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R-Matrix Codes for Charged-particle Induced Reactionsin the Resolved Resonance Region

H. Leeb, P. Dimitriou, I. J. Thompson

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

Summary Report of an IAEA Consultants' Meeting
IAEA Headquarters, Vienna, Austria
5-7 December 2016

Prepared by

Helmut Leeb,
Technische Universität Wien,
1040 Vienna, Austria

Paraskevi Dimitriou,
IAEA, Vienna, Austria

Ian Thompson
Lawrence Livermore National Laboratory
Livermore CA, U.S.A

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IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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International Atomic Energy Agency
Vienna International Centre
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Livermore CA, U.S.A

ABSTRACT

A Consultant's Meeting was held at the IAEA Headquarters, from 5 to 7 December 2016, to discuss the status of R-matrix codes currently used in calculations of charged-particle induced reaction cross sections at low energies. The meeting was a follow-up to the R-matrix Codes meeting held in December 2015, and served the purpose of monitoring progress in: the development of a translation code to enable exchange of input/output parameters between the various codes in different formats, fitting procedures and treatment of uncertainties, the evaluation methodology, and finally dissemination. The details of the presentations and technical discussions, as well as additional actions that were proposed to achieve all the goals of the meeting are summarized in this report.

January 2017

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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 5 to 7 December 2016, at the IAEA Headquarters in Vienna [1.1].

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.

The kick-off meeting of this coordinated project was held on 7-9 December 2015 at the IAEA in Vienna. The focus of that first meeting was on the specific capabilities of the existing R-matrix codes, R-matrix theory and its approximations, and how they are implemented in the codes, and finally, the translatability of R-matrix calculations produced by the various codes.

The purpose of this second meeting was to follow up progress on the above mentioned items, and propose necessary actions in order to establish a common evaluation methodology that would allow the joint production of evaluated cross-section data for charged-particle reactions in the resolved resonance region.

The meeting was opened by Arjan Koning, Section Head of the IAEA NDS, who welcomed the participants to the IAEA and emphasized the importance of their work for producing and disseminating reliable data to the Member States. Eight Participants from four countries attended the meeting: Ian Thompson, James deBoer, Mark Paris, and Goran Arbanas from the USA; Satoshi Kunieda (Japan), Zhenpeng Chen (PRC), and Helmut Leeb, Thomas Srdinko from Austria, including IAEA staff Paraskevi Dimitriou (Project Officer) and Roberto Capote. Ian Thompson (Lawrence Livermore National Laboratory) was elected chair of the meeting, and Helmut Leeb (TUW) agreed to act as rapporteur. The meeting began with individual presentations by the participants and was followed by lengthy discussions on a list of items covered in Section 3. Summaries of the presentations are given in Section 2 while the meeting Agenda, participant's list, links to the presentations and group photo are provided in Annexes 1 to 4, respectively.

References

[1.1] Summary Report of an IAEA Consultant's Meeting on R-matrix Codes for Charged-particle reactions in the Resolved-Resonance-Region, 7-9 December 2015, IAEA, Vienna, INDC(NDS)-0703.

2. Presentations by participants

Presentations made by the participants of the meeting are summarized in the following. Links to the presentations are provided in Annex 3.

2.1 Goals of the coordinated project 'R-matrix codes for charged-particle reactions in the resolved-resonance region', *P. Dimitriou (IAEA)*

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 the Ion Beam Analysis Data Library (IBANDL) [2.1]. Currently, IBANDL 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 available in different forms, either fine-tuned to the needs of the IBA community at SigmaCalc [2.2], or in point-wise cross section files (file 3) or resonance parameter files (file 2) in the ENDF database [2.3].

The emergence of new applications or developments in existing applications, however, necessitate complete and reliable evaluated charged-particle induced reactions cross sections at low energies, with proper treatment of uncertainties as is normally done within a complete and global evaluation.

To address these emerging data needs, 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.

The first meeting of this project was held on 7-9 December 2015, at the IAEA [1.1]. The aim was to assess the data needs, set the goals of the coordinated project, and recommend actions in order to achieve them. The meeting addressed (i) the capabilities of the existing R-matrix codes, and (ii) the implementation of R-matrix theory and its various approximations in the codes. The output was the creation of a new code, Ferdinand, to convert R-matrix parameters among the different codes and different formats. The code is in the final stages of development, and will be circulated to all project participants for testing with their codes on two different systems: ^{16}O+n, and ^{27}Al+p.

After the Ferdinand code has been tested and circulated, the next step in the project is the systematic comparison of actual R-matrix fits to experimental data. For this purpose, a simple and realistic test case should be discussed and adopted at this second meeting, and participants should run their codes, produce their fits, and then compare: 1) evaluated resonance parameters and their uncertainties, 2) evaluated cross sections and their uncertainties.

The third step, is to establish an evaluation methodology, outlining the criteria for accepting or rejecting experimental data, how to treat outliers, the statistical fitting (least-squares or generalized least squares), how to treat systematic uncertainties, and how to produce covariance matrices. This third step will be tackled in the third meeting to be held in 2017.

Ultimately, the project participants will undertake responsibility for the evaluation of certain compound systems, and will deliver their evaluated files in the adopted format (ENDF-6) [2.4] to the IAEA for broader dissemination. The long-term goal of this project is to provide reliable and complete evaluations of charged-particle reactions at low energies, starting from the resolved-resonance region, and extending to higher energies of unresolved resonances,

providing thus a smooth transition from the low energies to the higher energies of statistical models.

2.2 Theory Tools for R-matrix Fitting, *I.J. Thompson (Lawrence Livermore National Laboratory)*

After our meeting last December, we have learned what important theory components are needed for R-matrix fitting of nuclear reactions.

We recognize that, although approximations to R-matrix theory are sometimes convenient, they have to be treated with caution. For example, the *B*=*S* approximation for shift functions may be very useful in SAMMY as the poles are at the peak energies, but we find the cross sections are changed between resonances. We have long used the Reich-Moore approximation with diagonal damping, but now we hear from ORNL of a new approach with fewer approximations. Obninsk researchers have often used potential scattering for a baseline and adding R-matrix terms for extra resonances, but this makes specification of parameters more difficult for interchange. LANL researchers have argued for relativistic kinematics rather than non-relativistic, but it is still not clear how substantial the differences are in the approximations actually used.

To make exchange between R-matrix researchers and codes much easier, I have written a python code FERDINAND using the FUDGE processing for the GND format. It translates to and from GND, ENDF, SFRESCO, AZURE, HYRMA formats (see figure). It performs transformations to Brune's formalism, allowing the user to specify any energy-independent boundary condition *B* in the reverse Barker transform. At present a new POPS database being implemented ('Properties of Particles'), but previous versions have successfully translated results for n + ^{16}O, p + ^{27}Al R-matrix parameters.

Other tools are needed for the pointwise-reconstruction of cross sections from the R-matrix parameters (energies, widths, channels, *B* values). For charged-particle elastic scattering I prefer to use the numerical form for the difference with the Rutherford cross section, since elastic cross sections are not integrable. This reconstruction is not yet possible in RECENT in PREPRO, but it can be done with SAMMY and soon also in FUDGE from work by Caleb Mattoon and Dave Brown. In principle, any R-matrix fitting code can output the needed data, and so can check the reconstructions. We still need to establish international standards for formats describing the Brune parameterization. We propose SHF=2 in ENDF6 format, and a GND key word has been agreed. For ENDF6, in Nov 2017 we will make the case to CSEWG, and for GND in May 2017 we may have to make the case to the WPEC subgroup SG-B. It is already available in FERDINAND, HYRMA, and soon also in SAMMY.

