Surrey R-matrix mini-school: AZURE2 tutorial

May 9, 2013

School:	http://www.nucleartheory.net/NPG/Minischool_R-Matrix/index.htm
AZURE:	http://www.nd.edu/~azure
JINA:	http://www.jinaweb.org/events/matrix/lectures.html
NNDC:	http://www.nndc.bnl.gov/
TUNL:	http://www.tunl.duke.edu/nucldata/
IBANDL:	http://www-nds.iaea.org/exfor/ibandl.htm
EXFOR:	http://www-nds.iaea.org/exfor/exfor.htm
UNIX:	http://www.ee.surrey.ac.uk/Teaching/Unix/

1 Introduction and setup

The goal of this tutorial is to familiarise you with R-matrix analysis techniques, the relevant nuclear physics input and the general procedures behind making an R-matrix fit. Here we use the AZURE code, developed under support of the US Joint Institute of Nuclear Astrophysics (JINA). Specifically, we will use the C++ version AZURE (currently in beta-testing). The FORTRAN version is available on the AZURE website to registered users and has a similar graphical user interface. The two version have essentially the same capabilities [1]. The experienced gained should be generally applicable to other R-matrix codes that essentially all implement the same physical model [2, 3].

This tutorial will take you through the steps for setting up an R-matrix calculation with AZURE, running the calculations, fitting to data and interpreting the output. Since each calculation requires multiple input files and produces multiple output files, it is best to keep a separate directory for each analysis (i.e. set of calculations with a single compound nucleus).

Task 1: *Run shell script to set path and copy files.*

To run the codes you first need to type couple of commands in the terminal to make sure you have access. First, open a terminal via Applications > Accessories > Terminal. Then type

```
csh /user/phstf/es0011/azurebin/setup.sh
```

```
source .cshrc
```

These commands will add the executable to your path and copy over a number of prepared examples (directories and data files). You should now find a folder `azure2` in your home directory, within which should be a subfolder for each example, listed below.

Folder	Compound	Reactions
`o16`	^{16}O	$^{12}\mathrm{C}(\alpha,\alpha)^{12}\mathrm{C}$
`n14`	^{14}N	$^{13}\mathrm{C}(p,p)^{13}\mathrm{C}$
`mg22`	^{22}Mg	$^{21}\mathrm{Na}(p,p)^{21}\mathrm{Na}$

Within each directory you will find directories called `checks`, `data` and `output`. The first and the last of these will be empty, but the `data` directory will contain files containing the scattering and reaction data relevant to each example. These have been prepared for use with AZURE, though the format is relatively simple (see Appendix A). The first example will be considered in detail and forms the main part of the tutorial. The other examples may then be tackled or, if you have data of your own, feel free to start analysis on any case you like. In addition you should find a PDF version of this tutorial.

2 $^{12}\mathrm{C}(\alpha,\alpha)^{12}\mathrm{C}$

2.1 Configuration

We start with elastic scattering of alpha-particles on carbon-12, or $^{12}\mathrm{C}(\alpha,\alpha)^{12}\mathrm{C}$. In this case the compound nucleus will be ^{16}O. A level and threshold diagram can be found at the TUNL Nuclear Data website, also shown in Fig. 1.

^{12}C alpha-scattering is simple for a number of reasons. Firstly, the ground state spins of both ^{12}C and the alpha are both 0^+. This means that (a) only a single channel will contribute for each resonance state, with the resonance angular momentum equal to the channel spin $J = \ell$, and (b) only natural parity resonances, with $\pi = (-1)^\ell$ may be populated. Secondly, the α-particle-pair is the only one open - the only one energetically allowed - at the energies of interest here. Together, these facts mean each resonance is determined by just the resonance energy and a single width.

Task 2: *Open AZURE2 and set the output directories.*

The AZURE2 code has a graphical user interface (GUI) that allows you to set up, run and view the results of required calculations. Building the code from source requires certain external libraries: Qt, QWT, GSL and MINUIT2. Here, AZURE2 has been already compiled and installed on the local machines. If you haven't already, move into the `o16` directory by typing `cd o16` and then run the program by typing `AZURE2`. The AZURE2 GUI window should open.

