction

A Consultant's Meeting on 'R-matrix codes for charged-particle reactions in the Resolved Resonance Region' was held by the Nuclear Data Section (NDS) of the International Atomic Energy Agency, from 7 to 9 December 2015, at the IAEA Headquarters in Vienna. The purpose of the meeting was to gather experts from the international community who are developing R-matrix codes, discuss the main features and capabilities of their codes, and how they are employed to describe charged-particle-induced reactions in the low energy resolved resonance region.

Charged-particle reactions occurring at energies up to several MeV are resonant reactions that can be described by the R-matrix theory. The parameters of this theory are level energies, spins, parities, boundary conditions, and reduced width-amplitudes for each channel. The evaluation of the measured cross-section data is performed by suitably adjusting the R-matrix parameters to reproduce the observed resonance structure.

The IAEA Nuclear Data Section is coordinating an international effort to (i) evaluate charged-particle cross sections in the resolved resonance region, (ii) produce evaluated nuclear data files for further processing and finally (iii) disseminate these data through the general purpose evaluated nuclear data libraries.

This meeting was the first in a series aiming at setting the goals, recommending the actions and reviewing the results in order to achieve points (i) to (iii). The focus was therefore, on the capabilities of the existing R-matrix codes, the implementation of R-matrix theory in the codes, and establishing the translatability of the R-matrix fits produced by these codes. The latter would allow the conversion of the R-matrix fits between the codes and into appropriate data formats that could then be used by processing codes for broader applications.

The meeting was opened by Arjan Koning, Section Head of the IAEA NDS, who welcomed the participants and emphasized the importance of producing and disseminating reliable data files for charged-particle reactions in the resolved resonance region for applications. Ian Thompson (Lawrence Livermore National Laboratory) was nominated chair of the meeting, and participants James deBoer (Univ. of Notre-Dame), Satoshi Kunieda (JAEA), Mark Paris (Los Alamos National laboratory), and Paraskevi Dimitriou (IAEA) agreed to act as rapporteurs and contribute to the preparation of the summary report. The meeting began with a short introduction of the background and goals of the meeting by Roberto Capote, Head of the Data Development Unit, and Paraskevi Dimitriou (Scientific Secretary), followed by individual presentations by the participants (a group photograph and links to the presentations are provided in Annexes 3 and 4, respectively).

2. Importance of charged-particle data

Charged-particle induced reactions at low energies are important for Ion Beam Analysis (IBA) applications such as materials analysis, cultural heritage and preservation, environmental and climate control, and forensics, to mention a few examples. For over 10 years, the IAEA NDS has been serving as the international centre for the collection and dissemination of nuclear data for IBA. Through a series of Coordinated Research Projects (CRP) [2.1, 2.2], collaborations with expert scientists and staff efforts, it has created and maintained the Ion Beam Analysis Data Library (IBANDL) [2.3] that contains over 6000 datasets of differential and total experimental cross sections for charged-particle induced reactions in the low energy region below several MeV. Evaluated cross-section data are also

crucial for the implementation of the ion beam analytical techniques, since they are used in computer simulations of thick target which are then compared to measured spectra of the emitted radiation (particle or gamma). For many years the IBA community has been us relying on one single source of evaluated differential cross sections: the SigmaCalc online calculator. The cross sections available on this web site are R-matrix fits/evaluations performed by A. Gurbich [2.4].

On the other hand, the evaluated data files collected by nationally or internationally coordinated efforts (ENDF, JEFF, JENDL, CENDL) are to date, incomplete as far as charged-particle induced reactions in the resolved resonance region are concerned. The reason being that these reactions were not considered of importance for energy-related applications.

However, with the emergence of new applications or developments in existing applications, the need for reliable charged-particle induced reactions at low energies is growing and extending beyond the needs for IBA, therefore, the gap in the broadly used evaluated data files mentioned above needs to be filled. We briefly mention some of the applications where progress is leading to demands for reliable charged-particle data:

Management of reactor fuel in nuclear reactors involves the control of neutrons produced after the reactor operation is shutdown. For the most widely used fuel materials, UO2, UF6, PuF4 and PuO2, the dominant neutron producing reactions are (α,xn) reactions on isotopes of O and F. The alpha-particles are produced from the decay of the fissioning system and are stopped/re-absorbed in the reactor fuel through interactions with the lighter elements. At energies above the neutron emission threshold, (α,xn) reactions may occur in the resolved resonance region. A survey of the evaluated libraries reveals lack of reliable (α,xn) data in the low-energy resolved resonance region [2.5].

The National Ignition Facility at Lawrence Livermore National Laboratory, USA, with its main defined missions of global security, energy security, and basic science covering a vast spectrum of applications and data needs, will require reliable evaluated data for neutron, photon and charged-particle reactions over an extended energy range.

In nuclear astrophysics, the main stellar processes that produce the energy of the stars and lead to the synthesis of the light and medium-mass elements up to the iron nuclei, are fueled by thermonuclear reactions at temperatures of tens of millions of degrees Kelvin. In the earth laboratories these conditions translate into charged-particle induced reactions on light and medium-mass nuclei at energies of a few tens of keV. Significant effort has been made over the past decades to measure these cross sections at higher energies that are physically attainable at the available accelerators, and provide theoretical descriptions, R-matrix fits and/or evaluations of the data. The latter are important for extrapolating to the lower energies needed for the stellar nucleosynthesis models. Several astrophysics dedicated compilations (NACRE-I [2.6] and II [2.7]) and databases (REACLIB, BRUSLIB, KADONIS, NUCASTRODATA.ORG) have been made available as a result. The knowledge that has been accumulated over the years in measuring, fitting and modelling charged-particle induced reactions for astrophysics applications, could be extremely useful for other applications and should therefore, be integrated in the current effort to make complete and reliable evaluated nuclear data files for charged-particle induced reactions available to the broader user community.

Recently, there has been a recurrence of interest in charged-particle induced reactions over the entire energy region, including the low-energy resolved resonance region, at the Los Alamos National Laboratory.

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3. Presentations by participants

Presentations made by the participants of the meeting are summarized in the following. Links to the presentations are provided in Annex 4.

3.1 AZURE-2: an R-matrix code for nuclear astrophysics

R. J. deBoer (Univ. Notre-Dame, USA)

For low mass nuclear reactions important for determining the energy production in stars and nucleosynthesis that occurs there, a reaction model is often necessary in order to determine the cross section at stellar energies. The energy range of astrophysical interest, the Gamow energy, is determined by the convolution of the penetrability function of the cross section and the energy distribution of particles in the stellar environment. Stars burning hydrogen in their cores, main sequence burning, have core temperatures of tens of millions of degrees. This corresponds to a Gamow energy range of a few tens of keV. While these energies are trivially reached with particle accelerators, because of the Coulomb penetrability for interacting charged particles, the cross section at these energies is often too small to make them measurable with current techniques. Therefore, the tactic that is often chosen is to measure the cross section at higher energies and extrapolate down to the stellar energy range. Extrapolations are always dangerous unless a firm theoretical model is available that describes the function over the entire range of interest. For this reason a sound reaction theory is of the utmost importance.

Unfortunately fundamental physics driven nuclear models are not at the level of precision and accuracy desired by nuclear astrophysics for low mass reactions in the resolved resonance energy range. This has led to the development of phenomenological models that can be fit to perform the extrapolation. Over several decades, through the trials of many analysis, the most convenient and accurate model has been found to be R-matrix [3.1, 3.2].

