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# Evaluation of the implementation of the R-matrix formalism with reference to the astrophysically important $^{18}F(p,\alpha)^{15}O$ reaction

D.J. Mountford [a,*], R.J. deBoer [b], P. Descouvemont [c], A. St. J. Murphy [a], E. Uberseder [b], M. Wiescher [b]

[a] SUPA, School of Physics and Astronomy, University of Edinburgh, EH9 3JZ, UK
[b] Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA
[c] Physique Nucléaire Théorique et Physique Mathématique, C.P. 229, Université Libre de Bruxelles (ULB), B 1050 Brussels, Belgium

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ABSTRACT

*Background.* The R-Matrix formalism is a crucial tool in the study of nuclear astrophysics reactions, and many codes have been written to implement the relevant mathematics. One such code makes use of Visual Basic macros. A further open-source code, AZURE, written in the FORTRAN programming language is available from the JINA collaboration and a C++ version, AZURE2, has recently become available.

*Purpose* The detailed mathematics and extensive programming required to implement broadly applicable R-Matrix codes make comparisons between different codes highly desirable in order to check for errors. This paper presents a comparison of the three codes based around data and recent results of the astrophysically important $^{18}F(p,\alpha)^{15}O$ reaction.

*Methods* Using the same analysis techniques as in the work of Mountford et al. parameters are extracted from the two JINA codes, and the resulting cross-sections are compared. This includes both refitting data with each code and making low-energy extrapolations.

*Results* All extracted parameters are shown to be broadly consistent between the three codes and the resulting calculations are in good agreement barring a known low-energy problem in the original AZURE code.

*Conclusion* The three codes are shown to be broadly consistent with each other and equally valid in the study of astrophysical reactions, although one must be careful when considering low lying, narrow resonances which can be problematic when integrating.



## 1. Introduction

The field of nuclear astrophysics relies on the determination of low energy cross-sections from which the reaction rates important for nucleosynthesis are derived. In most cases, it has proved to be quite difficult to meet the desired level of accuracy for these reactions. This is primarily because, in the relatively low energy region of interest for thermonuclear reactions, cross-sections are suppressed by the Coulomb barrier making direct measurements difficult. Instead, measurements are often performed at higher energies where the cross-sections are correspondingly larger. These higher energy cross-sections must then be extrapolated down to the energies relevant for nucleosynthesis environments.

The R-Matrix formalism was generalised in the seminal work of Lane and Thomas [1]. The framework has proved indispensable for describing the cross-sections of reactions of interest to nuclear astrophysics, and is particularly useful for interfering broad resonances in low level density systems. Interfering or overlapping resonances in such a system render single resonance approximations invalid, and the R-matrix formalism provides a more robust solution. The theory parameterizes cross-sections in terms of the level properties of the compound nucleus by matching the nuclear force to the Coulomb force at the limit of its effect. Either the formal parameters of the theory [1] or the observed on-resonance parameters [2] may be used to calculate the cross-section.

The complexity of the formalism warrants the writing of computational codes for implementation. One such code is the AZURE code developed by a Joint Institute for Nuclear Astrophysics (JINA) collaboration [3]. The open source code, written in the FORTRAN programming language, is publicly available [4].

In parallel, several recent works on the study of the $^{18}F(p,\alpha)^{15}O$ reaction [5–7] have implemented a dual channel R-Matrix code

* Corresponding author. Present address: National Nuclear Laboratory, Central Laboratory, Sellafield, Seascale, Cumbria CA20 1PG, UK.
*E-mail address:* d.j.mountford86@gmail.com (D.J. Mountford).

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written by Descouvemont and known as DREAM, employing Visual Basic macros within the framework of Microsoft Excel. A summary of the mathematics used is given in the work of Descouvemont and Baye [8] and a recent work by Mountford et al. [7] on the astrophysically important $^{18}$F(p,$\alpha$)$^{15}$O reaction is an example of its use within a complicated system comprising entrance channels with non-zero intrinsic spin, various angular momentum transfers and a number of narrow and broad resonances.