I discussed several issues on the interpretation of data. We need to be sure whether the cross sections are at laboratory or center-of-mass angles and energies. I showed that interpretation of Nelson's 1984 data for p + ^{27}Al cross sections was much easier when they are taken as in the laboratory frame. The proton energy calibration must be examined as well, since it appears that the 'experimental' data in EXFOR database is *not* corrected for the energy calibration Nelson says he does using 991 and 1799 keV resonances as fixed points.

My strategies for fitting data included using existing tables of energies, spins and parities wherever possible, at least as starting points for iterations. It was very convenient to *start* as if Brune (or even B=S) energies. I have not yet found a good strategy for searching for E/J/π

values from scratch, or to make widths of new channels. I find it useful to focus on a specific resonance (or group) by keeping all R-matrix parameters in calculations, but to vary only those parameters near the resonance, and to calculate and plot only energies near resonance.

```
usage: ferdinand.py [-h] [-i INITIAL] [-o OUTPUT] [-z] [-v] [-g] [-R] [-r]
                    [-f FILTER] [-e ELASTIC] [-l LOWER] [-u UPPER] [-a] [-G]
                    [-b BOUNDARY] [-t TRANSFORM] [-c] [-E ENERGY] [-F FILE]
                    inFile finalformat

Translate R-matrix Evaluations

positional arguments:
  inFile                The input file you want to translate.
  finalformat           Output source format: fresco, sfresco, hyrma, endf,
                        azure, gnd=xml, ..

optional arguments:
  -h, --help            show this help message and exit
  -z, --zero            Omit zero widths
  -g, --nogamma         Omit gamma channels
  -R, --ReichMoore      Add a Reich-Moore gamma channel and convert to KRM=3
  -r, --noreac          Omit all nonelastic (reaction) channels
  -e ELASTIC, --elastic ELASTIC
                        Index (1,2,..) of elastic particle-pair
  -f FILTER, --filter FILTER
                        Filter of csv list of particle-pairs to include, e.g.
                        1,3,4 (no blanks). Overrides -g,-r options
  -a, --amplitudes      Convert intermediate gnd file stores to reduced width
                        amplitudes, not widths.
  -G, --Gammas          Convert intermediate gnd file stores to formal widths,
                        not reduced width amplitudes. Overrides -a.
  -b BOUNDARY, --boundary BOUNDARY
                        Boundary conditions for output file for EDA or FRESCO:
                        'C,X' where C=L,B,k,E or S, and X=float for B,k and E
  -t TRANSFORM, --transform TRANSFORM
                        Transform 'Brune' or 'Barker' of pole specification
```

FIG. 2.1. The principal arguments to Ferdinand.py.

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

2.3 R-matrix Needs in Nuclear Astrophysics, *R. J. deBoer (Univ. Notre-Dame, USA)*

AZURE2 is an R-matrix code for the nuclear astrophysics community built by the Joint Institute for Nuclear Astrophysics (JINA). It has been designed with the goal of analyzing near-threshold charged particle induced reactions in the resolved resonance region, in particular for capture. However, the code uses a general R-matrix framework, therefore it can make calculations for any two body reaction. AZURE2 is open source and can be obtained from azure.nd.edu.

As the amount of nuclear data increases and ever decreasing uncertainties are desired for reactions of interest to nuclear astrophysics, evaluations of nuclear data become increasingly important. With the mindset that new measurements will become part of ongoing comprehensive statistical analyses, a well-defined framework and repository, which is publically accessible, is highly desired. While the reactions important for nuclear astrophysics are limited, there is a large overlap with those of interest in ion beam analysis. Indeed, many of the tools of ion beam analysis are necessary for the accurate measurements desired by the nuclear astrophysics community. Therefore, while capture and transfer measurements are often the reactions of direct interest, accurate scattering data is often of nearly equal necessity for calibration of detector systems and target characteristics.

Further, R-matrix analyses are often performed for nuclear astrophysics reactions because the cross section needs to be extrapolated into a low energy region that is experimentally inaccessible. Experience has shown that the precision of these extrapolations can be significantly improved when data from all relevant reaction channels are analyzed simultaneously. This means that scattering data is always useful for the global R-matrix analysis of any reaction of interest for nuclear astrophysics.

In the intervening year since the last IAEA workshop on this topic, an R-matrix workshop was held in Santa Fe, NM. This workshop included about 50 attendees who spanned the nuclear physics community. It was clear that this kind of large scale nuclear data evolution is underway by multiple groups and that communication of the techniques and results is key for efficient and effective progress in several fields.

There is also nuclear data available that has often been overlooked by the nuclear astrophysics community. Part of the reason for this is that more complicated mathematical formalisms are required for their interpretation. However, many of these formalisms have been implemented in a limited number of codes. It is a main goal of the ongoing development of AZURE2 to include two of these kinds of data: polarization observables and unobserved primary observed secondary.

Following one of the tasks of the following year, progress has been made in the analysis of the ^{28}Si system. In particular, the ^{27}Al+p data of Nelson had two particular issues: an energy dependent offset of the data and a lack of detailed uncertainty information. For the energy calibration, a quadratic fit was made to several of the resonances whose energies are known to high precision from ^{27}Al(p,g) measurements. To partly address the uncertainty issue, the paper states that the scattering data have an uncertainty of about 3%. When this is applied to the scattering data it does seem like a reasonable estimate given the scatter of the data points. For the other reaction channels, where the cross sections are smaller and vary greatly, this is certainly not a good estimate. Since the data were taken simultaneously for all reaction channels at each energy, the uncertainty of the data points in these reaction data can be estimated based on the ratio of the cross sections. In particular, the thin target yield (Y) is $Y=\sigma N_t N_b \varepsilon$, where σ is the cross section, N_t is the number of active target atoms, N_b is the number of beam particles made incident on the target, and ε is the detection efficiency. If the uncertainties are assumed to be purely statistical, likely a good approximation in this case, then the uncertainty in the cross section proportional to the uncertainty in the yield. Then taking the ratio of the yields of a non-scattering (reaction) cross section to the scattering one at the same energy and angle gives dYreac = sqrt(Y_scat/Y_reac)*dY(scat), where dY is the percentage uncertainty. In Fig. 2.2, section a) represents a flat 3% uncertainty, while section b) shows the uncertainty scaled as described. It may also be useful to impose a lower limit on the observable cross section as some of the non-resonant regions may contain data that are really only upper limits.