Since the coding of the general R-matrix formalism is rather involved, over the years many R-matrix codes have been developed for ease of use. However, many of these codes are not freely available or are specialized for a specific reaction or kind of reactions. For this reason R. E. Azuma and M. Wiescher created the AZURE collaboration, sponsored by the joint

institute for nuclear astrophysics, with the goal of creating a general R-matrix code for the nuclear astrophysics community. This collaboration developed the AZURE code over about a ten year period from 2000 to 2010 at the University of Notre Dame. Dick Azuma led the development efforts and several graduate students were involved in the creation of the code. The code was published in Azuma et al. (2010) [3.3] and is freely available (open source) at azure.nd.edu. The code is written in FORTRAN77 and allows for the calculation of unpolarized cross sections coming from one particle entrance pair with multiple possible exit pairs. It can calculate two body (particle, particle) reactions using the standard R-matrix theory and can calculate (particle, γ) reactions using the methods found in Barker and Kajino (1991) [3.4].

While the AZURE code met several design goals, there were still several improvements, both in physics content and usability, that were desired. To meet several of these needs, the AZURE2 code was created by E. Uberseder over the period from 2010 to 2015. This code was completely rewritten in C++ to take advantage of the language's object oriented style and modern computational libraries. AZURE2's major physics improvement was that it now allowed for multiple entrance channels to be fit simultaneously. On the usability front, an improved GUI interface and dynamic memory allocation provide significantly easier use. In addition, AZURE2 also can calculate (β, particle) reactions as implemented in Barker and Warburton (1988) [3.5].

Even with the substantial improvements made in AZURE2, there are still several improvements underway. At the top of this list is the ability to calculate polarization observables. Other planned improvements are a more efficient comprehensive calculation of target corrections, calculation of differential cross sections for (particle, unobserved particle γ) reactions, and more robust and complete uncertainty analysis.

AZURE2's main achievements have been the analysis of nearly every reaction in the standard CNO cycle. These include several capture and (p,α) reactions. One of the main analysis improvements over those available previously, is the inclusion of many other possible reactions that populate the same compound nucleus over the energy range of interest. This allows for a cross check on the experimental calibrations of the different measurements both in energy and absolute magnitude. In particular the absolute magnitude of (particle, particle) reactions can be strongly constrained by the enforcement of unitarity in the theory.

The code also implements the alternate parameterization of C. Brune [3.6]. This allows for the direct fitting of observable parameters and allows for some of these parameters to be easily fixed during the fitting. For comparison with early works, the code can also take standard R-matrix parameters as input, but with the condition that the boundary condition be set equal to the shift function at the energy of the lowest resonance in each J^{π} group.

As AZURE is a freely available program and open source code, the AZURE website offers a user manual and tutorial to aid users in its use. As of December 18, 2015, about 250 people have registered on the AZURE website. The countries corresponding to their affiliations are summarized in Fig. 3.1.

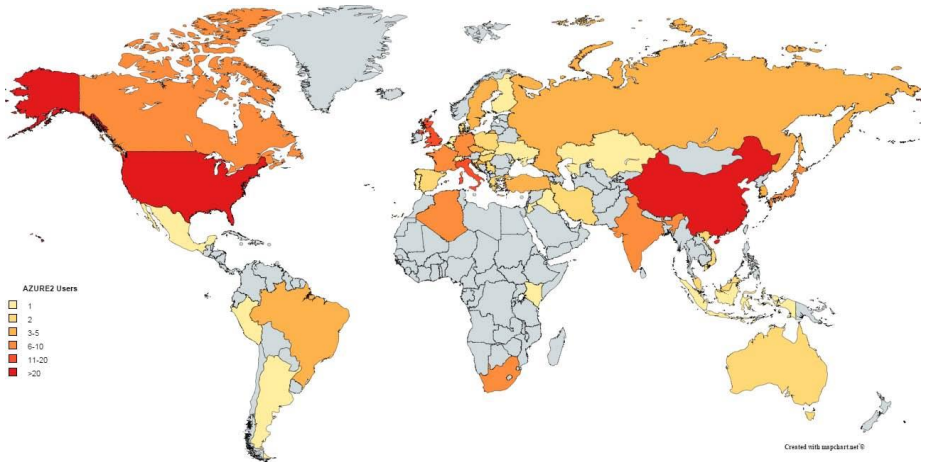

FIG. 3.1: *(Color online) Summary of number of AZURE2 users by the country of their affiliated institutions.*

3.2 Widening the Scope of R-matrix Methods

I.J. Thompson (Lawrence Livermore National Laboratory)

The R-matrix method for description of resonance cross sections has been a standard work-horse for many years. There has been a huge investment for modeling of neutron resonances, and excellent fits have been obtained. Resonances in charged-particle reactions have been described for light- and medium-mass nuclei, but not so comprehensively and transparently as for neutrons.

There are now still a few groups performing R-matrix fits, so we need to be clear about what might be some common issues for possible misunderstanding of each others' results. *First*, we need to clarify the R-matrix radius r_m: is it fitted or fixed, is it different for each channel and/or for each partial wave? Has it been made large enough to be outside the expected physical processes? *Second*, we need be sure of how widths are defined, since they may be given as reduced widths γ^2, reduced width amplitudes γ, full widths $2\gamma^2 P$, 'observed widths', or the eigenvalue widths. *Third*, we need to be clear which boundary condition β (or Bloch parameter $b = r_m\beta$). Is it a constant, set according to the partial wave, set for some eigenstate, or dependent on the scattering energy?

It is straightforward to generalize R-matrix theory in many ways: for complex scattering energies (e.g. looking for S-matrix poles), for non-integer l values (e.g. in hyperspherical expansions), for asymptotic couplings outside r_m , or for charged particles ($\eta \neq 0$: attractive or repulsive Coulomb potentials). Thus resonances of charged particles should be describable with equal accuracy as for neutrons, provided the codes are written to allow for Coulomb forces.

In Fig. 3.2 a preliminary calculation of resonances in p + ^{27}Al scattering is shown, where an attempt to reproduce the published fit of Ref. [3.7] by using their published resonance energies and reduced widths (though as yet without the mixing angles) was made. In order to get reasonable results, a boundary condition depending on the shift function in each partial wave at the scattering energy: $b = S(E_p)$ was used. In the figure we see that this fit is not perfect, with some discrepancies especially at the end of the energy ranges. Subsequently it was discovered that the calculation did not convert lab to cm cross sections correctly (only the

lab angles to cm angles), and that if these were done properly the fit at 160 degrees would be much better at low energies. The (p,α) data from the same publication can also be fit to the (rather low) accuracy of the data.