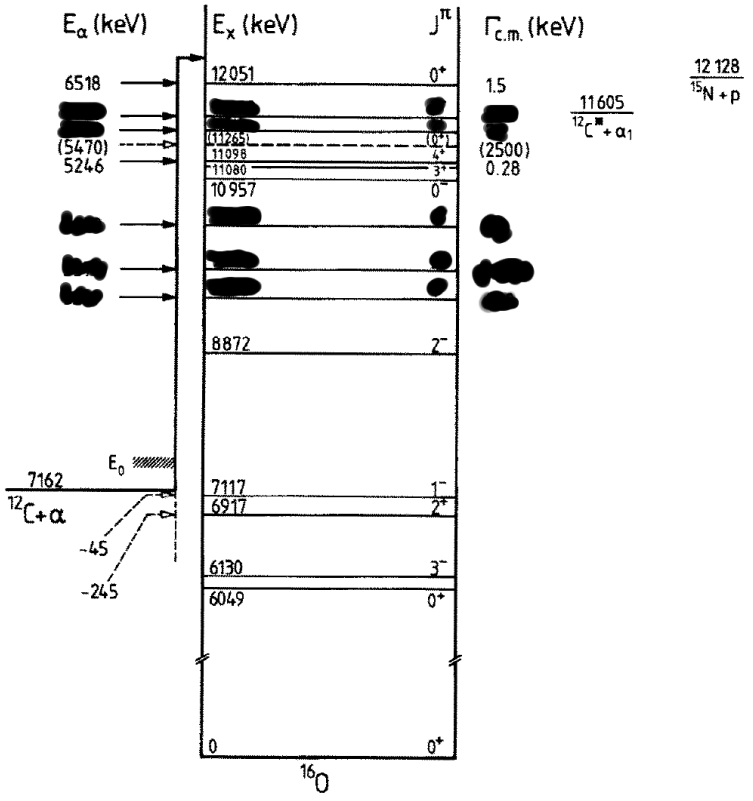

Figure 1: Energy level schematic for the ^{16}O compound nucleus (taken from Plaga *et al.* [4]). (States used later in the tutorial have had their properties redacted!)

The GUI consists of a number of tabs that let you edit the input files, run calculations and view the results. The first thing to do is configure the output directories. Click Configure > Directories, and the window shown in Fig. 2 will open. This allows us to set where the output and checking files will go. Add in "output" and "checks" where appropriate.

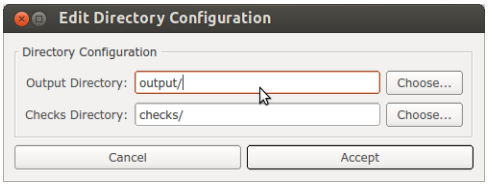

Figure 2: Configure directories.

2.2 Particle pairs

On the Particle Pairs tab, shown in Fig. 3, the properties of the different particle pairs involved in the reactions of interest can be defined. The reactions of interest themselves are later defined when data is added to the calculation - each set of data is assigned an initial and final particle pair. For the present case, we need only define the ^{12}C+α particle pair.

Task 3: *Add the ^{12}C+α particle pair to the compound nucleus.*

Particle pairs can be added or removed by clicking the plus and minus buttons in the bottom left-hand corner. Clicking the plus button opens the add particle pair screen, shown in Fig. 4. Boxes for the light and heavy particle are shown. Fill in the spin J, parity, mass M and charge Z for each particle. The g-factor or dimensionless magnetic moment is relevant for very particular particle capture reactions, and for the present can be left at zero. Next fill out the channel properties. The excitation energy (e.g., excitation of final state in ^{12}C) here is zero. The separation energy is the energy used to separate the ground state of the compound nucleus into the light and heavy particle defined by this particle pair. Separation energies for protons and neutrons are widely tabulated. Others can be calculated from the respective masses, taken from the TUNL energy level diagrams, or by finding the Q-value for the related light-particle capture reaction (x, γ) (see e.g., at the NNDC Q-value calculator). Finally, the channel radius should be set, typically $a = 1.4(A_1^{1/3} + A_2^{1/3})$. In principle the final fits should be independent of the channel radius chosen, though this should always be checked. The result should look like Figs. 4 and 4 (except perhaps for minor differences in the channel radius).

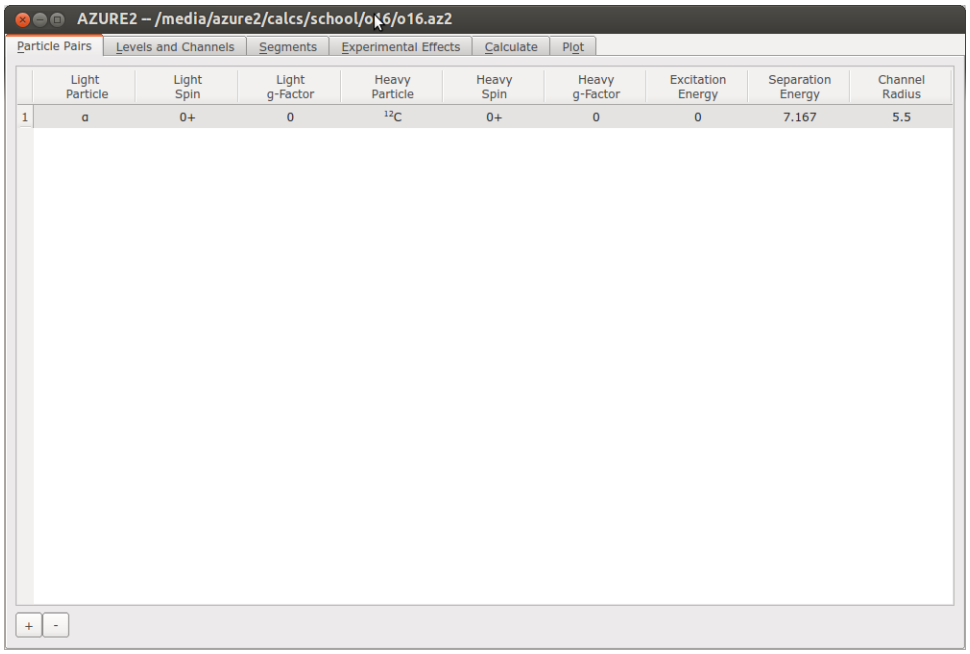

Figure 3: Particle pairs tab.