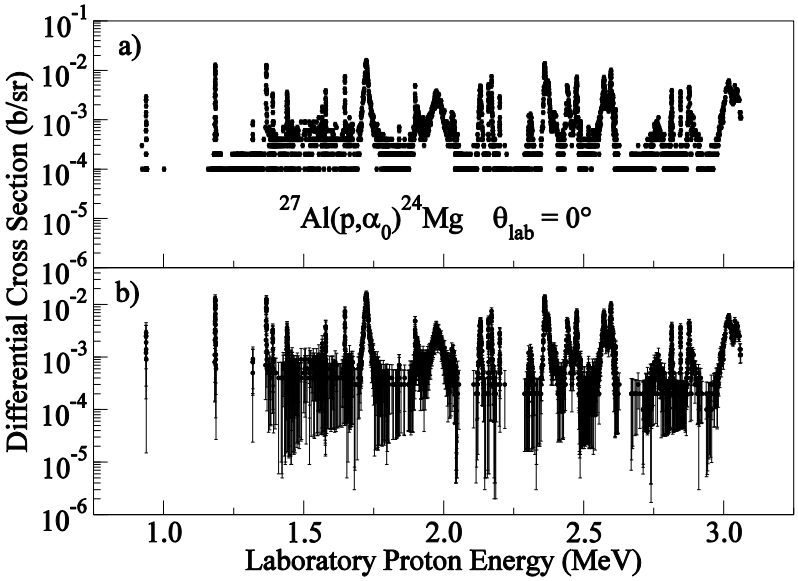

FIG. 2.2. Uncertainty estimates for the $^{27}Al(p,a_0)^{24}Mg$ reaction cross section based on a) a flat 3% estimate and b) uncertainty scaled to that of the scattering cross sections.

2.4 Recent Progress on AMUR Code, *S. Kunieda (Japan Atomic Energy Agency)*

The status of the AMUR code was presented together with its preliminary use in an analysis for the ^{17}O system. AMUR is a multi-channel, multi-level R-matrix code base on the Wigner-Eisenbud's formalism except for the γ-ray channels which are calculated by the Reich-Moore approximation. The code can be applied to the analysis of cross sections, differential cross-sections including those for charged-particle reactions. In addition to the R-matrix parameters such as boundary parameters, energy eigenvalues and reduced-width amplitudes, experimental parameters such as the re-normalization and the resolution can be deduced from the shape analysis of measured cross sections. The fitting method adopted is equivalent with that of the KALMAN/SOK code, which is also able to estimate the covariance matrix of the parameter values, and hence of the cross sections.

The unitarity of the S-matrix constrains the behavior of the R-matrix parameters so much that it could be used to reduce the uncertainty of evaluated cross sections. It was demonstrated on a simultaneous analysis of measured ^{16}O(n,tot), ^{16}O(n,n), and ^{13}C(α,n) cross-sections, where the re-normalization parameters introduced for each measurement were uniquely determined by the fitting procedure. By studying the correlation matrix of the cross sections, it was also suggested that features of the unitarity were visualized through the sensitivity/covariance analysis of the cross sections.

Recent developments in the code include the addition of a new capability to analyse polarized measurements. This functionality has been validated through a comparison of the experimental and calculated analysing powers of the ^{16}O(n,n) reaction. A preliminary approach to reduce a large difference between the R-matrix calculations and the measured ^{13}C(α,α) differential cross sections was also presented. Through simultaneous analysis of the measured ^{16}O(n,tot), ^{16}O(n,n), ^{13}C(α,n) and ^{13}C(α,α) cross sections, it was pointed out that large theoretical backgrounds are necessary not only for the n+α channels but also for the n- and α-only channels independently, to reduce the discrepancy. Furthermore, if the channel radius and hard-sphere radius are fitted separately, much better fits could be obtained (however, this approach may be inconsistent with the standard R-matrix theory, i.e. it violates unitarity).

2.5 A Modern Theoretical Approach to the R-Matrix and the EDA6 Los Alamos Implementation, *M. Paris (Los Alamos National Laboratory)*

The Los Alamos National Laboratory R-matrix code, Energy Dependent Analysis (EDA), is a 'full' multichannel unitary R-matrix analysis code that handles all observables – integral and differential, inclusive and polarization – for two-body particle and electromagnetic channels. Its theoretical foundation is based on the modern, Bloch approach to the R-matrix method, which encompasses the treatment of Lane & Thomas. It stresses a self-consistent formalism that takes into account the requirements of multichannel unitarity which ensures a parametrization of the S-matrix that is consistent with the requirements of analyticity and causality. In particular, the boundary condition parameters (channel radii and boundary values) used are energy independent, as is required in order to interpret the parametrization as the physical, unitary scattering matrix. We have emphasized that the R-matrix level parameters (energy levels and reduced widths) are functions of the boundary condition values, which are not physical quantities but rather are *regulators* of the theory.

The EDA code parametrizes the R-matrix in a manner consistent with relativistic two-body kinematics. This is important for systems that furnish very narrow resonances, which would not be properly located across channels in a non-relativistic parametrization. An example is provided by the ^{17}O system: There is a narrow 3/2+ resonance at E_n = 3.0071 MeV having a center of mass width of 0.33 keV. Relativistically, this resonance would show up at a laboratory energy of 0.802717 MeV. Non-relativistically, it would be at 0.803041 MeV. So, the difference is 0.324 keV, or 0.248 keV in the center of mass, which is a significant fraction of the width of this resonance.

The current version of EDA (EDA5) has been used to evaluate about 30 compound systems of up to 10's of thousands of data points per system. Recent updates have been performed for the NN, ^{7}Li, ^{8}Be, ^{10}Be, ^{11}B, ^{13}C, ^{14}C and ^{17}O systems.

Current work is focused on the development of a Fortran2008 version of EDA5 (EDA6) which will extend EDA5 capabilities to include improved data handling, covariance analyses, resonance parameter (e.g., the Brune alternative parametrization and model-independent S-matrix poles) and output formats. EDA6 intends to allow users to employ planned implementations of resonance parameter exchange formats but we recommend that the complex-energy S-matrix parameters are employed in comparisons to ensure observable-equivalent unitary parametrizations.

2.6 SAMMY modernization, *G. Arbanas (Oak Ridge National Laboratory)*[1]

SAMMY is a code developed by Oak Ridge National Laboratory (ORNL) for Bayesian fitting of R-matrix resonance parameters to neutron, proton, and α-particle differential cross sections data in resolved and unresolved resonance energy ranges. SAMMY provides facility-specific multi-component experimental resolution functions, including resolution functions of

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commercially available detectors, and it accounts for Doppler broadening of cross sections, multiple scattering effects, etc. For several decades SAMMY has been the foremost tool for R-matrix resonance parameter evaluations in the U.S. and abroad contributing many evaluated resonance parameter sets and their covariance matrices to nuclear data libraries. A coupling to integral benchmark experiments to inform evaluation of R-matrix parameters recently implemented in the SAMINT module of SAMMY will be outlined. SAMMY modernization efforts are progressing in the path of an ongoing and successful modernization of ORNL's neutron transport code suite SCALE and its nuclear data processing unit AMPX, in a broader context of ORNL's adoption of standardized software quality assurance practices. Consequently, the SAMMY code version control, bug-tracking system, automated build and test system have been upgraded to that of SCALE and AMPX. Furthermore, the anticipated module sharing among SAMMY, AMPX, and SCALE will be leveraged for modernizing SAMMY.

This work has been presented at the 2016 Workshop on R-matrix methods and applications, 27 June-1 July 2016, Santa Fe, NM.