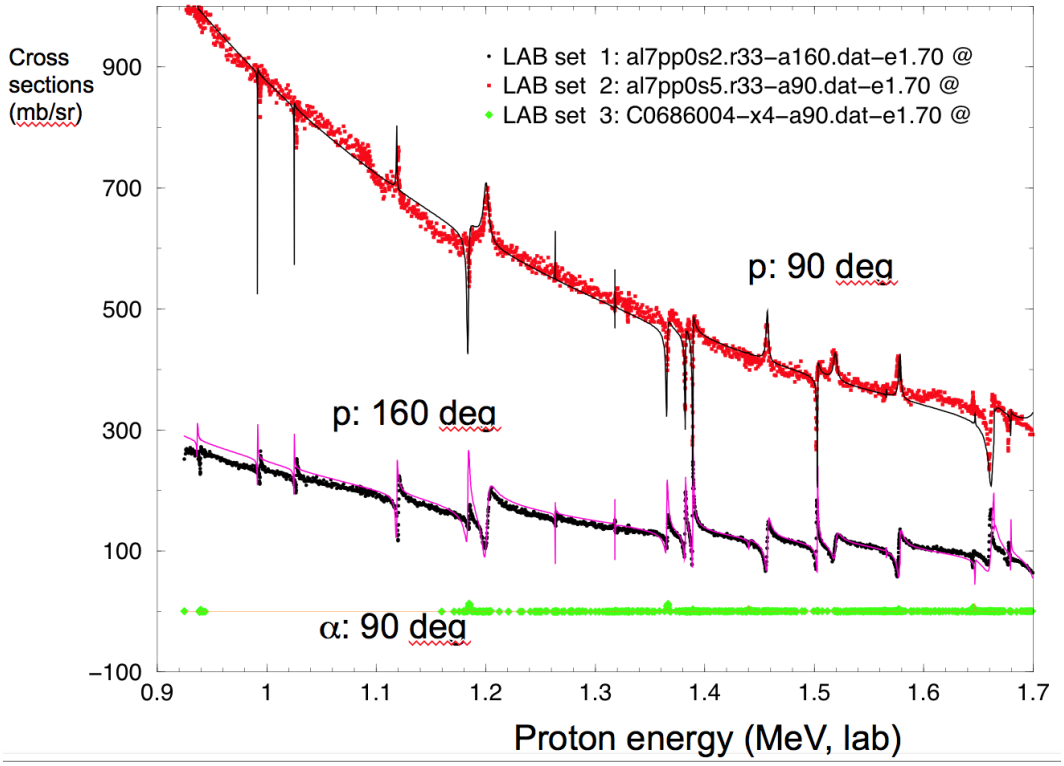

FIG. 3.2: *Attempt to describe the data of Nelson et al (1984) for p+^{27}Al elastic scattering using the published R-matrix parameters.*

This simple calculation can be easily extended to include channels for excited states of the target, and also of the residual ^{24}Mg after α emission. Capture channels (p,γ) can also be included explicitly as another R-matrix channel, or collectively in the Reich-Moore approximation as an imaginary addition to the pole energy. However, going to energies that are above the resolved resonances is more difficult, as is going above any three-body breakup threshold.

In the remaining part of the presentation, 'calculable' R-matrix methods for solving quantum scattering problems starting from a Hamiltonian were presented. These methods have been used extensively for coupled-channels systems (I.J. Thompson), while Lagrange-mesh R-matrix methods based on microscopic Hamiltonians have often been used to solve light-ion scattering problems (Sofia Quaglioni, LLNL). In these approaches we use the orthonormal basis for interior wave function $r < r_m$, and produce R-matrices as a step to giving S-matrix and cross section results. In principle, two- and three-body channels can be simultaneously used (though not orthogonal) to give results above breakup thresholds.

The calculable methods may be combined with phenomenology, either by explicitly adding in R-matrix terms for resonances missing from the model Hamiltonian, or by 'fine-tuning' the calculated R-matrix energies and widths to improve fits to experimental data.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

3.3 AMUR code

S. Kunieda (Japan Atomic Energy Agency)

The status of the AMUR code was presented including some results from preliminary analyses of the ^{8}Be and ^{17}O systems.

AMUR is a multi-channel, multi-level R-matrix code based on the Wigner-Eisenbud formalism except for the γ-ray channels which are calculated by the Reich-Moore approximation. The code is based on object-oriented programming to facilitate continuous management and further development. Apart from the R-matrix parameters, the experimental parameters (such as for the re-normalization, resolution, etc) could also be deduced from the shape analysis of the measured cross sections. The fitting method adopted is equivalent to that of the KALMAN/SOK code which is also able to estimate the covariance matrix of the parameter values, and the cross-sections.

A preliminary analysis of the ^{17}O system for the evaluation of n+^{16}O cross-sections was also presented. Using the unitarity-constraint from R-matrix theory, we may solve the discrepancies among the different measurements by introducing experimental parameters such as re-normalization to each measurement.. This is very relevant to the estimation of the uncertainty and covariances of the cross sections. The analysis of ^{8}Be system is also ongoing for the evaluation of the p+^{7}Li cross sections. In the preliminary analysis, the energy eigenvalues are fixed to those taken from ENSDF, while the reduced-width amplitudes, channel radii and boundary condition numbers are varied for each channel. It was pointed out that there could be some missing levels in ENSDF which are necessary to fit the measured cross sections. Besides, the channel radii obtained are larger than the experimental rms radii for the nucleus. This may be consistent with the well-known picture of the nucleus because the nucleus has a diffuseness around the surface and the companion (particle) is not a "point-particle".

The code is still under development as it has some drawbacks such as the lack of relativistic corrections, the non-explicit handling of the γ-ray channels, missing function for polarization/analysing power

3.4 The p+^{27}Al system using SAMMY

P. Dimitriou (IAEA)

R-matrix fits to proton-induced reaction cross sections on ^{27}A using the SAMMY code [3.8] were presented. Three open channels were considered in the fits: the elastic (p,p$_0$), and the two inelastic channels (p,p$\gamma_{1\text{-}0}$) and (p,p$\gamma_{2\text{-}0}$). Photons were treated in the Reich-Moore approximation (see [3.8]).

The experimental cross sections were taken from IBANDL [2.3]. For the elastic channel, the fit was performed on the data of Nelson et al [3.7], while for the inelastic channels all the available data were taken into account.

The fits used the R-matrix parameters of Nelson et al [3.7] as initial values of the resonance parameters. The SAMMY code was used with ISHIFT=0 which enforces S = B at all scattering energies and for all channels (with S the shift parameter and B the boundary condition number).With this assumption the resonance parameters in the input/output files are identical to those observed in the cross-section data. The fits to the different differential cross section data sets were performed sequentially. For the elastic channel, the fits to the different angles were possible using different energy-dependent background normalizations.

3.5 R-Matrix Analyses of Multichannel Reaction Data with EDA

M. Paris (Los Alamos National Laboratory)

The Energy Dependent Analysis (EDA) code has been developed at Los Alamos National Laboratory to provide a unitary description of the scattering and reaction of neutron and charged particle reactions since the 1970's. EDA is a general and versatile code supporting a variety of reaction parameters (scattering energies, charge and spin states, electromagnetic channels, etc.). It employs the Wolfenstein trace formalism to handle *any* states of polarized or unpolarized nuclei for initial and/or final states of two nuclei. It also handles electromagnetic channels composed of a single photon and a nucleus. EDA has been used to study a variety of light compound systems with $A \leq 20$. It employs a relativistic parameterization of the R-matrix elements and has additional features such as the ability to fit reaction data of isobaric compound systems (eg. ^{7}Li and ^{7}Be) simultaneously. EDA is under continuous development and is currently being recoded in modern Fortran90/95.

We briefly summarize the approach to obtaining the accurate and unitary scattering/reaction amplitudes with EDA that we typically employ at LANL. This is the approach that is used in the determination of ENDF data files for light compound systems. The R-matrix is the Green function in the presence of the Bloch operator for the compound system of A-nucleons. The Bloch operator enforces boundary conditions determined by the set of two-body channels that couple to the given compound system. The boundary conditions are determined at the channel radius, which should be regarded as regulator of the theory (and therefore observables should be *independent* of the channel radius) by the form of the scattering wave function at distances comparable to or beyond the range of polarizing interactions. The boundary conditions in EDA are chosen in accord with those of Wigner & Eisenbud, which are scattering-energy independent, and therefore give rise to scattering-energy-independent R-matrix parameters (level energies and reduced widths). The R-matrix is related to the transition (T) matrix in the standard way; by translating to Kapur-Peierls (outgoing) boundary conditions and including the penetrability factors for charged-particle channels, if appropriate. R-matrix level energies and reduced widths are varied to minimize the χ^2-per-DOF of data sets that span sets of scattering and reaction data (polarized or unpolarized) for all two-body channels (and some quasi-two-body channels that approximate three- or more-body channels) that couple to the given compound system (or systems, if we may invoke isospin conservation) under consideration. Typically, we consider compound systems which couple to many partitions (somewhere around 5 partitions and 50 channels is not unusual) and include on the order of 10^4 data points. A solution is reached when the derivative of the χ^2 function with respect to the R-matrix parameters is zero to a user-defined precision typically 10^{-3}.