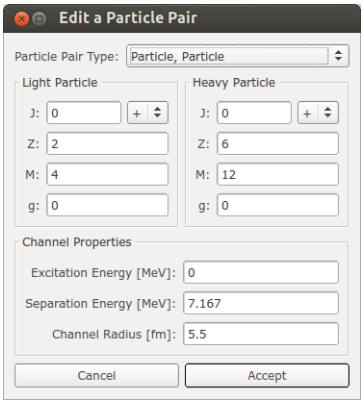

Figure 4: Add particle pairs screen.

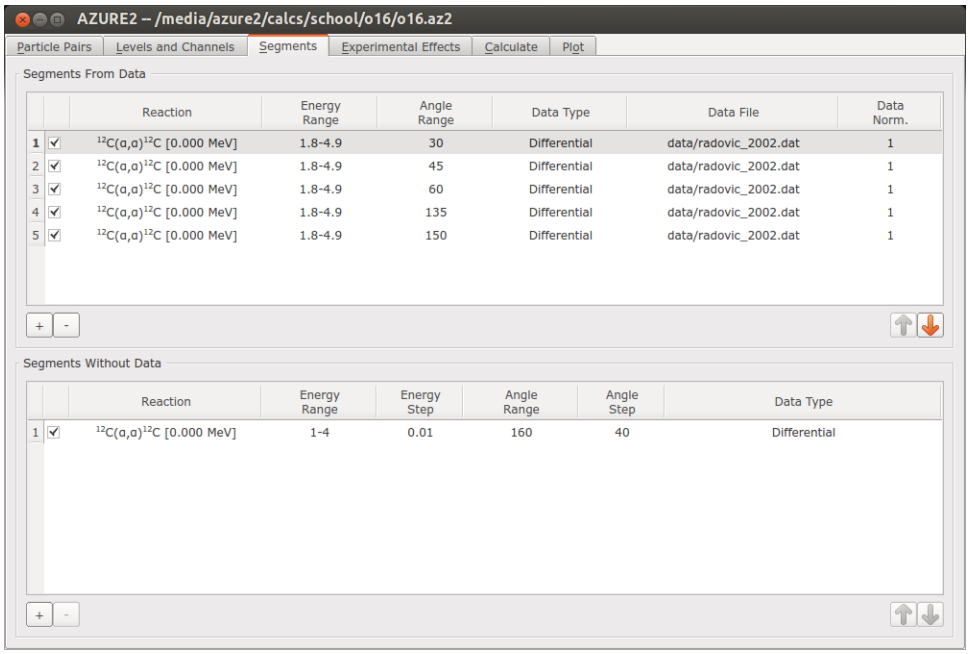

Figure 5: Data segments tab.

2.3 Data segments

AZURE divides the input data into segments. A segment represents a series of data points, usually from one specific source, and usually at either a single angle for a range of energies (a yield curve), or a range of angles for a single energy (an angular distribution). The GUI makes these very easy to add and edit. Clicking on the Segments tab should show something similar to Fig. 5. Sometimes it is useful to have a single data point present in two different segments. For example, when fitting scattering data, it might be convenient to have segments for angular distributions at particular energies, as well as yield curves at different angles. The segments concept allows for this, but in any fitting you must ensure sure any given data point appears only once. Including more than once would mean that the error bar for the data point is artificially reduced.

Task 4: *Add the data files for the Bogdanovic-Radovic data set.*

Here we (initially) consider only a single data set, from Bogdanovic-Radovic *et al*[5]. The data we will use here is provided in a format already compatible with AZURE2, in a file name `radovic_2002.dat`. This single file contains data covering laboratory energies of 1.8-4.9 MeV, at laboratory angles 30, 45, 60, 135 and 150 degrees. We will divide this data into five segments, one for each of the five angles. (See Appendix A at the end of the tutorial for information on the precise data format required.)

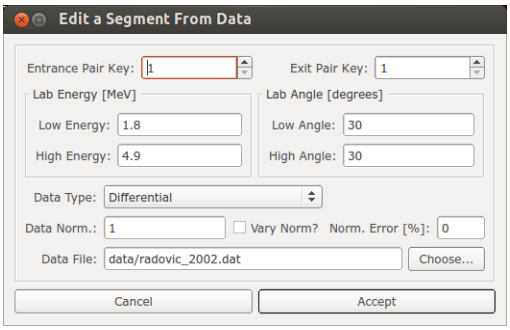

Figure 6: Data segments tab

Data segments can be added by clicking the plus and minus buttons in the bottom half of *the upper half of the tab*. The add data segment should open, shown in Fig. 6. If the pop-up looks different to this, check you clicked the plus button in the *upper half* of the window. The controls in the lower half are there for controlling the extrapolation segments.