2.7 Generalized Reich-Moore R-matrix Approximation, *G. Arbanas (Oak Ridge National Laboratory)*[1]

A conventional Reich-Moore approximation (RMA) of *R*-matrix is generalized into a manifestly unitary form by introducing a set of resonant capture channels treated explicitly in a generalized, reduced *R*-matrix. A dramatic reduction of channel space witnessed in conventional RMA, from $N_c \times N_c$ full *R*-matrix to $N_p \times N_p$ reduced *R*-matrix, where $N_c=N_p + N_\gamma$, N_p and N_γ denoting the number of particle and γ-ray channels, respectively, is due to $N_p << N_\gamma$. A corresponding reduction of channel space in generalized RMA is from $N_c \times N_c$ full *R*-matrix to $N_{c'} \times N_{c'}$, $N_{c'} = N_p + N_\lambda$ and N_λ is the number of *R*-matrix levels. This reduction, although not as dramatic as in the conventional RMA, could be significant for medium and heavy nuclides where $N_\lambda << N_\gamma$. The resonant capture channels defined by generalized RMA correspond to level-level interference (via capture channels) neglected in conventional RMA. The expression for total capture cross section in generalized RMA is formally equal to that of the full $N_c \times N_c$ *R*-matrix. This suggests that generalized RMA could yield improved nuclear data evaluations in the resolved resonance range. This would come at a cost of introducing N_λ (N_λ -1)/2 resonant capture width parameters. Manifest unitarity of generalized RMA justifies a method advocated by Froehner and implemented in the SAMMY nuclear data evaluation code for enforcing unitarity of conventional RMA. Capture widths of generalized RMA are exactly convertible into alternative R-matrix parameters via Brune tranform. Applying idealized statistical methods to generalized RMA shows that variance among conventional RMA capture widths could be used to estimate variance among off-diagonal elements neglected in conventional RMA. Significant departure of capture widths from an idealized distribution may indicate the presence of underlying doorway states.

This work has been presented at the International Conference on Nuclear Data for Science and Technology, ND2016, 11-19 Sept. 2016, Brugges.

2.8 Adaptive R-Matrix Approach for Light Nuclei, *T. Srdinko (Technisches Universität Wien)*

The consistent description of reaction cross sections of light nuclear systems suffers from the limited applicability of statistical model calculations as well as from the lack of microscopic models providing quantitatively reliable cross sections. The former can only be applied at

higher energies for which the level density of the compound nucleus is almost continuous. At lower energies the R-matrix formalism allows an excellent description of experimental data, but allows neither predictions nor physics interpretations. The R-matrix formalism and the statistical model are conceptually different and therefore a smooth transition between the two approaches is not obvious.

The adaptive R-matrix approach is aimed to provide an almost continuous transition between statistical model and R-matrix calculations. The method makes use of the R-matrix formalism as a tool for the solution of coupled-channel equations. Therefore it describes the low-energy range by a coupled-channel system which contains all channels up to a certain transition energy, thus satisfying unitarity. In order to provide a smooth transition to the statistical model regime, a background pseudo-potential is introduced which is set initially to be the real part of the optical potential with adequately chosen coupling terms. This assumption is based on the idea that the flux loss into the open channels of the coupled channel-system will be equal to the one reflected in the transmission coefficients at the transition energy.

The background pseudo-potential is defined in relative channel-coordinates representing a projection of the mean field generated by the microscopic interactions. Introducing this background pseudo-potential into the coupled-channel system and solving the equations within the R-matrix formalism leads to a well-defined spectrum of poles with widths.

We implemented the adaptive R-matrix approach into our new coupled-channel code GECCCOS and applied the method to the ^{17}O system with n+^{16}O as entrance channel. Starting with the Woods-Saxon shaped real volume term form the RIPL3 library for (n+^{16}O), the structure of the total cross section could be fairly well reproduced and approaches smoothly the corresponding statistical model calculations performed at higher energies with TALYS.

For a proper description of the experimental data additional R-matrix poles must be introduced in order to include narrow resonances which cannot be accounted for by the background pseudo-potential. In order to describe the experimental cross sections the additional pole parameters as well as the background poles must be varied simultaneously. The latter lead to small variations of the pole parameters which clearly indicate a *J*,*L*-dependence of the background mean field. The dependence and the necessity of variation are not unexpected as they would account for neglecting the real part of the polarization potential in our ansatz.

For the energy region 0.2 to 3.0 MeV the total cross section was fairly well reproduced. At higher energies the R-matrix representation requires further optimization. The pole spectrum associated with the background pseudo-potential represents the mean field, while additional pole terms may be attributed to the residual interaction. Interference effects between the two groups of poles can occur making the fitting procedure challenging. The proper adaption of the fitting procedures and the inclusion of further channels at higher energies are currently ongoing.

2.9 Introduction to RAC-CERNGEPLIS, *Z. Chen (Tsinghua University of Beijing)*

A new evaluation method RAC-CERNGEPLIS has been developed, which includes：

RAC—R-matrix Analysis Code with multi-levels and multi-channels theory [2.5];

C—Covariance statistics and generalized least squares fitting are used [2.6];

E—Error propagation law is used to get accurate Covariance Matrix [2.7];

R—Relativistic calculation for energy;

N—Normalization for relative data (Scaling factor) and absolute data (Normalized factor);

G—Global database for a nuclear system is used;

E—Elimination of channel is used to expended energy range [2.5];

P—PPP modification is considered [2.8];

L—Lett's criteria is used to minimize the effect from occasional 'outliers';

I—Iterative fitting procedure is used to get expectation values [2.9];

S— Systematic error is updated according to the errors of fitted values.

In 'General least-squares method' fitting, the question is which kind of systematic error should be used finally? For any data set (Y), in the fitting procedure it is modified by a normalization factor (or scaling factor) (n) to minimum χ^2. If the N is good enough, then nY is the data set actually used. But then, what is the systematic error of nY (ε)? If it should not be the original one absolutely, then it should be a new one, i.e. the residual of the original systematic error. In this case maybe there exists the following relation:

$$E-k\sigma< nY < E+k\sigma, \quad 1<k<2$$

Where E is the expectation value, and σ is the error of the evaluated value. In 'General least-squares method' fitting, Perl's Pertinent Puzzle (PPP) is a very big problem. Experience shows that if the systematic error is larger than 40% of statistical error, the PPP will occur obviously. The majority of experimental papers often give a rather small statistical error and a rather larger estimate of the systematic error. With this kind of data, the 'General least-squares method' fitting can't be used absolutely. So at first the 'Least-squares method' fit is used, whereby PPP does not occur when the following χ^2 is minimized:

$$\chi^2=\sum_{i=1}^{i=n}[\ (X_i(\mathrm{P}) - \mathrm{n}R_i)\ /((\varepsilon_s+\varepsilon_t)\mathrm{n}R_i)]^2 \Rightarrow \text{minimum}$$

After obtaining very good evaluated values and very good R-matrix parameters $\overrightarrow{\theta_a}$, the 'General least-squares method' fitting is used (see p. 187 of Ref. [2.6]):

$$\chi^2 = \ (\vec{\theta} - \overrightarrow{\theta_a})^+ V_a^{-1} \left(\vec{\theta} - \overrightarrow{\theta_a}\right) + \ (\vec{\eta} - \vec{y})^+ V_a^{-1} \ (\vec{\eta} - \vec{y}) \Rightarrow \text{minimum}$$

is used, in which the kσ has to be taken as the systematic error, the V is the full covariance matrix of database, and V_a^{-1} is the reverse matrix of V, the $\overrightarrow{\theta_a}$ is the prior knowledge of $\vec{\theta}$. This method needs to be applied iteratively, so that at each iteration the experimental data have an impact on the determination of the expectation value, and the experimental data are improved by the normalizing factor and systematic error. This iterative procedure is applied until all parameters, all normalization factors, and all calculated values become very stable, so that the final evaluated value can be very near the expectation value. In this way using different priors will lead to the near same final results.