We performed a preliminary analysis of the ^{28}Si system including only elastic data from the p-^{27}Al partition, which includes 9109 excitation function data points. Using the (not consistently defined) resonance parameters from the Nelson (1984) R-matrix parameterization, we obtained a poor description of the data with a χ^2-per-DOF of about 4.6. A preliminary optimization of this data, obtained by varying 121 R-matrix parameters improved this to 1.05.

(Further optimization to achieve a solution gave χ^2-per-DOF of 0.57.) This test problem was a useful exercise for the application of EDA to compound systems with significantly higher numbers of nucleons (A=28, here) than usual. (Typically, EDA has been applied to systems with A$\leq$ 20.) Further work on ^{28}Si is planned to incorporate the α-^{24}Mg reaction data.

Significant activity has recently been pursued on other compound systems such as ^{5}He, ^{7}Be, and ^{17}O. We discussed this and our work on spectra of particles in final states with more than two particles.

3.6 Charged-Particle Resonance Data in ENDF-6 Format

A. Trkov (IAEA)

Very few evaluated data files for incident charged particles are available that extend in energy down into the resonance range. A comprehensive compilation of experimentally measured resonance parameters for incident charged particles has been compiled many years ago by Soukhoruchkin [3.8], but no evaluated data files of resonance parameters exist, although the ENDF format can accommodate such data even for incident charged particles. The SAMMY code can analyse charged-particle resonance data and store them in ENDF-6 format, but no standard data processing code can handle such data, for example by converting them to an equivalent tabular representation (MF6/LPT12 in ENDF terminology) that is easier to handle by the users and is used in the few evaluated data files in ENDF format that are currently available.

Assuming that resonance parameters are evaluated, a possible interim solution is to use SAMMY to generate simple tables of cross sections at densely-spaced angles. The IBAEND code was developed at the IAEA that can re-format such data into MF6/LPT12 representation. Such data can be processed with the ENDVER package and with the on-line graphical display tools of the ENDF interface on the IAEA-NDS web site.

The plan is to process all charged particle resonance evaluations obtained through contracts from the IAEA and upload them into the ENDF database. This will allow graphical display of the data and easier access to a broader community of data users.

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4. Technical discussions

4.1 Interchange of R-matrix fits

The issue of translatability of the resonance parameters input and output information between the codes was one of the issues considered at the meeting. Participants discussed how the resonance parameters (E_R, Γ_R) and R-matrix fitting parameters (E_λ, Γ_λ) are defined and how the boundary conditions and channel radii are determined in the different codes. It was agreed that the optimum way of comparing the fitted resonance parameters provided by the various codes was to convert the standard R-matrix resonances parameters into the alternative parameters of Brune [4.1], which have the advantage of being independent of the boundary conditions, however not the channel radii. In view of the latter, in the inter-change of R-matrix fits, information of channel radii should also be included.

Action on Thompson, deBoer: prepare a stand-alone code to inter-convert standard R-matrix code parameters with the Brune [4.1] parameters following the prescription implemented in AZURE2 and provide to other participants for use. The draft proposal for the development of such a code, named Ferdinand, was prepared by I. Thompson and is included in Appendix 1. The proposal will be circulated to R-matrix code developers who were not present at the meeting for their advice.

Discussions also evolved around the use of channel radii as fitting parameters in R-matrix analyses. The variation of the channel radius as a fitting parameter implies that this 'parameter' has an uncertainty or variance determined in the optimization. However, the channel radius is merely a regulator of the R-matrix approach. Equivalent R-matrices with different channel radii (and level structure) can give equally good descriptions of the data. Therefore, quoting error bars/variance for such an object may be difficult to interpret.

Recommendation for future evaluations: evaluators should keep the same radius within the mass partition.

Action on Paris, Kunieda: to prepare a report on the arguments against and in favour of varying the channel radius (as a fitting parameter) within a mass partition.

4.2 R-matrix codes comparison

An inter-comparison of the capabilities of the R-matrix codes EDA, AZURE2, AMUR, FRESCO and SAMMY was discussed. As these codes were developed initially for the solution of different problems, each one has its particular features, strengths and weaknesses. A summary of the specifications is given in Table 1. [Sec. note: the information in Table 1 for the SAMMY code were completed after the end of the meeting by Goran Arbanas (ORNL). The specifications for code HYRMA were also added after the meeting by Sofia Quaglioni (LLNL).]

Action on Paris, Thompson, Kunieda, Dimitriou: Use the deBoer code to convert standard R-matrix parameters to alternative parameters of Brune and use them as input to the EDA, FRESCO, AMUR and SAMMY code, and compare the results.

In the near future, in addition to R-matrix parameters and cross sections, R-matrix parameter covariances will also be compared.

4.3 R-matrix calculations for the ^{28}Si system

Prior to the meeting participants were asked to study the system p + ^{27}Al --> ^{28}Si using the resonance parameters measured by Nelson et al [4.2] and the experimental differential cross section data available in IBANDL [4.3].

From the comparison of the results, it became clear that not all of the details needed to interpret the resonance parameters of [4.2] were available in that work (i.e. exact channel radius, boundary conditions, and transformation method from reduced widths to partial widths). Furthermore, from the ensuing extensive discussion on boundary conditions, there was a consensus that, the approach for boundary conditions which sets S-B=0 for each resonance level (where S is the energy shift and B the boundary constant) separately, is a simplified one that is generally incorrect. For channels where there is a single resonance level, this simplified approach poses no problem. But in the case where there is more than one resonance level, one cannot simply set the energy shift of the level (that is, set S-B=0) for each of the resonance levels in that channel simultaneously. To do so is inconsistent with the mathematical formulation of the R-matrix approach. In particular, it gives reaction amplitudes that do not satisfy unitarity.

Participants agreed to continue studying this system, by applying suitable boundary conditions and by using the Brune [4.1] description of resonance parameters to obtain a consistent set of input parameters. That way it would be possible to investigate any remaining differences in the cross section calculations between the different codes.

Once the differences in the codes are clearly understood, a complete evaluation of the ^{28}Si system can begin. This will start with the data of Nelson [4.2] which cover the range from E_p = 0.92 to 3.05 MeV and include all open particle channels.

4.4 Evaluation Methodology

Though different approaches may be employed by different groups for the evaluation of the experimental data, it is standard practice that an evaluation should provide the evaluated quantity (cross sections, resonance parameters etc) with its uncertainty and correlations of the uncertainties (covariance matrix).

Participants agreed that a thorough comparison of the different approaches would be the second important step –the first being described in Sections 4.1, 4.2 herein- in forming a broader international collaboration, to produce R-matrix evaluations of charged-particle induced reactions. This second step will be the subject of a follow-up meeting.

Evaluation approach

In all evaluation methodologies, the first common step is undoubtedly a thorough literature search to find the existing experimental data and analyses for the reaction and/or compound system of interest. To complement this, a literature search is also performed for data and analyses for all the reactions that form the same compound nucleus. These are usually limited to the same excitation energy range, but often one tries to begin at threshold for each reaction channel. This additional information can put stringent constraints on the adjustable parameters of the R-matrix fit if unitarity of the scattering matrix is to be fulfilled.

The steps following the literature search can vary among the evaluators. A general outline of the steps normally taken was described by deBoer, while Kunieda listed the specific steps he followed in the evaluation of the ^{7}Be and ^{17}O systems:

J. deBoer:

1.) Evaluate the data based on experimental information provided for each data set. Does the data have well defined uncertainties, both statistical (point-to-point) and systematic? If not, summarize any more limited information that is available.

2.) Perform an initial R-matrix calculation based on the level parameters in the literature and the selected data sets. This may involve multiple calculations since different analyses may have conflicting results for the level parameters.

3.) If a good set of parameters can be found that gives a reasonable description of all the data in all the different reactions channels under consideration, try to perform an actual fit. If not, try to perform an independent analysis to see if a solution can be found.