A new implementation of the JINA collaboration's R-Matrix code, AZURE2, has recently been developed. This open source code has been written in the C++ programming language and allows multiple entrance channel analysis with a much improved user interface. In addition, mathematical processes are now performed using modern computational libraries such as the GNU Scientific Library (GSL) for differentiation [9].

It is very useful, and important for overall comparison of R-matrix parameters, to critically compare the results of the different codes so that any discrepancies may be discovered and corrected. Such discrepancies can arise, for example, through the choice of numerical algorithms or the treatment of mathematical operations in the transformation between formal R-matrix and physical parameters. Hence, the aim of the present work is to use the experimental data of Mountford et al. [7] to check the consistency between the different R-matrix codes.

## 2. Theoretical background

The R-matrix formalism was introduced in 1948 by Wigner and Eisenbud [10] and was generalised for use in the study of nuclear reactions by Lane and Thomas in 1958 [1], with Barker and Warburton including the capability to consider $\beta$-decay in 1988 [11] and Barker and Kajino [12] adding radiative capture treatment in 1991. The formalism has developed further since, with Brune introducing an alternative parameterisation in 2002 [2] making the theory more directly related to experimental observations.

This evolution over time leads us to the complex formalism used today for the interpretation of experimental nuclear physics data. This complexity and the success of the formalism has led to the development of standard computer codes which are now used extensively in the study of nuclear reactions.

The formalism is well described by papers associated with the three codes to be investigated in this paper. The theory behind the extraction of parameters from the DREAM code is described in the work by Descouvemont, who developed the code, and Baye [8] while the calculations in the original AZURE code are described in Azuma et al. [3]. The new code developed by the JINA group, AZURE2, follows the same processes.

These three codes are consistent in their calculation of the R-matrix and scattering matrix. Despite differing methods of calculation of spin-coupling coefficients, the values extracted have also been observed to be consistent. For this spin-coupling, AZURE makes use of existing FORTRAN code, while AZURE2 makes use of the GSL 3j and 6j functions [9]. The Visual Basic code has a built in function for the calculation of Clebsch-Gordan, Racah and 6j coefficients which are then combined to calculate the total angular coupling coefficients.

The Coulomb wavefunctions, also critical to the calculation of the final cross-section, are calculated in AZURE through legacy FORTRAN code using several approximations, while AZURE2 uses the routines published in the work of Michel [13]. Finally DREAM makes use of the well-tested Barnett method [14]. The reaction cross-section is fully derived in Lane and Thomas [1].

Furthermore, the three codes use slightly different minimization routines. AZURE uses the original MINUIT [15] code, while AZURE2 uses the updated C++ MINUIT2 [15]. Again, DREAM has its own function for the minimization procedure, based on the Marquardt Method [16].

## 3. Previous analysis

The work of Mountford et al. [7] on the $^{18}$F(p,$\alpha$)$^{15}$O reaction extracted experimental parameters from new experimental data using the Visual Basic R-Matrix code of Descouvemont. These calculations were based upon previous spin-parity assignments reported in the review paper of Nesaraja et al. [17] and the more recent works of Murphy et al. [5] and Dalouzy et al. [18]. The main result of the work was the observation of a predicted broad *s*-wave resonance at $E_{c.m.}=1.455$ MeV [19], consistent with the measurement of Dalouzy et al. [18] and the recent work of Adekola et al. [20]. A 2013 study by Laird et al. [21] has further re-assigned the spin and parity of some low energy resonances, stimulating further interest in this reaction.

An experiment was carried out where a secondary $^{18}$F beam ($J^{\pi}=1^{+}$), produced by bombarding a thick carbon target with a 95 MeV/A primary $^{20}$Ne beam, was degraded from 4 MeV/u to $\sim$2 MeV/u and impinged upon a thick polyethylene target. Emitted protons and $\alpha$-particles were then detected in a 50 mm $\times$ 50 mm double sided silicon strip detector positioned downstream on the beam axis. For a more complete description of the experimental setup, the interested reader is referred to the work of Mountford et al. [7].