It should be emphasized that only when there exists good enough evidence to explain that the final evaluated value can be very near the expectation value, the kσ can be taken as the systematic error of the normalized experimental data used finally. It should be emphasized

too that if one wants to use the 'General least-squares method' in evaluation, the systematic error have to be reduced by this approach, whereas the original rather lager systematic error which was obtained by using 'archaeological skills' (see p. 134 of Ref. [2.6]) or was given arbitrarily (e.g. 5% to 10%) can't be used anymore, because then PPP will occur.

The RAC-CERNGEPLIS method has been used to complete 'A Global Evaluation for ^{7}Li system', and the evaluated results have been used to construct the Neutron standard for ^{6}Li(n,t) in IAEA-2016 version. An important finding of this work is that the evaluated cross sections of ^{6}Li (n, tot) in ENDF/B-VII.1 deviate systematically from the experimental data, something that could be improved.

The RAC-CERNGEPLIS method has also been used to complete 'A Global Evaluation for ^{11}B system'.

The RAC-CERNGEPLIS method has been used to complete 'A Global Evaluation for Astrophysical S factor and Reaction Rate of ^{12}C $(\alpha,\gamma)^{16}$O with Reduced R-matrix Theory'. This work is of scientific significance because of the following: The astrophysical S factors of ^{12}C $(\alpha,\gamma)^{16}$O are the most important fundamental data for determining the abundances of the elements produced by nucleosynthesis. The determination of accurate values of the S factors (error < 10%) has been regarded as the 'holy grail' of nuclear astrophysics for decades. In spite of the tremendous efforts made worldwide over 40 years, this goal has not been reached. In our approach, we skillfully combine the formulae of the classical R-Matrix theory and the γ transition theory, with the coordination of covariance statistics and error propagation theory, a global fitting for almost all available experimental data of ^{16}O system formed by ^{12}C+α have been done. A set of reliable, accurate S factors and reaction rate of ^{12}C $(\alpha,\gamma)^{16}$O have been obtained. At E = 0.3 MeV total S factor is 161.74±8.61 keVb with error 5.3%, at T_9 = 0.2 Reaction Rate is 7.56±0.41 mol.s-1.cm-3 with error 5.5%, for the first time meet the required precision.

In theory, the 'Conventional least-squares' fitting ignore the correlation of statistic error and systematical error, therefore it cannot provide an unbiased estimate for a complex sample, nor can it evaluate correct covariances. According to the 'maximum likelihood principle', only the 'General least-squares' method can provide an unbiased estimate for a complex sample, and correct covariances for the parameters and the evaluated values. So using the 'General least-squares' fitting should be encouraged.

2.10 Uncertaintiy quantification in (α, N) Neutron Source calculations in an Oxide Matrix, *M. Pigni (Oak Ridge National Laboratory)*[2]

The most recent version of the R-matrix code SAMMY [2.11] allows the study of the ingoing and outgoing charged-particle channels in the low-energy interaction range. Although the SAMMY code system is mainly used in nuclear data evaluations for incident neutrons in the resolved resonance region (RRR), built-in capabilities also allow the code to describe the resonance structure produced by other incident particles, including charged particles.

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ENDF/B-VII.1 nuclear data library [2.12] contains no evaluated data for α-induced reactions. However, (α, n) data provide fundamental information that underpins nuclear modeling and simulation software, such as ORIGEN [2.13] and SOURCES4C [2.14], used for the analysis of neutron emission and source emission processes.

The ultimate goal of this work is to carry out evaluations of charged-particle-induced reaction cross sections in the RRR. The SAMMY code was recently used in this regard to generate a Reich-Moore parameterization of the ^{17,18}O(α,n) available experimental cross sections in order to estimate the uncertainty in the neutron generation rates for uranium oxide fuel types [2.15].

The presentation provided a detailed description of the SAMMY evaluation procedure for the treatment of (α, n) reaction cross sections applied to ^{17,18}O isotopes.

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3. Technical discussions

Two more R-matrix code developers joined the project at this meeting (RAC-developed by Z. Chen, GECCCOS-developed by H. Leeb and T. Srdinko) adding to the variety and richness of R-matrix codes, methods and approaches considered by this project.

3.1 Theory-Approximations-Codes

It was realized from the first meeting [1.1] that although all the codes under discussion are based on the standard R-matrix theory, as described in [2.5], in practice they assume certain approximations that ultimately make the inter-comparison of resonance parameters they produce unfeasible. These approximations include treatment of boundary conditions, channel radii, unitarity, and relativistic kinematics. These issues were discussed further at this meeting and the conclusions/decisions that were taken are mentioned in the following.

R-matrix theory: Meaning of Approximations

B=S approximation: 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 [3.1], which have the advantage of being independent of the boundary conditions, however not the channel radii. At this meeting it was clarified that the B=S approximation adopted in SAMMY cannot be exactly converted to standard R-matrix representation. It can only approximately be converted through the Brune transformation, but then the resulting resonance parameters need to be refitted to the data to best accuracy.

Variation of the R-matrix radii: Some of the codes treat the R-matrix radii as adjustable parameters while others determine the optimum radius parameter starting from a formula and keep it constant throughout the fitting procedure. 'Observable equivalent' analyses are possible with analyses that employ different sets of channel radii in the fitting procedure. Comparisons based on R-matrix parametrizations, however, necessarily require using the same set of channel radii. One rather approximate approach would be to vary the sets of channel radii by keeping the 'observed widths' unchanged (e.g. with fixed $\Gamma=2\cdot\gamma^2\cdot P$). The latter will have to be checked and verified during the fitting procedure.

Unitarity: this issue has been discussed at considerable length due to the important constrains it imposes on R-matrix fits to experimental data. The expression for the S-matrix in terms of (symmetric and real) standard R-matrix satisfies unitarity by default. However, the Reich-Moore approximation for eliminated γ-channels yields a complex R-matrix (due to resonant capture widths appearing in denominator) that is reduced to particle-channel space. The S-matrix corresponding to the Reich-Moore R-matrix in particle channel space is not unitary, however, the complete S-matrix (that includes the eliminated capture channel) can be made unitary by equating capture cross section to the deviation from unitarity of the Reich-Moore R-matrix in particle channel space. This prescription has been suggested by F. Froehner [3.2], and it has been implemented in SAMMY since its inception. A more general perspective on unitarity of Reich-Moore is provided by a generalization of Reich-Moore approximation (Sec. 2.7) that is shown to be manifestly unitary since its R-matrix is real and symmetric.