4) If a good fit can be achieved, perform an uncertainty analysis. In principle the uncertainty analysis should include uncertainties on all of the fit parameters and the cross sections as a function of both energy and angle. In practice the analysis may be limited to the specific quantity of interest for the analysis.

The above represent a rather idealized procedure for the data analysis. Often it is found that data sets disagree with each other or a satisfactory fit cannot be achieved. Perhaps because the level structure is not known that well over the range of the data. In many cases there may be only a single set of data for a given reaction channel and that data may be incomplete, lacking even statistical uncertainties. This often happens when older data must be used. For example, in many cases scattering data is only available from a very old measurement. Then the evaluator must assign uncertainties to the data in some way, which may have a strong influence on the outcome of the uncertainty analysis. Additionally, aside from the basic R-matrix fit, different target effect corrections often need to be supplied. Sometimes these are given but often the evaluator must try to calculate these themselves based on the limited information at hand, this can also have a significant effect on the final uncertainty analysis.

While often a tedious task, the model uncertainties inherent in any R-matrix fit should also be investigated to gauge their effect on the parameters of the fit and any other derived quantities. Specifically, the sensitivity of the fit to the channel radius and possible background poles should be investigated.

S. Kunieda:

In implementing the standard R-matrix analysis for light-nuclei, Kunieda fixed the energy eigenvalues E_λ and corresponding J^π to those given in ENSDF (Evaluated Nuclear Structure Data File) [4.4] as a first approach. The assumption being that in ENSDF, the level energies and J^π have been "evaluated" from a number of experimental studies performed over the years. This first step allowed him to estimate reasonable values of boundary parameters such as channel radii R_c and boundary condition numbers B_c together with the initial value of reduced-width amplitudes γ_c (including those for the instant levels). Once reasonable boundary parameters were obtained, they were fixed, and E_λ was varied together with γ_c simultaneously. If some energy levels seemed to be missing in ENSDF, levels with the value of J^π which gave reasonable fit to the experimental cross-sections were added. Several iterations were performed to obtain the required convergence.

The uncertainty/covariance of the cross-section was estimated by the deterministic approach, the KALMAN/SOK method [4.5, 4.6], in which the covariance of the R-matrix parameters is propagated to the cross-sections through the sensitivity matrix. In this approach, the question

is how one tackles the unknown uncertainty in the measurements, i.e. the systematic effects that are not or cannot be quantified by the experimentalists. For example, systematic differences arise among different measurements due to a large uncertainty in the sample thickness. In such cases, we used the useful recipe of introducing a re-normalization parameter for each measurement included in the R-matrix analysis, following the prescription of the LANL group (Hale and Paris) [4.7, 4.8].

4.5 ENDF-6 format

Independent of the formats that are already used by the different codes to output resonance parameters and cross sections, it was decided that all the R-matrix evaluations produced within this coordinated effort will also be prepared in the ENDF-6 format [4.9] used for the Evaluated Nuclear Data File (ENDF) libraries [4.10].

This would allow these charged-particle evaluated data files to be processed by the widely used data processing codes before being eventually included in the libraries of transport codes and other simulation codes used in various applications.

The ENDF-6 format is well defined for storing resonance parameters for neutrons in the incident channel (File 2). Though this format can easily be used for incident charged particles, the standard data processing codes are currently unable to process these data in order to reconstruct the charged-particle cross sections.

A temporary solution to this problem is to produce ENDF files that include point-wise cross-sections for charged-particles (File 6) instead of resonance parameters (File 2). PREPRO processing code and ENDVER (plotting) could easily process these files.

Participants agreed to adapt the ENDF-6 format to allow the inclusion of Brune's alternative R-matrix parameterization [Ref] to facilitate the exchange of resonance parameters among them. For this purpose they suggested introducing a value of SHF=2. In addition, we recommend using LRF=7, LRP=1, LRU=1, KRM=3 or 4, KRL=0, APE=APT, IFG=1, and having the same R-matrix channel radius within each mass partition. KRM=3 should be used for Reich-Moore, with its inclusive gamma channel, and KRM=4 for standard R-matrix calculations with all channel quantum numbers given explicitly.

Action on Thompson, DeBoer: circulate a code to convert resonance parameters to File=2 ENDF-6 format. [Sec. note: Subsequent to the meeting, a first draft of the proposal for the development of the code, called Ferdinand, was prepared by I. Thompson and was circulated to meeting participants. Further solicitation will be sought from other experts.]

4.6 Work program

Codes development

Participants discussed their plans for further developing their codes, such as the addition of relativistic kinematics in AMUR (Kunieda), and treatment of polarization observables by AZURE2 (deBoer) and AMUR (Kunieda).
Following the discussions on R-matrix parameters inter-change, and the physics and uncertainties analysis required for creating evaluated nuclear data files for charged-particle reactions, it was agreed that code capabilities should be extended where needed to:

- perform transformations between Brune parameters and standard R-matrix parameters.
- calculate (p,p'γ) angular distributions.
- use the covariances of the fitted R-matrix parameters to generate uncertainties on the observables.

Evaluations

It was agreed that the enormous amount of work that has already been performed on evaluating charged-particle induced reactions should also become available to the user community, especially if the results of the evaluations have already been published in peer-reviewed journals, internal laboratory reports, or IAEA reports. Table 2 contains a compilation of the various light and light-medium mass compound systems that have been evaluated by participants of this meeting, including those available from the SigmaCalc online calculator mentioned in Section 2. The highlighted numbers indicate the number of differential cross-section datasets available in IBANDL for the specific channels.
As can be seen from the table, there is overlap between IBANDL data and evaluations in the light-mass region only, while for masses larger than A=23 the only existing evaluations are those from SigmaCalc.

Participants agreed to make efforts to release their existing evaluated R-matrix parameters for comparison and discussion. The ultimate goal is to construct resonance parameter files in ENDF-6 format for further processing by the major processing codes and eventually, for broader dissemination through the ENDF database.

Concerning the mass region A>23, for which very few evaluations are available, the consensus was that it would require a coordinated effort that would involve more R-matrix experts including the training of new experts through suitable training programs.

The following actions were adopted to help achieve the above-mentioned goals:

Action on Dimitriou: find previous R-matrix fits and publications of evaluations of compound systems shown in Table 2 that provide information on spins and parities.

Action on Trkov: explore procedure used for reconstructing cross-section covariance File 33 from R-matrix covariances stored in File 32.

Action on Thompson and Trkov: contact D. Cullen about processing charged-particle data with PREPRO (RECENT module).

Compound system ^{28}Si

The evaluation of this compound system will be completed once (i) the inter-changeability of R-matrix fits has been established and a computer code to convert R-matrix resonance parameters between the forms used as input in the various R-matrix codes is available for different code developers and users to use, and (ii) the differences between the different R-matrix codes are well understood.

In addition, there has to be an agreement on the uncertainties of the experimental data.

An effort will be made by participants to complete their evaluations of 28Si and compare the evaluations at the R-matrix Workshop which is to be held in Santa Fe, 27 June – 1 July 2016.

References

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[4.9] ENDF-6 Formats Manual, Eds. A. Trkov, M. Herman and D. A. Brown, CSEWG Document ENDF-102, Report BNL-90365-2009 Rev.2, December 2011.
[4.10] Evaluated Nuclear Data File libraries, https://www-nds.iaea.org/exfor/endf.htm

5. Conclusions

A Consultant's Meeting of R-matrix code developers was held at the IAEA from 7 to 9 December 2015. The meeting discussed the capabilities and specific features of six different R-matrix codes, namely, SAMMY, AZURE2, FRESCO, AMUR, EDA, and HYRMA, that are currently used to perform R-matrix fits of charged-particle-induced reactions in the resolved resonance region.