This allowed center of mass excitation functions to be extracted for both the $^{18}$F(p,$\alpha$)$^{15}$O and $^{18}$F(p,p)$^{18}$F reactions. The cross-sections were then normalized to the most well-known resonance in the $^{18}$F+p system, at a center of mass energy of 665 keV [22], to provide an absolute cross-section calculation across the center of mass energy range. The extracted spectra were then entered into DREAM. The analysis initially assumed the nuclear level parameter assignments from a review by Nesaraja et al. [17] and more recent published works by Murphy et al. [5] and Dalouzy et al. [18]. An iterative technique was then adopted that explored modifications to the parameter set driven by improved matching between the experimental data and the R-Matrix-calculated cross-section. The final extracted parameters are discussed at length in Mountford et al. [7] and presented in Table 1.

## 4. AZURE analysis

R-Matrix calculations made with the parameters of Mountford et al. [7], using the two JINA codes, were found to show excellent agreement in the calculated cross-section of the $^{18}$F(p,$\alpha$)$^{15}$O reaction, for both individual partial waves and combinations of all partial waves bar one; an alternative relative interference between the $J^{\pi}=1/2^{+}$ and $J^{\pi}=5/2^{+}$ partial waves was observed. Reversing this relative interference gave a consistent calculation. This discrepancy was attributed to the Coulomb contribution being omitted in the cross-section calculation of the Visual Basic code. Such a difference only occurs in the case of broad low-angular momentum partial waves and had consequently previously been missed. The broad nature of the $J^{\pi}=1/2^{+}$ resonance has brought this discrepancy to our attention. As a result, the observed *s*-wave state requires the opposite interference term relative to the $J^{\pi}=5/2^{+}$ resonances and the resulting differential cross-section calculations are then in excellent agreement. It should be noted that the integrated cross-section, however, is unaffected by interference effects between different $J^{\pi}$ groups and so the astrophysical implications of Mountford et al. [7] are unaffected.

**Table 1**
Tabulation of results presented in Mountfoord et al. [7], with the corresponding parameters extracted by the JINA FORTRAN (AZURE) and C++ (AZURE2) codes. $J^\pi$ values are unchanged while a discrepancy arising in the relative interference between states is discussed in the text. An asterisk denotes a parameter which is not well constrained by the data and so no uncertainty could be extracted.

| Mountford et al. [7] | | | | AZURE results | | | AZURE2 results | | |
|---|---|---|---|---|---|---|---|---|---|
| $E_{c.m.}$ (MeV) | $J^\pi$ | $\Gamma_p$ (keV) | $\Gamma_\alpha$ (keV) | $E_{c.m.}$ (MeV) | $\Gamma_p$ (keV) | $\Gamma_\alpha$ (keV) | $E_{c.m.}$ (MeV) | $\Gamma_p$ (keV) | $\Gamma_\alpha$ (keV) |
| 0.665 | $\frac{3}{2}^+$ | 15.2 | 23.8 | 0.665 | 15.2 | 23.8 | 0.665 | 15.2 | 23.8 |
| 0.759(20) | $\frac{3}{2}^+$ | 1.6(5) | 2.4(6) | 0.755(77) | 1.7(17) | 3.3(33) | 0.756(2) | 1.7(17) | 1.1(5) |
| 1.096(11) | $\frac{5}{2}^+$ | 3(1) | 54(12) | 1.097(29) | 3.3(20) | 71(45) | $1.096(^{+42}_{-63})$ | $3.4(^{+34}_{-29})$ | $71(^{+71}_{-63})$ |
| 1.160(34) | $\frac{3}{2}^+$ | 2.3(6) | 1.9(6) | 1.149(14) | 2.5(25) | 2.1(21) | 1.156* | 4.5* | 1.1(4) |
| 1.219(22) | $\frac{3}{2}^-$ | 21(3) | 0.1(1) | 1.211(17) | 27(17) | 0.2(2) | 1.210(5) | $20(^{+12}_{-2})$ | 0.1(1) |
| 1.335(6) | $\frac{3}{2}^+$ | 65(8) | 26(4) | 1.339(23) | 65(13) | 31(27) | 1.338(20) | 59* | $30(^{+19}_{-23})$ |
| 1.455(38) | $\frac{1}{2}^+$ | 55(12) | 347(92) | 1.50(18) | 44(23) | 310(150) | $1.486(^{+55}_{-48})$ | 44(9) | 304(66) |
| 1.571(13) | $\frac{5}{2}^+$ | 1.7(4) | 12(3) | 1.569(30) | 1.7(12) | 8(6) | 1.570(2) | 1.8(18) | $6(^{+3}_{-6})$ |

Upon applying the above correction, the same data were then fitted using the same procedure as in Mountford et al. [7] to extract parameters. The spin and parity assignments assumed from the review paper by Nesaraja et al. [17] remain valid and the results are presented in Table 1.