Relativistic kinematics: wave numbers and momenta are affected by the type of kinematics, be it relativistic or non-relativistic. However, it remains to be demonstrated through mathematical formulae how the employed relativistic kinematics will affect the pole positions or even the relative pole positions of the R-matrix.

Alternate R-matrix forms:
Action on I. Thompson: Propose CSEWG [3.3] to represent Brune transformation in the ENDF-6 format [2.4] because it is independent of the boundary B and the poles are close to the peaks in the cross section. It is an objective alternative to the standard R-matrix presentation. Also propose to WPEC to include it in GND [3.4].

Cross sections at exactly the R-matrix pole energies: As the R-matrix is not defined at the pole energy, an approach is needed to deal with this and compute the cross sections at these energies. A question was raised regarding the various approaches used by the different codes and how these can affect the R-matrix calculations and fits overall. This matter will be further discussed at a next meeting.

Calculating Observables
Angular distributions of decay γ's: the calculation of the angular distributions of the γ's emitted from a given excited state of the nucleus following inelastic scattering (X,X'γ) or a nuclear reaction (X,Yγ) where X,Y = p,n,d, α, is straightforward and a detailed prescription is given in [3.5]. The Los Alamos group has an auxiliary code, called SPECT, which handles angular distributions of photons in three-body (two particle and one photon) final state channels. The other code developers (SAMMY, SFRESCO, AZURE2, RAC) agreed to look into this and incorporate it in their codes.

Particle polarization: several of the codes already calculate polarization observables (see an update of Table 1 of [1.1] in Appendix 2). An effort will be made by the other code developers (AZURE2, GECCCOS) to include calculations of such observables.

Unresolved resonance region (URR): how to treat the higher energy region of unresolved resonances (URR) is an open question which however needs to be addressed when trying to connect the lower resolved-resonance region with the region of strongly overlapping resonances that are normally treated with statistical methods. In a first step one can use an averaged R-matrix cross section and extrapolate to higher energies, or extrapolate trends of R-matrix pole densities and widths to higher energies. Another method is to use the URR averaging formulae (derived in the literature) to give the average cross sections from R-matrix pole densities and widths. The approach presented at this meeting (Sect. 2.8) uses real potentials to generate poles that link the higher energy region to the lower resolved-resonance region (GECCCOS). More development and discussion is needed in this area however the results of Sect. 2.8 are quite promising.

Low-energy predictions: With regard to astrophysical S-factors one should take care of subthreshold states which may have a strong impact on the low-energy behaviour as pointed out in R.J. deBoer's presentation (see Sect. 2.3).

Fits above 3-body thresholds: these are done only approximately by simulating the breakup component by using discrete states for the successive decay steps, and summing over such products to improve the accuracy where needed.

Closed channels: Closed channels can have a very strong effect on cross sections near the threshold as was demonstrated at the meeting. In R-matrix theory closed channels arise when there are poles with partial widths in channels where the pole energy there is sub-threshold. For example, in elastic scattering, closed channels may exist as subthreshold states in

channels coupled to the scattering channel of interest. This would mean there are R-matrix poles with non-elastic widths and some non-zero elastic widths. Having both gives rise to the coupling of the elastic to non-elastic channels. But the pole energies are excluded in this case from being sub-threshold in the elastic channel of interest. This discussion was meant as a reminder to the beginners in R-matrix fitting of cross sections in the low-energy region.

FERDINAND: update

The FERDINAND Code is a stand-alone code developed by I. Thompson after the first meeting [1.1] to provide an inter-translation between different R-matrix code formats. It has been tested on SFRESCO, AZURE2, and HYRMA, and with ENDF-6 [2.4] and GND [3.4] data formats. It is however still in a preliminary state, but will be fixed and completed in the next 2 months after the meeting. One issue to be solved is the relativistic kinematics (KRL key in ENDF-6 [2.4]: KRL=0 nonrelativistic, KRL=1 relativistic). It will be distributed to all code developers with a working version of FUDGE [3.6] (new version in February 2017) with ENDF files for the systems n+^{16}O and p+^{27}Al. In this complete version it will also include pointwise reconstruction of cross sections from resonance parameter files.

Action on all: test the FERDINAND+FUDGE code on n+^{16}O and p+^{27}Al systems and report the results back to I. Thompson by end of May 2017.

3.2 Experimental Data

Some useful comments were made when discussing how to use experimental data in R-matrix fits.

Using EXFOR Data: Evaluators should check the EXFOR corrections system [3.7] for improvements on data submitted by evaluators which should be taken into account.

Resolution and Broadening: Resolution and thermal Doppler broadening should be taken into account. The resolution broadening should reflect the specifics of the experimental setup.

In general broadening should account for angular and energy resolution. This should apply for both resolution and thermal Doppler broadening.

User Requirements: IBANDL user requirements include the evaluation of p+^{7}Li -> 2α channel. Angular distribution for n+^{7}Be -> 2α may be available from Andy Bacher. These evaluations should also become available in ENDF.

3.3 Formats/Data processing

LRF=7: It was concluded that the limited R-matrix format (LRF=7) is adequate for accommodating standard R-matrix theory fits in ENDF-6 format [2.4].

Pointwise reconstruction of cross sections:
PREPRO [3.8] cannot handle charged-particle elastic scattering. FUDGE will do this in the near future. SAMMY is currently the only code that can process ENDF-6 resonance parameter files (file 2) for charged-particle elastic scattering and reconstruct pointwise cross sections (file 3).

3.4 Coordination-Allocation of effort:

The successful outcome of the coordinated project on R-matrix codes for charged-particle reactions in the resolved-resonance region relies entirely on the commitment of the contributing code developers and evaluators. The following participants re-affirmed their strong interest and frim commitment to the work proposed at this meeting:

SFRESCO (Thompson), HYRMA (Quaglioni)
EDA (Paris, Hale)
AZURE2 (deBoer)
SAMMY (Arbanas, Pigni), Dimitriou
RAC (Chen) – letter of support of the collaboration between Chen and IAEA requested
AMUR (Kunieda)
GECCCOS (Leeb, Srdinko)

3.5 R-matrix fits

In addition to comparing the R-matrix codes with respect to their specifications various approximations incorporated in them (see table in Appendix 1), participants also agreed to compare the R-matrix fits they produce for a given realistic case. A test exercise was therefore defined by participating code developers (SFRESCO, AZURE2, EDA, SAMMY, AMUR, RAC, GECCCOS), the details of which are described in the following.

3.6 Definition of Test Case

The objective of the exercise is to compare the fits produced by the different R-matrix codes for a realistic case. Specifically, the comparison will cover

- evaluated parameters and their uncertainties,
- evaluated cross sections and their uncertainties-including covariances

Description of test case

R-matrix fits will be performed for the ^{7}Be system. Cross sections will be calculated for incident energies up to 12.8 MeV to include the following open channels:

$\alpha(^{3}He, ^{3}He)\alpha$, $^{4}He(^{3}He,p_0)^{6}Li$,,$^{6}Li(p,\alpha)^{3}He$, $^{6}Li(p,p_0)^{6}Li$, $^{6}Li(p,p_1)^{6}Li$*

The R-matrix calculations will use the following parameters:

1. Real symmetric R-matrix
2. B_c=-L_c values fixed (B is partial wave dependent, but energy independent)
3. Channel radius a_c=1.4 [fm] ($A_1^{1/3} + A_2^{1/3}$)
4. Maximum L: L_{max}=4 (^{3}He+^{4}He), L_{max}=1 (p+^{6}Li)
5. No energy broadening or resolution corrections will be needed.