Participants agreed that a necessary condition to perform useful comparisons of R-matrix calculations was the interchangeability/translatability of R-matrix input and output parameters between the various codes. The development of a code to convert R-matrix fits between several formats, including ENDF, GND, and the various formats used for the input and output of the above-mentioned R-matrix codes was recommended.

Once the translatability between the different codes is established, and the inter-comparison of the codes is completed, participants will work together on the evaluation of the 28Si compound system. In the meantime, efforts will be made to make existing evaluations of charged-particle reactions in the resolved resonance region available to the user community.

For purposes of preserving the expertise in R-matrix analyses participants recommended the organization of dedicated training workshops.

The next meeting to review progress will be held in 2016.

6. Tables

Table 1. R-matrix codes comparison.

Feature	**EDA**	**AZURE2**	**AMUR**	**FRESCO**	**SAMMY**	**HYRMA**
R-matrix	Full	Full	Limited (for gammas)	Full	SLBW, MLBW, RM, Full[1]	Only particle channels
Derivatives	Analytic	Numerical	Numerical	Numerical	Analytical for $\sigma_{T=0K}$ Numerical otherwise[2]	Numerical
Kinematics	Relativistic + non-relativistic	Non-relativistic	Non-relativistic	Relativistic+ non-relativistic	Non-relativistic	Non-relativistic
Reference frame	Lab/CM	Input Lab /output CM	Lab/CM	Lab/CM	Lab/CM	Lab/CM
Channel Radii	Varied	Varied	Fitted (option)	Fixed	Varied	Fixed
Photons	In/Out	Out	Out	In/Out	Out	No
Observables: cross sections (energy and energy-angle differential)	All	All	All	All	All	All
Observables: polarization, tensor analysing power etc	All	No	No	All	No. SAMINT links to IBE	No

[1] Full R-matrix in SAMMY is achieved by treating γ-channels as reaction channels.

[2] Analytic derivatives of cross sections at T=0 K, numerical derivatives of Doppler broadened and resolution broadened cross sections.

Feature	EDA	AZURE2	AMUR	FRESCO	SAMMY	HYRMA
Inverse reactions	Yes	Yes	Yes	Yes	Yes	No
Decay gammas	Post-processing	No	No	Post-processing	No	No
Isobaric reactions simultaneously	Yes	No	No	No	No	No
Doppler broadening	No	No	No	No	Yes	No
Resolution broadening	Yes	Yes	Yes	No	Yes	No
Normalization	Yes	Yes	Yes	yes	Yes	No
Background subtraction	No	No	Yes	No	Yes	No
Background R-matrix terms	Energy-dependent	Distant poles	Distant poles	Distant poles	Yes	Distant poles
Sample-size corrections	No	Yes	No	No	Yes	No
Closed-geometry Q-corrections	No	Yes	No	No	Yes	No
Fitting procedure	L-SQ	MINUIT2	KALMAN	MINUIT1	Bayesian i.e. GLS	MINUIT
Multiple data sets	simultaneously	simultaneously	simultaneously	Simultaneously	Simultaneously	simultaneously
Uses data covariances	No	No	Yes	No	Yes	No
Uses prior parameter covariances	Yes	No	Yes	No	Yes	No

Feature	EDA	AZURE2	AMUR	FRESCO	SAMMY	HYRMA
Produce evaluated data covariances (MF 32)	No	No	No	No	Yes	No
Brune parameter output	No (planned)	Yes	No	No	No (planned)	Yes
ENDF-6 format output	Yes	No	Yes	No	Yes	No
ENDF-6 input	No	No	No	No	Yes	Yes
Number of resonances	To be filled				>3,000 for U-235	
Code language	F77	C++	C++	F90	F77[3]	F90
Availability	Export controlled	yes	no	yes	RSICC Export Control[4]	Export controlled
Documentation	no	yes	no	yes	Online	no
Parallelized	no	yes	yes	no	No	no
Interactive fitting	yes	no	no	Yes	Yes	no
Maintainer	Hale/Paris	DeBoer/ Uberseder	Kunieda	Thompson	Arbanas	Quaglioni

[3] SAMMY modernization in progress: the SAMRML code has been modernized into C++.

[4] SAMMY may have its export-controlled classification removed.

Table 2. Reaction channels evaluated by different groups.

Target	Projectile						SigmaCalc (IPPE)	EDA (LANL)	AZURE (ND)	AMUR (JAEA)	ECPL (LLNL) [Evaluated Charged Particle Library]
	p	d	3He	a	6Li	7Li					
H-1	20	-	2	33	-	2	(a,p)	(p,p),(d,d), (^{3}He,^{3}He), (a,a), (t,t),(t,n),(t,d)			(p,p), (d,d), (t,t), (t,n), (t,d), (t,a), (^{3}He,^{3}He), (a,a),
H-2	5	-	4	20	-	-		(p,p), (d,d), (d,n), (d,p), (^{3}He,^{3}He), (a,a), (t,a)			(p,p), (p,np), (d,d), (d,n), (d,p), (t,t), (t,n), (t,aγ), (^{3}He,^{3}He), (a,a), (a,n), (a,p)
H-3	1	-	-	1	-	-		(p,p), (p,n), (p,d), (d,d), (d,n), (^{3}He,^{3}He), (^{3}He,d), (a,a), (a,n)	(a,a),(a,γ)		(p,p), (p,n), (p,d), (p,a), (d,d), (d,n), (t,t), (t,nn), (^{3}He,^{3}He), (^{3}He,n), (^{3}He,d), (a,a)
He-3	1	3	-	-	-	-		(p,p), (d,d),(d,p), (t,t), (t,d), (^{3}He,^{3}He), (^{3}He,p), (a,a), (a,p)			(p,p), (d,d), (d,p), (t,t), (t,np), (t,d), (^{3}He,^{3}He),(^{3}He,pp), (a,a)
He-4	14	-	-	-	-	-	(p,p0)	(p,p), (p,d), (d,d), (d,t), (t,t), (t,n),			(p,p), (d,d), (d,np), (t,t), (^{3}He,^{3}He),

								(^{3}He,^{3}He), (^{3}He,p), (a,a), (a,p),(a,n), (a,d)			(a,a)
Li-6	88	100	17	9	-	-		(p,γ), (p,p), (p,^{3}He), (d,d), (d,n), (d,p), (d,a), (t,t), (t,d), (t,n), (^{3}He,γ), (^{3}He,^{3}He), (^{3}He,p), (^{3}He,d), (a,a), (a,^{3}He), (a,p)	(p,p0),(p,a)	(d,p0), (d,p1), (d,n0), (d,n1),(d,a)	(p,p), (p,^{3}He), (d,d), (d,p), (d,n), (d,a), (t,t), (t,n), (t,p), (t,nn), (t,d), (^{3}He,^{3}He), (a,a)
Li-7	89	2	-	1	-	-		(p,p), (p,n), (p,d), (p,a), (d,d), (d,n), (d,t), (t,t), (t,n), (t,nn), (t,a), (^{3}He,^{3}He), (^{3}He,p), (^{3}He,a), (a,a), (a,n), (a,t)		(p,p0), (p,p1), (p,n0), (p,n1),(p,a)	(p,p), (p,d), (p,a), (d,d), (d,n), (d,nn), (d,p), (d,t), (t,t), (t,n), (t,nn), (t,nnn), (^{3}He,^{3}He), (^{3}He,np), (^{3}He,p), (^{3}He,t), (^{3}He,a), (^{3}He,a1), (a,a)
Be-7	9	-	-	-	-	-		(d,d),(d,p),(d,^{3}He), (t,p), (t,^{3}He), (t,a), (a,a), (a,p),			
Be-9	82	34	25	14	-	-		(p,p), (p,^{3}He), (p,a), (d,n), (d,t), (d,a), (^{3}He,p), (^{3}He,a), (a,n)			
B-10	81	117	18	11	-	-		(p,p), (p,a), (d,p), (d,a), (t,n)			
B-11	69	16	19	11	-	-		(p,p), (p,a), (d,n), (t,n), (a,p), (a,n), (a,a)			