## 5. Uncertainty analysis

The code used by Mountford et al. [7], DREAM, extracts parameter uncertainties from the covariance matrix as described in Descouvemont et al. [23], relying on a diagonal covariance matrix for accurate calculations of parameter uncertainties. A non-diagonal covariance matrix, as often occurs, results in the quoted uncertainties not providing a complete solution unless simultaneously presented with the full covariance matrix.

As noted in Ref. [23], the parameter uncertainty estimates calculated by DREAM are underestimated when the minimum $\overline{\chi}^2$ is greater than 1; the suggested procedure for correction to the uncertainties has been applied, *i.e.* the error bars on data points are increased to give the best fit solution a $\overline{\chi}^2 = 1$ and, the error analysis procedure was performed. The errors extracted are presented with their parameters in Table 1. For a full discussion of the parameters extracted and their uncertainties in relation to the covariance matrix, the interested reader is referred to Mountford et al. [7].

The AZURE error analysis is carried out by the MINOS package within CERN's MINUIT [15], where the code searches the parameter space for the $\chi^2 + \Delta\chi^2$ contour and $\Delta\chi^2$ is defined as the $1\sigma$ confidence limit as in Descouvemont et al. [23]. For this case $\Delta\chi^2 = 23.5$ for 24 free parameters. The uncertainty on the broad $J^\pi = 1/2^+$ resonance energy was extracted from AZURE independently of the other parameters in order to constrain its effect within the limits of the experimental.

The resulting parameters extracted from the different codes are, mostly, within $1\sigma$ of one another, implying a consistency between the fitting mechanisms and R-Matrix calculations of the Visual Basic code, AZURE and AZURE2. The more extensive error analysis of AZURE and AZURE2 has resulted in larger uncertainties on most of the extracted parameters, as expected [15], except for in the case of the final resonance which has a very small uncertainty, most likely due to the narrow width and, hence, well-defined energy.

As an aside, if an error bar becomes too large, the C++ version of MINOS assumes that the parameter in question is unconstrained by the available data and, therefore, no uncertainty can be extracted. These parameters are marked with an asterisk in the table.

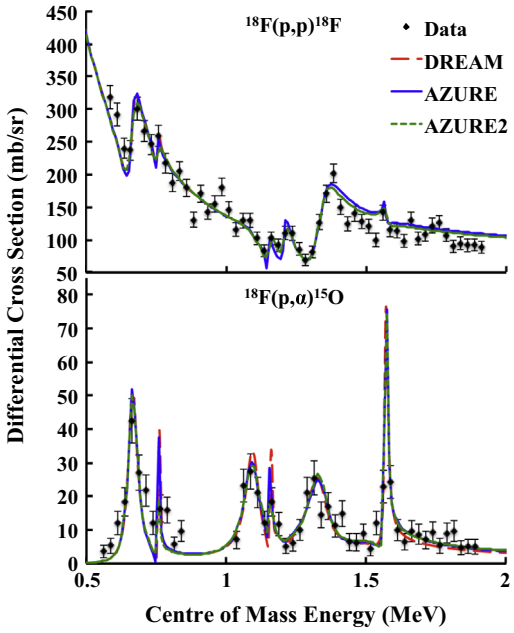


**Fig. 1.** The cross-sections from the fit to the data of Mountford et al. ($\overline{\chi}^2 = 1.634$) by DREAM (red long-dashed lines), the AZURE code ($\overline{\chi}^2 = 1.435$) of the JINA collaboration (blue solid lines) and the AZURE2 code ($\overline{\chi}^2 = 1.569$) of the JINA collaboration (green short-dashed lines). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

Furthermore, it should be noted that a complete error analysis would include systematic errors and R-matrix model space considerations. That is to assess contributions such as open channels and resonances to be included while also varying the channel radius to obtain a complete uncertainty analysis.