First set the entrance and exit particle pairs. These numbers refer to the particle pairs defined on the Particle Pairs tab. In this case we have only one and the entrance and exit particle pairs are the same. Set the low and high energies to 1.8 and 4.9 MeV respectively. Next, change the Data Type drop-down-list to Differential - this tells AZURE that the segment is differential with respect to the angle θ. This then allows us to fill in the low and high angles; set these both to 30. Leave the Data Norm at 1 and the Norm Error at 0. Finally, type `data/radovic_2002.dat` into the Data File box. Click Accept to finish. The segment should appear in the upper panel. Now repeat the above sets to create data segments for the other four angles (45, 60, 135 and 150 degrees). You should finish up with five segments. Note that in the segments list each of the segments has a checkbox on the left-hand side, that determines if a particular segment is included in the calculation. This is very useful when there are many segments or where some segments contain the same data points (i.e. yield curves and angular distributions).

2.4 Levels and channels

Before running any calculation we need to add some levels to our compound nucleus. These can be added on the Levels and Channels tab, shown in Fig. 7. The screen consists of three columns. From left to right, these will list (i) the compound nucleus levels, (ii) the allowed channels for a given level, and (iii) the details of a particular channel.

Task 5: *Add levels to the compound nucleus.*

Because of the way AZURE is designed, you *must* manually add a resonance for each allowed $J^\pi$when you're considering elastic scattering data. The primary purposes is that all appropriate hard-sphere scattering terms will then be included. If placed above the energy window

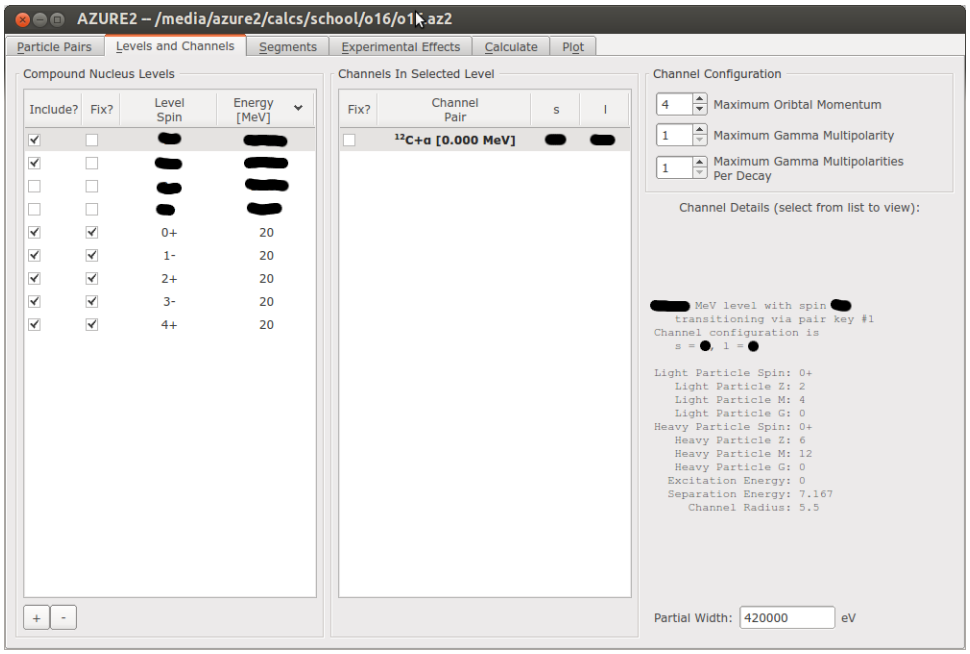

Figure 7: Levels and channels tab.

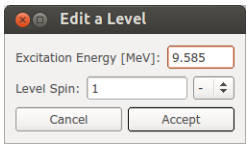

Figure 8: Add a level.

of interest, these resonances can be also be used as background resonances if required, either to mimic the effect of higher-lying resonances or, in the case of elastic scattering, to improve the description of the non-resonant hard-sphere scattering.

Start by adding background resonances with zero widths for each J^π. They should be ~ 5 MeV above the energy range of interest. The energies specified are excitations in the compound system, so for this case place these background resonances at 15 MeV. To add a level click the plus symbol in the bottom left-hand corner of the tab. The Add Level window should pop up. Edit the spin, parity and energy to add a 0^+ state at 15 MeV. Click Accept to finish. To edit a resonance, double click on the entry in the left-hand column.

We need to add resonances for the other spin parities, but first we investigate this resonance further. If we left-click on the entry in the left hand column, the allowed channels should appear in the central column. The allowed channels are automatically determined by AZURE according to angular momentum coupling rules and by the limits set in the top right-hand corner of this screen. Here we can adjust the maximum orbital (channel) angular momentum

Calculate segments from data	Runs the R-matrix calculation without fitting resonance parameters. Fast, and useful for establishing a good initial parameter set.
Fit segments from data	Use MINUIT to fit all resonance energies and widths (aside from those zeroed and specifically fixed) to obtain the best fit to the data via χ^2 minimistion. The fitting time and the quality of the final fit are sensitive to the starting parameter set.
Calculate segments without data	Perform an extrapolation based on the current input parameter set and the defined extrapolation segments.
Perform MINOS error analysis	Use the MINOS component of MINUIT to investigate sensitivity of input parameters (used after best fit obtained)
Calculate Reaction rate	Calculate the astrophysical reaction rate for the calculated cross section (computationally demanding, particularly for capture reactions with external contributions).

Table 1: List of calculations types.