B-nat	-	-	-	1	-	-					
C-12	92	150	43	128	1	1	(a,a) (d,d0) (d,p0) (p,p0)	(t,p), (t,n), (t,a), (a,γ), (a,a)	(p,p0),(p,γ), (p,a1), (a,a0),(a,γ)		
C-13	26	25	9	6	-	-	(p,p0)	(d,p), (d,n), (d,a), (^{3}He,γ), (^{3}He,a), (a,a), (a,n)	(p,p0),(p,γ)	(a,n0)	
N-14	68	70	20	47	-	-	(a,a0) (d,a0) (d,a1) (d,p0) (p,p0)	(d,γ), (d,a), (t,n), (t,a), (a,p), (a,a)	(a,a0),(p,p0),(p,γ)		
N-15	15	6	-	8	-	-		(p,γ), (p,a), (d,n), (d,a), (^{3}He,p), (^{3}He,a)	(p,p0),(p,a0), (p,γ),(a,a0)		
O-16	40	95	20	59	-	1	(a,a0) (d,a0) (d,d0) (d,p0) (d,p1) (p,p0)	(d,p), (d,a),	(p,p0), (a,a0)		
O-17	2	-	-	-	-	-		(p,p), (p,a)	(a,n)		
O-18	23	4	-	17	-	-	(p,a0)		(p,p0), (p,γ),(a,n)		
F-19	206	30	-	17	1	-	(p,p0)				
Ne-20	9	3	-	3	-	-	(a,a0) (p,p0)		(p,p0),(p,γ)		
Ne-22	2	-	-	-	-	-			(a,n)		
Na-23	65	28	-	1	-	-	(p,p0) (p,pg1-0)		(p,p0)		

Mg-24	56	55	-	7	-	-	(a,a0) (p,p0)				
Mg-25	39	15	-	-	-	-					
Mg-26	52	6	-	-	-	-					
Mg-nat	5	6	-	1	-	-	(p,p0)				
Al-27	118	51	-	8	3	4	(p,p) (p,pg1-0)				
Si-28	14	51	-	15	-	-	(a,a0) (p,p0)				
Si-29	20	-	-	-	-	-					
Si-30	5	8	-	-	-	-					
Si-nat	28	-	-	20	2	2	(a,a0) (p,p0)				
P-31	26	26	-	2	-	-	(p,p0)				
S-32	17	33	-	9	-	-	(p,p0)				
S-33	2	-	-	-	-	-					
S-34	4	-	-	-	-	-					
Cl-35	11	3	-	-	-	-					
Cl-37	23	2	-	-	-	-					
Cl-nat	1	-	-	1	-	-					
Ar-36	14	-	-	-	-	-					
Ar-38	1	-	-	-	-	-					
Ar-40	8	-	-	1	-	-	(p,p0)				

K-39	9	9	-	8	-	-	(p,p0)				
K-41	14	-	-	-	-	-					
K-nat	5	-	-	-	-	-					
Ca-40	17	3	3	30	-	-	(p,p0)				
Ca-41	-	-	-	9	-	-					
Ca-42	1	-	-	-	-	-					
Ca-43	2	-	-	-	-	-					
Ca-44	10	-	-	-	-	-					
Ca-46	2	-	-	-	-	-					
Ca-48	3	15	-	3	-	-					
Ca-nat	6	-	-	2	-	-					
Sc-45	22	-	-	-	-	-					
Ti-46	13	-	-	-	-	-					
Ti-48	16	-	-	-	-	-	(p,p0)				
Ti-50	12	-	-	-	-	-					
Ti-nat	3	-	-	-	2	2	(p,p0)				
V-51	4	-	-	-	-	-					
Cr-50	8	-	-	-	-	-					
Cr-52	11	-	-	-	-	-	(p,p0)				

Cr-nat	5	-	-	-	-	-	(p,p0)				
Fe-54	5	-	-	-	-	-					
Fe-56	2	-	-	1	-	-	(p,p0)				
Fe-58	1	-	-	-	-	-					
Fe-nat	16	-	-	-	-	-	(p,p0)				
Cu-nat	-	-	-	2	-	-					

Code Proposal

Version 0.1: 10 Dec 2016

I.J. Thompson, M. Paris, S. Kunieda, R.J. deBoer and P. Dimitriou

FERDINAND

The Vienna R-matrix Interchange Code

1. A Code Proposal

We propose to write and use a code (or suite of codes) to convert R-matrix fits between several formats, including ENDF, GND, and the various formats used for the input and output of fits by R-processing codes (SAMMY, AZURE2, FRESCO, AMUR, EDA, HYRMA, and others). The aim is to enable the results of any R-matrix fit to be used as input to any other code and produce the same quality of fit, and also to convert the results of these fits to international data formats for use by processing codes for many different applications.

This proposal arises from discussions at the IAEA consultants meeting *R-matrix codes for Charged-particle Reactions in the Resolved Resonance Region* held at Vienna, 7-9 Dec 2015. It will apply of course to neutron as well as charged-particle reactions.

2. Documentation Files

Each fit in each format will also include a text **documentation file** that will list:

1. the authors of the original fit, and of any later modifications,
2. the dates and code versions used,
3. the sets of experimental data used in the fit, with, for each set:
    a. X4 or IBANDL reference names, numbers, and/or URL of the data source,
    b. the statistical and systematic uncertainties assumed (if not given in the data source),
    c. the absolute normalization of the data obtained as the result of the fit,
    d. any energy calibration shifts or resolution functions used,
    e. a description of which (if any) experimental data points were either given larger uncertainties, or excluded from the fit altogether,
4. the chi-squared per degree-of-freedom for the final fit using the data as possibly modified according to the descriptions of (3)
5. whether any of the R-matrix parameters were fixed by prior information and not included in the searches. The Reich-Moore gamma widths are often fixed like this. Such fixings should be reflected in the covariance matrix of the fit.
6. any other relevant comments
7. references to relevant publications for the codes and versions, experimental data, and publication(s) of this fit as evaluated data.

3. R-matrix fit parameter formats

The following **fit parameter formats** that will be able to be read and written. The *first* format (1) listed is our preferred international exchange format for communication between R-matrix evaluators. It is not (yet) a data distribution format.

(1) **ENDF6+ format with Brune parameters** for pole energies and reduced width amplitudes in non-relativistic kinematics. This format will be identified by SHF=2 (a extension not defined in the ENDF-6 specification). The files will include at least documentation (MF=1), R-matrix parameters (MF=2), and covariances of R-matrix parameters (MF=32). Only data for the specified energy range (EL, EH) need be included. If any background cross section is needed, then a point-wise background cross section (MF=3) may be included in that energy range for some of the reactions MT that are included in the R-matrix fit.

(2) **ENDF6 format for standard R-matrix parameters**. This similar to (1.), but with SHF=1, and now using the boundary condition number *B*=BND that needs to be specified by the user for each partial-wave channel in MF=2.

(3) **ENDF6 format for 'Sammy' R-matrix parameters calculated assuming *B*=S.** This similar to (2.), but with SHF=0, and ignores the boundary condition numbers BND. (Until further research, this is only an output format for all codes except SAMMY).

(4) **AZURE2 format with Brune parameters** for pole energies and reduced width amplitudes in non-relativistic kinematics. This is the ND code of R.J. deBoer.

(5) **EDA format for standard R-matrix parameters**. This is for the LANL code of G. Hale, M. Paris, et al.

(6) **FRESCO format for standard R-matrix parameters**. This is the code of I.J. Thompson at LLNL, for both the public code FRESCO and the LLNL development code FRESCOX.