## 6. Calculation of resulting cross-section

The resulting cross-section calculated from these parameters by each program is presented in Fig. 1 and is shown to be consistent. Insignificant discrepancies remain due to some minor differences in the calculation process, such as AZURE2 requiring that the resolution be fixed across all energies while it can be allowed to vary linearly in DREAM. For example, the experimental resolution was found to vary from 3 to 5 keV in this $^{18}$F(p,p)$^{18}$F measurement and 7–13 keV in the $^{18}$F(p,$\alpha$)$^{15}$O measurements, and so the average values, 4 keV and 10 keV respectively, were taken for the AZURE calculations. Due to the strong agreement, it is

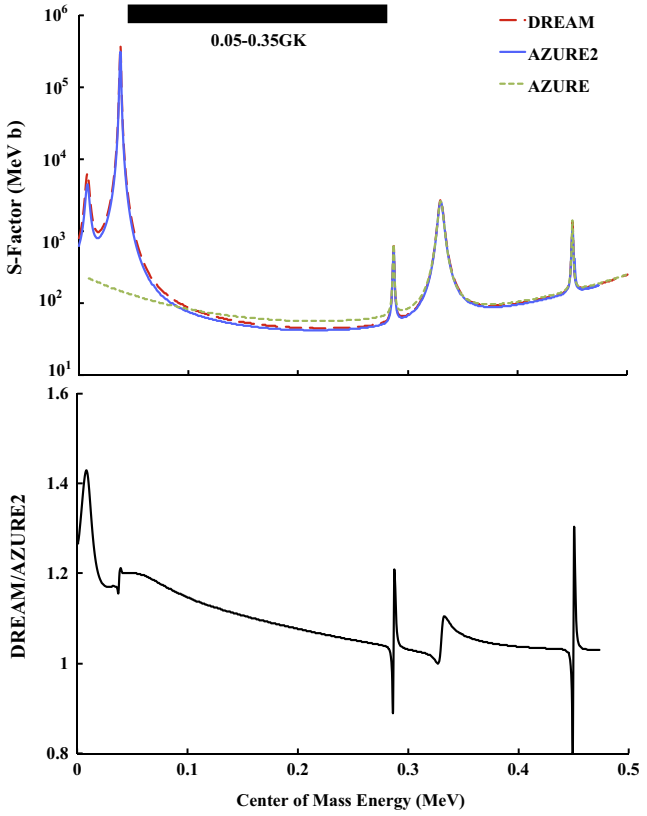


**Fig. 2.** Top panel:Astrophysical S-factor of the $^{18}$F($p$,$\alpha$)$^{15}$O reaction based on the parameters of Iliadis et al. [24] as calculated by DREAM (red long-dashed line), AZURE (green dashed line) and AZURE2 (blue solid line). Bottom panel: The ratio of the DREAM output to the AZURE2 output. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