ℓ, the maximum gamma multipolarity L and the maximum number of allowed gamma-decay multipolarities per level. Here, change the allowed channel angular momentum to 4. Then, clicking on one of the channels shows further details in the lower half of the right-hand column. Below this, a text box is shown where you can change the partial width Γ_c (in units of eV) for this channel. For now, leave this width at zero.

Note the various columns headed Include? and Fix?. The Include? checkbox sets where a resonance will be included in the calculation. Unchecking this box is an easy way to temporarily remove a resonance from a calculation. This can be useful when trying to understand the interferences of broad resonances for instance. The Fix? checkbox fixes a particular parameter when a fit is made. This is useful for reducing the number of free parameters in a fit or where particular parameters are taken from the literature.

2.5 First calculations and plotting

Task 6: *Run the first calculation and look at the results.*

We are now in a position to perform the first calculation. Click on the Calculate tab. There are multiple types of calculation AZURE can perform, selectable in the drop-down list labelled Calculation type, and these are listed in Table 1.

Make sure Calculate segments from data is selected click Save and Run. The calculation will run and present some information in the text box, including progress on the calculation and the final χ^2 for each of the segments.

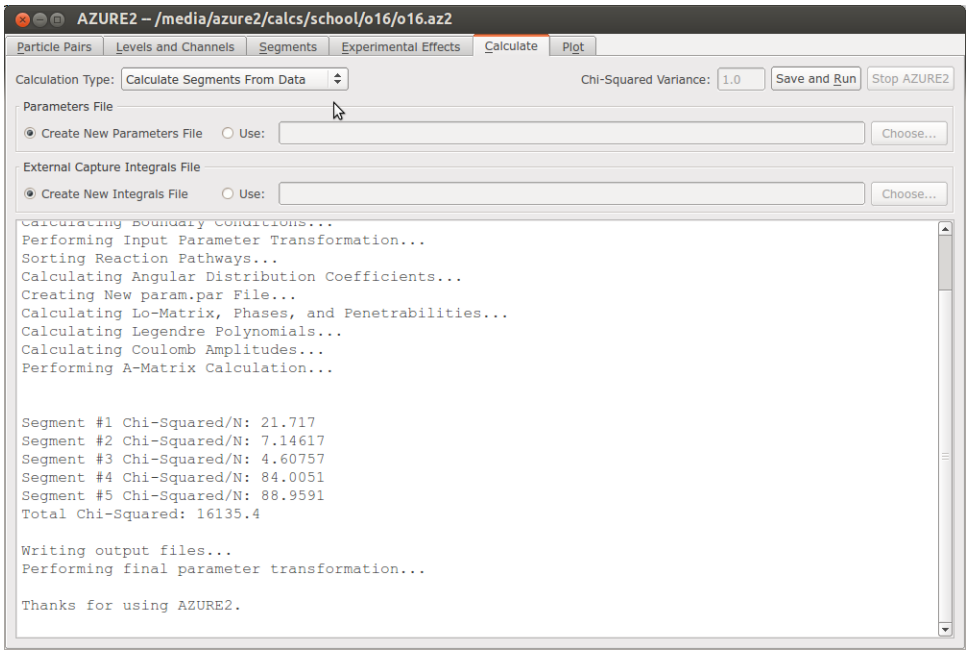

Figure 9: Calculate tab.

The results of the calculation are output (in the centre-of-mass system) to files in the `output` directory. The resonance parameters of the final fit can be found in the file `parameters.out` in that directory. For the present calculation these are just the input parameters, but if a fit had been performed they would be different. A full list of the output files can be found in Table 2.

Once the calculation is finished, click on the Plot tab. This allows us to plot the results for each individual segment as a function of the centre-of-mass energy, the compound nucleus excitation energy, or light-particle exit angle. You should see a list of five data segments in the top-left box. Select the first and last data segments and then click Draw in the bottom left-hand corner. The resulting graph should look like that shown in Fig. 10. The calculation

`parameters.out`	Final transformed resonance parameters.
`param.par`	Initial parameter list sent to MINUIT.
`param.sav`	Final parameter list from MINUIT.
`chiSquared.out`	Lists final χ^2 for each data segment.
`AZUREOut_aa=X_R=Y.out`	Output data and calculations for entrance particle pair X and exit particle pair Y.
`AZUREOut_aa=X_R=Y.extrap`	Extrapolations for entrance particle pair X and exit particle pair Y.

Table 2: Output files (all found in the output directory).