(7) **AMUR format for standard R-matrix parameters**. This is the code of S. Kunieda at JAEA.

(8) **HYRMA format for standard R-matrix parameters**. This is the LLNL code of S. Quaglioni.

(9) **Full evaluations in ENDF6 format with standard R-matrix parameters**. This is the merged file that combines an output file of format (2.) above with all the other MF files of a full evaluation from a previous ENDF6-formatted file such as from ENDF/VII.1. The merge will replace all the previous data in all MF sections of the evaluation in the energy range (EL, EH) of the R-matrix fit. The documentation files will be concatenated.

(10) **Full evaluations in ENDF6 format with 'Sammy' R-matrix parameters *B*=S**. This is the merged file that combines an output file of format (3.) above with all the other MF files of a full evaluation from a previous ENDF6-formatted file such as from ENDF/VII.1. The merge will replace all the previous data in all MF sections of the evaluation in the energy range (EL, EH) of the R-matrix fit. The documentation files will be concatenated. (Output format only, except for SAMMY)

(11) **GND format**. All of the ENDF6 or ENDF6+ formatted files above can also be converted to the GND format developed at LLNL, and converted back from GND format, without loss of information. These conversions will be performed by separate Python scripts that call the FUDGE library.

(12) **Pointwise ENDF6 or GND formats**. All of the above ENDF or GND formatted files can have their MF=2 R-matrix parameter sets expanded to point-wise data (along with any MF=3 background terms). The resulting cross sections will be in MF=3 and the angular distributions will be in MF=6. This requires specifying some accuracy for using the point-wise data with linear interpolation. The MF=32 parameter covariances will also be converted to MF=33 cross-section covariances. This is an output format only.

The international exchange format [see (1) above] will (ideally) use the following options (specified for convenience here in terms of the parameters in the ENDF6 manual):

LRU=1: resolved resonance parameters are given

NER=1: prefer just one energy range for all the data

LRF=7: R-matrix limited (RML)

NRO=1: R-matrix radius is energy independent

NAPS=1: use AP in the penetrabilities and shift factor as well as in the phase shifts?

KRM=3: Reich-Moore, *or* KRM=4 (full R-matrix)

KRL=0: non-relativistic kinematics

PNT=1: calculate penetrability

SHF=2: assume Brune input energies and widths (ENDF6 manual only has SHF=0, 1)

APE=APT: use the same radius for phase shifts, shifts, and penetrabilities

KBK=0: no background R-matrix terms, rather use distant poles if needed in fits

KPS=0: calculate hard-sphere phase shifts, rather than tabulate them

IFG=1: input widths are reduced width amplitudes γ, *not* γ^2 *or* Γ *or* observed Γ.

All formats take the partial waves to be specified in the channel-spin representation. The Reich-Moore option (KRM=3) needs to separately treat the gamma channel, so that channel should be listed as the first partition.

All files are ascii text files, with some maximum number (e.g. 200) of characters per line.

My recommendation is that all formats be chosen so that some indicator within some number of first lines of the file indicates the chosen format and its version. Another recommendation (not quite so good) is to agree on a unique file extension name for each format. Or use both, with the first overriding the second if they conflict, or if the file extension cannot be determined.

4. Methods of Conversions

The inter-conversions will not change the R-matrix radius. This radius may have been varied in the different mass partitions, but will be assumed to be constant for all partial waves within each partition, and for all scattering energies. We will assume that the R-matrix radii are *not* included in the detailed fit minimization (and so do not enter into the chi-squared or the covariance data), since they are not physical quantities.

Conversion to any of the 'standard R-matrix parameter' formats requires as additional input the specification of your preferred boundary condition number *B* for each partial-wave channel. This is always energy-independent.

The point-wise expansion of R-matrix parameter data to grids of cross sections and angular distributions for charged-particle scattering is not yet widely implemented. At present only SAMMY and SIGMACALC do this. The other fitting codes can be easily extended to output point-wise data in some fine grid, but ideally the standard pre-processing codes RECENT (in PREPRO) and FUDGE should expand this themselves independently, as well as the standard processing codes NJOY, AMPX and GIDI. (Some of these may need to be extended to handle charged-particle elastic scattering by including the Coulomb amplitude, and to generate numerical LTP=12 elastic scattering angular distributions.)

5. Starting the Code

This code FERDINAND will be started by R.J. deBoer using perhaps the C++ AZURE2 modules for converting between Brune and standard R-matrix parameters. It will then be extended by I.J. Thompson (in F90) to input and output the parameters in ENDF6 formats.

The authors of the various R-matrix codes will then write additional processing modules for the code to read and write the specification files for their own fitting codes. If their input and output formats are different, then both need to be coded in FERDINAND, or else local conversions performed. The output files from FERDINAND will of course need to be supplemented by files with further search specifications to actually run new searches, but ideally the previous fits should be reproduced in the first step with no extra input.

Initial versions of FERDINAND will only translate R-matrix parameters, not covariances.

6. Solicitation of Further Comments

Additional contributions to this document will be solicited from:
M. Pigni, ORNL; G. Arbanas, ORNL; D. Cullen; G. Hale LANL; N. Uberseder, LANL; L. Leal, IRSN; S. Quaglioni, LLNL; C. Mattoon, LLNL, and others.

APPENDIX II

Consultants' Meeting on
"R-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region"

IAEA, Vienna, Austria
7-9 December 2015
Meeting Room VIC A0534

PROVISIONAL AGENDA

Monday, 7 December

08:30 – 09:30 Registration (IAEA Registration Desk, Gate 1)
09:30 – 10:00 Opening Session
Welcoming address (Arjan Koning, NDS Section Head)
Administrative matters
Election of Chairman and Rapporteur
Adoption of the Agenda

10:00 – 17:30 Presentations by participants
1) Motivation for IAEA meeting (P. Dimitriou, R. Capote)
2) R-matrix analyses of multichannel reaction data with EDA (M. Paris)
3) AZURE2: An R-matrix code for Nuclear Astrophysics (R. DeBoer)
4) Present status of R-matrix code AMUR and analyses for ^{8}Be and ^{17}O systems (S. Kunieda)
5) Widening the scope of R-matrix methods (I. Thompson)
6) R-matrix fits for p+^{27}Al using SAMMY" (P. Dimitriou)
7) Charged-particle resonance data in ENDF-6 format (A. Trkov)

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

19:00 Dinner at a local restaurant (see separate information in folder)

Tuesday, 8 December

09:00 – 17:30 Round Table Discussion

R-matrix codes comparison
Evaluation methodology
Discussion of 28Si system
Charged-particle data in ENDF-6 format
How to proceed?
Future of R-matrix calculations/codes

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Wednesday, 9 December

09:00 – 13:00 Drafting of the Summary Report
Closing of the Meeting

Coffee break as needed

APPENDIX III

Consultants' Meeting on
"R-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region"

IAEA, Vienna, Austria
7-9 December 2015

LIST OF PARTICIPANTS

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APPENDIX IV

Consultants' Meeting on
"R-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region"

IAEA, Vienna, Austria
7-9 December 2015

Links to Online Presentations

#	Author	Title	Link
1	P. Dimitriou	Motivation-Background information; p+^{27}Al using SAMMY	PDF
2	R.J. deBoer	AZURE2: An R-matrix Code for Nuclear Astrophysics	PDF
3	M. Paris	R-Matrix Analysis of Multichannel REaction Data with EDA	PDF
4	I.J. Thompson	Widening the Scope of R-matrix Methods	PDF
5	L. Leal	Brief descriptions about the SAMMY Code	PDF
6	A. Trkov	Charged-Particle Resonance Data in ENDF-6 Format	PDF
7	S. Kunieda	Present status of R-matrix code AMUR and analysis for ^{8}Be and ^{17}O systems	PDF

APPENDIX V

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