Regular checks for unitarity for all particle channels, especially if the B=S approximation is used, are advised.

The data sets for this test case, along with starting resonance parameters, will be prepared and distributed to participants by R.J. deBoer. The details of the exercise including the data are given in Appendix 3.

Deadlines

- data files and parameter files will be distributed to participants by the end of 2016 (Action on R.J. deBoer)
- exercise will be completed by May 2017
- results will be discussed at the next meeting to be held in June 7-9, 2017

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4. Conclusions and perspectives

The long term goal of this coordinated effort is to produce evaluated data files for charged-particle reactions in the resolved resonance region for the user community at large. To do so will require the joint efforts of all participating R-matrix code developers and evaluators, as well as a clearly-defined common evaluation methodology that would include treatment of uncertainties. The first steps in this direction were taken at the first meeting of December 2015, where an inter-comparison of the codes was held, and subsequently at this meeting with the discussion of R-matrix theory and approximations, the adoption of Brune transformation and the development of the Ferdinand code for inter-changing resonance parameters between different formats and R-matrix codes. The next important step is to compare and understand the fitting capabilities of the various codes, before establishing the joint evaluation methodology. These two issues will be the subject of the third meeting which will be held on 7-9 June 2017 at the IAEA, in Vienna. In preparation for this third meeting, participants will carry out a joint exercise that consists of fitting a realistic system with a well-defined set of data (see Sect. 3.2.1).

In view of the long-term goals of this coordinated project, it is inevitable that the group will also have to address the treatment of breakup channels, e.g in the ^{24}Mg compound system there is a 3-body channel ^{16}O+α+α at 2.6 MeV; in other systems there will be even 4-body exit channels.

Finally, in the period leading to the 3rd meeting in June 2017, the IAEA will carry out a survey of the ENDF/B-VII data base for existing charged-particle evaluations, and on the basis of its findings and the current status of IBA-related evaluations (Table 2 of INDC(NDS)-0703), it will produce a list of priority evaluations that need to be provided by the participating evaluators.

Topics for Consideration in R-matrix Consultants' Meeting
5-6 December 2016

(Ian Thompson in collaboration with Vivian Dimitriou, 28 Nov 2016)

(in green what can be postponed to later)

1. Theory-Approximations-Codes

— ***R-matrix theory***
Angular distributions of decay gammas (i.e. residual polarization)
Particle polarization (incoming, exit)
Relativistic kinematics
Alternate R-matrix forms (Brune, Holcomb)
Unitarity
Unresolved-resonance region (URR
Low-energy predictions
    Astrophysical S-factors
    Thermal neutron scattering
S-matrix poles (complex)
Fits above 3-body thresholds:
    Two-step products of R-matrices (e.g. Hale+Brune)
    Democratic 3-body decays
    Discretized continuum (PS, CDCC, HO, THO)
    Hyperspherical-harmonic basis (HH)

— ***Meanings of Approximations:***
B=S approximation
How to convert to standard R-matrix theory (with B specified)?
Reich-Moore approximation with vanishing gamma widths
Brune transformation (SHF=2)
Generalized Reich-Moore Approximation (Arbanas, Holcomb)
Variation of R-matrix radii (e.g. with fixed Gamma = 2*gamma^2*P)

— ***Ferdinand:***
distributed with Fudge!
translation between R-matrix-code formats: ENDF, Fresco, AZURE, HYRMA
transformations IFG=0,1
transformations SHF=0,1,2
adding/removing channels (e.g. gammas)

— ***Testing transformations and Ferdinand results:***
n + 16O
p + 27Al
+ others !!

2. Fitting experimental data (evaluation)

— ***Using experimental data***
Using Exfor data
Lab and cm angles
Lab and cm cross sections

Resolution and broadening
Beam energies
Scattering angles
Renormalizing experimental data
Calibration to Rutherford at low energies
Experimental energy calibrations

— ***User requirements***
High resolution measurements
Energy calibrations
Low resolution measurements
How much averaging is appropriate? Angles? Energies?

— ***Fitting procedures***
Closed channels
Known levels (bound states)
New levels (fits need sub-threshold levels)
Choice of R-matrix radii
Trying different J/pi for resonances
Manual or automatic?
Energy range
Segment fits
Single-resonance fits
Fitting entire range?

— ***Code bases***
Pointwise reconstruction of cross sections
Yes: Sammy, Fresco, Fudge (soon).
No: Prepro
Relativistic kinematics
Chi-squared and Bayesian methods

— ***Covariances:***
Parameter covariances
Data covariances from parameter fits
Using analytic derivatives
Using numeric derivatives

3. Formats

— ***Data formats***
ENDF option SHF=2 for Brune transformation
GND options (being implemented)
Non-Reich-Moore evaluations (no gamma channel)
What is 'limited' about RML?
Writing covariances to evaluation files (MF=32 in ENDF)

4. **Coordination**

— ***Manpower for Fitting Reactions***
ND (de Boer)
LANL (Paris, Hale)
LLNL (Thompson, Quaglioni)
ORNL (Pigni, Sobes, Arbanas)
IAEA (Dimitriou)
+ others!

— ***Publication/dissemination of evaluations***
WITH R-matrix parameters and approximations listed!
Showing fits in slides for talks
CSEWG for ENDF/B-VIII.x
LLNL for GND
IAEA for IBA databases (see Table 2 of INDC(NDS)-0703)

— ***Allocation of effort***

Table. R-matrix codes comparison-revised

Feature	EDA	AZURE2	AMUR	FRESCO	SAMMY	HYRMA	RAC
R-matrix	Full	Full	Limited (for gammas)	Full	SLBW, MLBW, RM, Full[3]	Only particle channels	Full
Derivatives	Analytic	Numerical	Numerical	Numerical	Analytical for $\sigma_{T=0K}$ Numerical otherwise[4]	Numerical	Analytic
Kinematics	Relativistic + non-relativistic	Non-relativistic	Non-relativistic	Relativistic+ non-relativistic	Non-relativistic	Non-relativistic	Relativistic+non-relativistic
Reference frame	Lab/CM	Input Lab /output CM	Lab/CM	Lab/CM	Lab/CM	Lab/CM	Lab/CM
Channel Radii	Varied	Varied	Fitted (option)	Fixed	Varied	Fixed	Varied
Photons	In/Out	Out	Out	In/Out	Out	No	In/Out
Observables: cross sections (energy and energy-angle differential)	All	All	All	All	All	All	All
Observables: polarization, tensor analysing power etc	All	No	Yes	All	No. SAMINT links to IBE	No	All