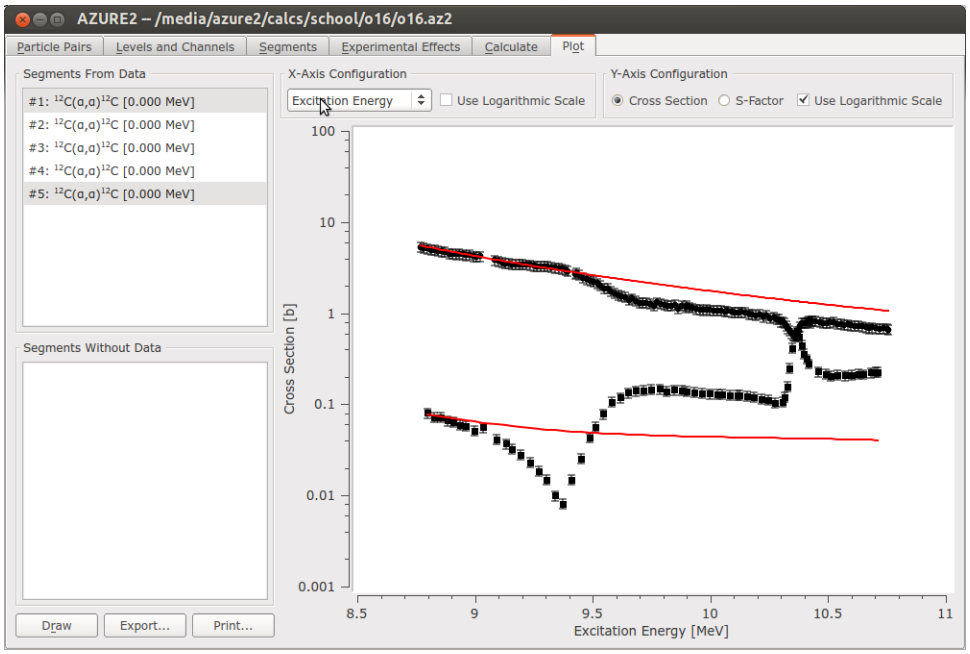

Figure 10: First results - Coulomb and $\ell = 0$ hard-sphere.

essentially just includes the Coulomb (Rutherford scattering) and $\ell = 0$ hard-sphere scattering contributions, but this looks like a good start.

However, these results do not contain all the possible hard-sphere contributions, as we've only added in a single $J^\pi = 0^+$ resonance. Go back to the Levels tab and add in resonances at the same energy as the 0^+ state for each of the natural parity cases - 1^-, 2^+, 3^- and 4^+, and check the Fix checkbox to fix their energies (useful for later fitting). Then go back to the Calculate tab and re-run the calculation. You might notice that the χ^2 values change marginally. If you then go back to the Plotting tab, the previous calculation is still displayed. The plot will not change until you click Draw. Do so now, and note how the red calculation changes slightly due to the additional hard-sphere components. In general the significance of the hard-sphere component will increase for higher energies and backward angles. Later, we will use the levels we've just added as background resonance contributions, but for now leave their widths set at zero.

2.6 Adding resonance states

> **Task 7**: *Using the Plotting tab, identify any resonances and estimate their (a) energy in laboratory system for incident α particles E_R, (b) energy in the centre-of-mass of ^{12}C+α E_{cm}, and (c) excitation energy in the compound nucleus E_x.*

One handy feature of the AZURE2 plotting tab is that the data can be plotted either by centre-of-mass energy, or by excitation in the compound nucleus. By plotting by excitation

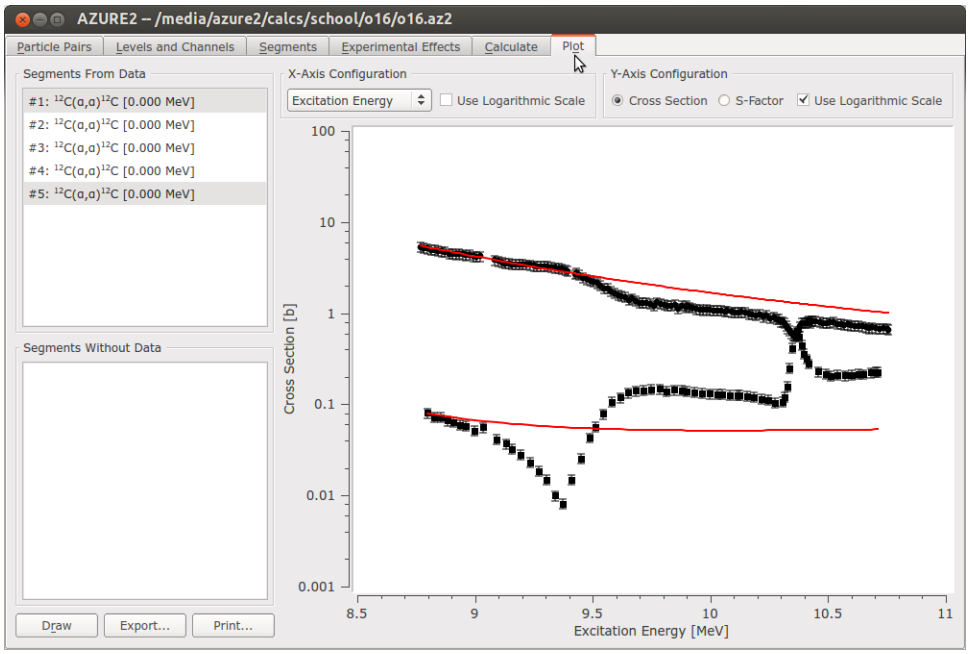

Figure 11: Second results - Coulomb and $\ell = 0 - 4$ hard-sphere. The difference is small, but not insignificant.

energy, resonances in different channels line up in the same place when different channels are simultaneously plotted. This helps determine which resonances are relevant to which channels and makes identifying states from the literature more simple. Now we wish to add in the two resonance states that can be seen. These resonances are known, but this will not always be the case and here we will determine the resonance parameters from the data.