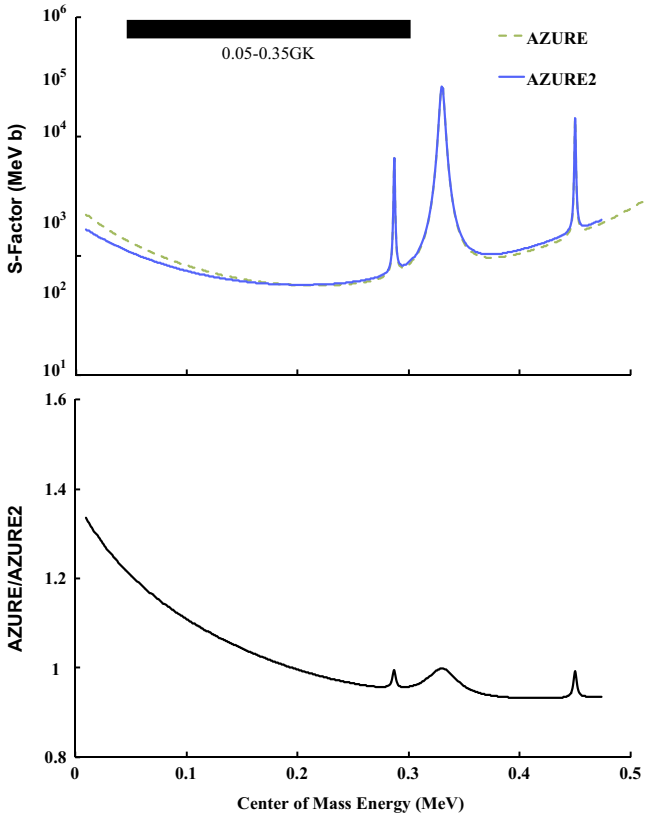


**Fig. 3.** Top panel: Astrophysical s-factor of the $^{18}$F($p$,$\alpha$)$^{15}$ O reaction based on the parameters of Iliadis et al. [24] as calculated by AZURE (green dashed line) and AZURE2 (blue solid line). The lowest energy resonances have been removed as they are too narrow to be included in the calculation by AZURE. Bottom panel: The ratio of the AZURE output to the AZURE2 output. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

difficult to distinguish between the calculations of each code shown in Fig. 1.

One of the plots presented in Fig. 4 from Mountford et al. [7] is reproduced in Fig. 2. In this figure, the astrophysical $S$-factor of the $^{18}$F(p,$\alpha$)$^{15}$O reaction in the temperature region of interest for nova explosions is plotted based on recommendations made by Iliadis et al. [24], which includes a sub-threshold resonance. There are a range of possible $S$-factors in the region of interest due to the alternative interference effects between two $3/2^+$ resonances, although only the case of constructive interference is shown in this work. It should be noted also that resolution effects are omitted in the calculation of the astrophysical s-factor presented in Fig. 2. The resulting plots, shown in Fig. 2, show good agreement between DREAM and AZURE2 despite some narrow discrepancies around resonances.

The three resonances at low energy in the S-factor calculation feature proton widths of $10^{-11}$ eV or less. The numerical precision of the AZURE code is, unfortunately, limited when transferring from physical parameters to R-matrix parameters, such that any widths below $10^{-10}$ eV cannot be processed. Therefore, to illustrate the consistency between all other aspects of the calculation, the treatment of sub-threshold resonances most importantly, AZURE and AZURE2 calculations are given in Fig. 3. These plots are in very good agreement above $E_{cm}$=0.2 MeV, generally varying from each other by around 5%. As the energy decreases, an increasing divergence is observed between the calculations because of inaccurate numerical derivatives of the Whittaker functions in AZURE. This affects the transformation of Asymptotic Normalisation Coefficients (ANCs) [25] to reduced widths for levels that are close to threshold (see Eqs. 31, 33, and 34 of Azuma et al. [3]). In this case the proton ANC for the broad level ($\Gamma \sim 231$ keV) at $E_x$=6.001 MeV ($J^\pi = 1/2^+$), ~0.4 MeV from threshold ($S_p$=6.411 MeV) is not transformed correctly resulting in a difference in the energy dependence. It should be noted here that these discrepancies lie in the transformation between parameters and not in the cross-section calculation itself, which remains consistent. Aside from the issues with levels near threshold using AZURE, there is good consistency between the three codes.

## 7. Conclusions

The R-Matrix formalism is an extremely important tool in the study of nuclear astrophysics, both in extraction of experimental parameters from data and extrapolation of cross-sections to an experimentally challenging region. Three codes used to implement the formalism have been tested through the analysis of data obtained in the study of the astrophysically important $^{18}$F(p,$\alpha$)$^{15}$O reaction [7]. Given the importance of using adequate analysis techniques, it has been demonstrated that the parameters extracted from these codes are broadly consistent and cross-section calculations are, for the most part, consistent. One must use caution when making calculations at energies close to reaction thresholds, as shown in Figs. 2 and 3 and the associated text. These minor discrepancies should be considered when integrating to obtain reaction rates. AZURE2 has addressed many of the limitations of the AZURE code such that the agreement with DREAM is much improved, as such it is shown that AZURE2 has now superseded the original AZURE code.

The broad agreement between cross-section and $S$-factor calculations, and the consistency between extracted resonance parameters are welcome developments for research in this area.

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