[3] Full R-matrix in SAMMY is achieved by treating γ-channels as reaction channels.
[4] 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	RAC
Inverse reactions	Yes	Yes	Yes	Yes	Yes	No	Yes
Decay gammas	Post-processing	No	No	Post-processing	No	No	Included
Isobaric reactions simultaneously	Yes	No	No	No	No	No	Yes
Doppler broadening	No	No	Yes	No	Yes	No	No
Resolution broadening	Yes	Yes	Yes	No	Yes	No	No
Normalization	Yes	Yes	Yes	yes	Yes	No	Yes
Background subtraction	No	No	Yes	No	Yes	No	No
Background R-matrix terms	Energy-dependent	Distant poles	Distant poles	Distant poles	Yes	Distant poles	Distant poles
Sample-size corrections	No	Yes	No	No	Yes	No	No
Closed-geometry Q-corrections	No	Yes	No	No	Yes	No	No
Fitting procedure	L-SQ	MINUIT2	KALMAN	MINUIT1	Bayesian i.e. GLS	MINUIT	G-SQ
Multiple data sets	simultaneously	simultaneously	simultaneously	Simultaneously	Simultaneously	simultaneously	Simultaneously
Uses data covariances	No	No	Yes	No	Yes	No	Yes
Uses prior parameter covariances	Yes	No	Yes	No	Yes	No	Yes

Feature	EDA	AZURE2	AMUR	FRESCO	SAMMY	HYRMA	RAC
Produce evaluated data covariances (MF 32)	No	No	No	No	Yes	No	Yes
Brune parameter output	No (planned)	Yes	No	No	No (planned)	Yes	No
ENDF-6 format output	Yes	No	Yes	No	Yes	No	Yes
ENDF-6 input	No	No	No	No	Yes	Yes	No
Number of resonances	To be filled		No limit		>3,000 for U-235		No limit
Code language	F77	C++	C++	F90	F77[5]	F90	F77
Availability	Export controlled	yes	no	yes	RSICC Export Control[6]	Export controlled	Export controlled
Documentation	no	yes	no	yes	Online	no	No
Parallelized	no	yes	yes	no	No	no	No
Interactive fitting	yes	no	no	Yes	Yes	no	No
PPP modification			fit within the logarithmic space (limited Box-Cox method)	no			yes

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

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

Feature	**EDA**	**AZURE2**	**AMUR**	**FRESCO**	**SAMMY**	**HYRMA**	**RAC**
Error propagation law			KALMAN method	none			Yes
How to deal with systematical error			use experimental value/ normalization-free (both options)	use experimental value/ normalization-free (both options)			The STD of evaluated value
Lettes criteria			No	No			yes
Elimination of channel Γ_λ^e			No	Yes			yes
Maintainer	Hale/Paris	DeBoer/ Uberseder	Kunieda	Thompson	Arbanas	Quaglioni	Chen

ANNEX 1

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

IAEA, Vienna, Austria
5-7 December 2016
Meeting Room VIC A2411

ADOPTED AGENDA

Monday, 5 December

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

09:30 – 17:00 Presentations by participants
1) Short review of project, goals and current status (P. Dimitriou, IAEA)
2) Theory and Tools for R-matrix Fitting (I. Thompson, LLNL)
3) R-matrix needs in Nuclear Astrophysics (R. DeBoer, Notre-Dame U.)
4) Recent progress of an R-matrix code (S. Kunieda, JAEA)
5) A Modern Theoretical Approach to the R-matrix and the coming EDA6 Los Alamos implementation (M. Paris, LANL)
6) SAMMY modernization, generalized Reich-Moore approximation and its relevance to unitarity and alternative R-matrix parametrization of Brune (G. Arbanas, ORNL)
7) An Adaptive R-Matrix Approach for Light Nuclei (T. Srdinko, TUW)
8) Evaluation of 17,18O(alpha,n) reaction (M. Pigni, ORNL)- Skype connection
9) Introduction to RAC (Z. Chen, Tsinghua University)

Coffee break(s) as needed
(12:30 – 13:30 Lunch break)

ANNEX 1

Tuesday, 6 December

09:00 – 17:30 Round Table Discussion

Coffee break(s) as needed
(12:30 – 14:00 Lunch break)

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

Wednesday, 7 December

09:00 – 13:00 Round Table Discussion cont'd - Drafting of the Summary Report
Closing of the Meeting

Coffee break as needed

ANNEX 2

Consultants' Meeting on

R-Matrix Codes for Charged-Particle Reactions in the Resolved Resonance Region

5-7 December 2016

A24-11, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS

AUSTRIA

Helmut LEEB
Technische Universität Wien
Arbeitsbereich Kernphysik und nukleare Astrophysik
Wiedner Hauptstrasse 8-10
1040 VIENNA
E-mail: leeb@kph.tuwien.ac.at

Thomas SRDINKO
Technische Universität Wien
Atominstitut der Österreichischen Universitäten
Wiedner Hauptstrasse 8-10
1040 VIENNA
E-mail: tsrdinko@ati.ac.at

CHINA

Zhenpeng CHEN
Tsinghua University
Department of Physics
Tsinghua Garden
BEIJING
E-mail: zhpchen@mail.tsinghua.edu.cn

JAPAN

Satoshi KUNIEDA
Nuclear Data Center
2-4 Shirakata Shirane, Naka-gun
TOKAI 319-1195
Tel: + 81 029 282 5482
E-mail: kunieda.satoshi@iaea.go.jp

UNITED STATES OF AMERICA

Richard J. DEBOER
Notre Dame University
225 Nieuwland Science Hall
Notre Dame, IN 46556
E-mail: richard.j.deboer.12@nd.edu

Ian J. THOMPSON
Lawrence Livermore National Laboratory
P.O. Box 808, L-414,
Livermore, CA 94551
E-mail: thompson97@llnl.gov

Mark PARIS
Los Alamos National Laboratory
Theoretical Divisaion, MS B283
Los Alamos, NM 87545
E-mail: mparis@lanl.gov

Goran ARBANAS
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge TN 37831
E-mail: arbanasg@ornl.gov

ANNEX 2

Roberto CAPOTE NOY
Tel. +43-1-2600 21713
E-mail: Roberto.CapoteNoy@iaea.org

Andrej TRKOV
Tel. +43-1-2600 21712
E-mail: a.trkov@iaea.org

Arjan KONING
Section Head
Tel.: +43-1-2600-21709
E-Mail: a.koning@iaea.org

All:
IAEA/NAPC / Nuclear Data Section
Wagramer Strasse 5
1400 Vienna

ANNEX 3

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

IAEA, Vienna, Austria
5-7 December 2016

Links to Online Presentations

#	Author	Title	Link
1	P. Dimitriou	Review of the projects, goals and persepctives	PDF
2	R.J. deBoer	R-matrix needs in Nuclear Astrophysics	PDF
3	M. Paris	A Modern Theoreticak Approach to the R-matrix and the coming EDA6 Los Alamos implementation	PDF
4	I.J. Thompson	Theory and Tools for R-matrix fitting	PDF
5	G. Arbanas	Sammy Modernization Generalized Reich-Moore approximation and relevance to unitarity and Brune parametrization	PDF PDF
6	Z. Chen	Global evaluation of 7Li system Introduction to RAC code	PDF PDF
7	T. Srdinko	An adaptive R-matrix approach for Light Nuclei	PDF
8	S. Kunieda	Recent progress in the R-matrix code AMUR	PDF
9	M.T. Pigni	Evaluation of 17,18O(alpha,n) reaction	PDF

ANNEX 3

ANNEX 4

Group Photo

ANNEX 4

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21710
Web: http://www-nds.iaea.org