Task 8: *By looking at the data, estimate how wide the lower energy resonance is.*

By default, AZURE2 takes observed resonance properties as input and converts them formal reduced width amplitudes with a boundary condition $B_c = S_c(E_\lambda)$. With a Breit-Wigner resonance, the (observed) width Γ is defined as the full width of a resonance at half the maximum cross section. With scattering data, the non-resonant Coulomb component makes identifying the width by eye harder. In this case, the width of the state is approximately 400-500 keV. We will determine this more precisely later by fitting the width as a parameter.

Task 9: *Assume the resonance has* $J^\pi = 0^+$. *By taking a resonance width of* $\Gamma = 450$ *keV, add the resonance at the appropriate energy on the Levels and Channels tab. Calculate the cross section and look at the results.*

Once you've added the state, be sure to edit the width for the channel. Click on the channel in the middle column and edit the width in the bottom right-hand corner. Note that when

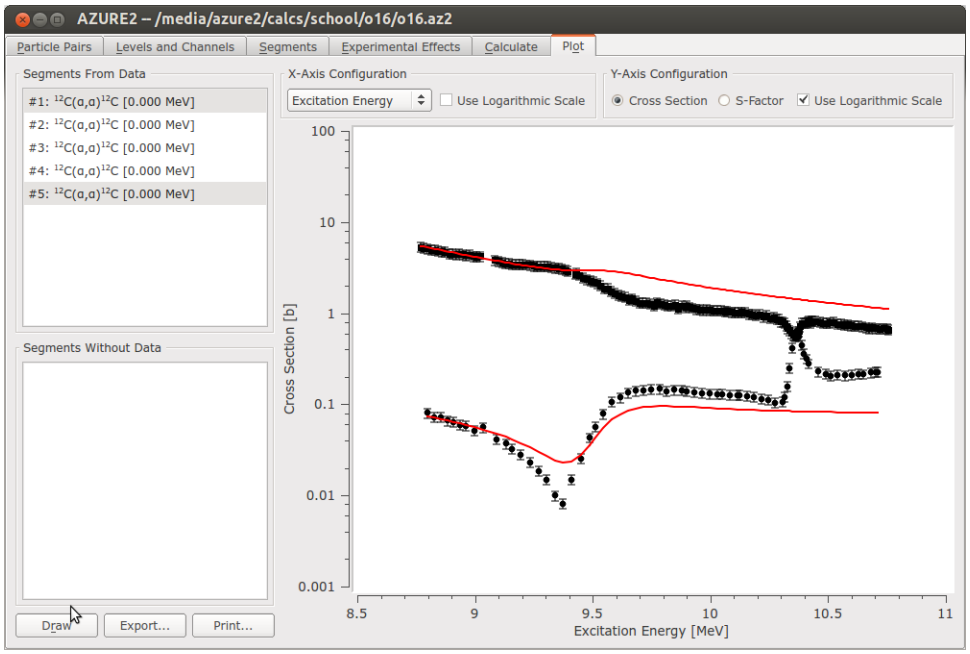

Figure 12: Results with 0^+ resonance

the width for a channel is non-zero, the channel is shown in bold font in the channels list. If you look at the results and the energy isn't quite right, just go back and edit the level in the Levels and Channels tab, but don't worry about finding very precise agreement yet. Crucially, the angular distribution depends sensitively on the $J^\pi$of the resonance and with good data over a range of angles the J^πcan be determined.

On the Plot tab, look at each of the angles (the different data segments) individually. The results for the smallest and largest angles are shown in Fig. 12. How is the agreement for the assumption of a J^π=0^+ state? For the larger angles the shape of the resonance seems basically correct, but for the small angles the trend is definitely wrong. This suggests that the resonance is not 0^+.

> **Task 10**: *Edit the level and change the spin-parity, first for positive parity states (2^+ and 4^+) then for negative parity states (1^- and 3^-). For each case, assess the quality of agreement with the experimental data. Which is the correct J^π?*

Note that each time you change the spin-parity of a level, the allowed channels will change and the widths will be reset unless the new and old resonances happen to share the same channel. You'll need to edit the width and set it to 450 keV each time. Once you've identified the correct J^π, you should have a result that looks like Fig. 13.

> **Task 11**: *Follow the same procedure for the second resonance; identify the energy and estimate the width. Then change the J^π to identify which will fit best.*

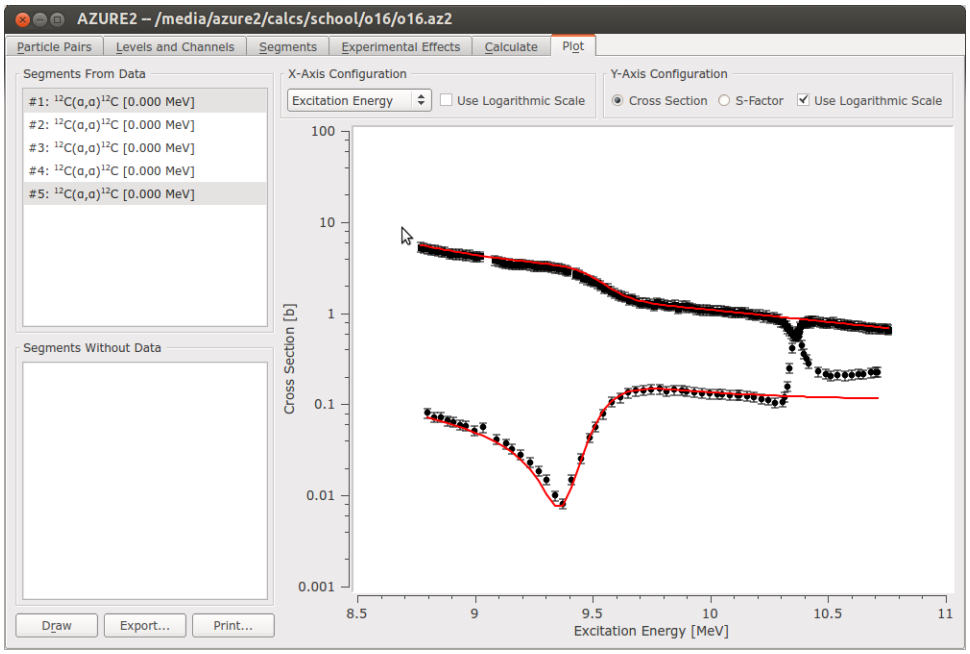

Figure 13: Results with a resonance of the correct spin-parity

This case is particularly simple, as the resonance only has a single channel, the width of which can easily be estimated by eye. When multiple channels contribute to a single resonance and the density of states increases, things can become considerably more complicated. However, in this case at least we can firmly assign the J^π of the state.

2.7 Fitting

With the likely spin-parities of the states established, we now can fit the resonance energies and widths to obtain a best fit to data, and then compare the results to literature values.

> **Task 12**: *On the Calculate tab, change the drop down to "Fit segments from data". Now click "Save and Run". You may be asked to enter a file name. The text area will show the progress of the fit.*

Once the fitting is complete, switch to Plotting, and admire the quality of the fit (shown in fig. 14). The fit at low energies and between the resonance is, on the whole, very good. The only deviations come at high energies above the second resonance. This could be an indication of higher lying states that need to be accounted for.

> **Task 13**: *Compare the results of the fit to values from the literature.*

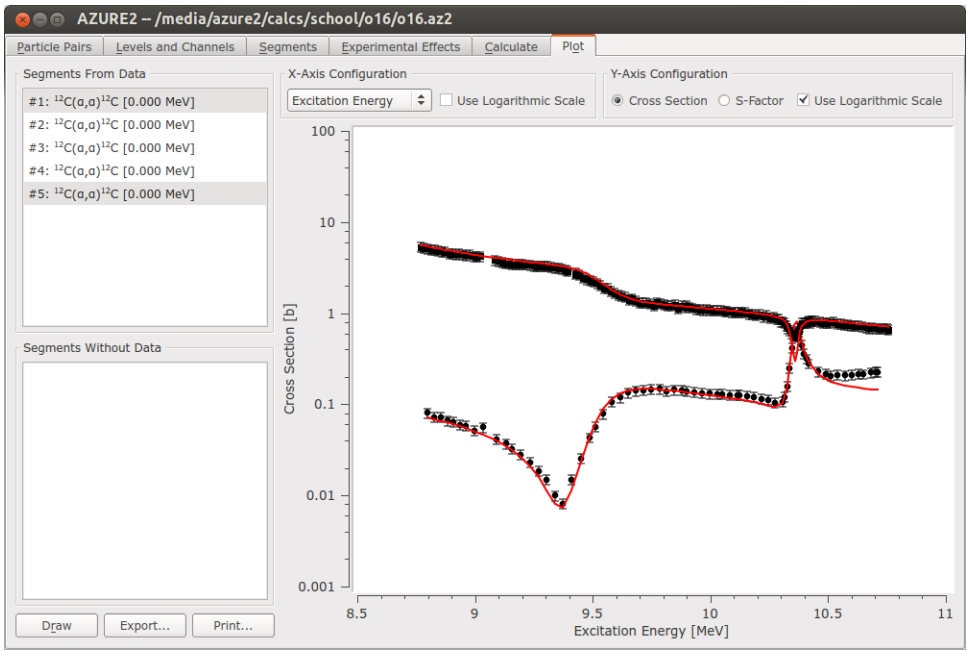

Figure 14: Results of a fit with two resonances.

The parameters resulting from the fit can be viewed in an output file, `output/parameters.out`. There are numerous online databases that tabulate resonance parameters. Two good examples are the TUNL Nuclear Data Project which is very comprehensive for light nuclei, or the more general US National Nuclear Data Centre. The resonances identified in the fit match those given by NNDC as:

$$\begin{array}{lll} 9.585 \text{ MeV} & 1^- & \Gamma_\alpha = 420 \text{ keV} \\ 10.356 \text{ MeV} & 4^+ & \Gamma_\alpha = 26 \text{ keV} \end{array}$$

Note that AZURE2 does not automatically transfer the results of a fit (i.e. the resonance energies and widths) back to the input file; if you start a calculation afresh, your original input parameters will be used. The results in `parameters.out` can be used to improve the quality of your initial parameter set, but should be adopted wholesale with caution.

2.8 Extrapolations

With the resonance parameters fitted, we then may be interested in calculating the cross section at angles or energies for which we don't have data. For example, for an astrophysical application, we may wish to calculate the cross section at low energies. With elastic scattering

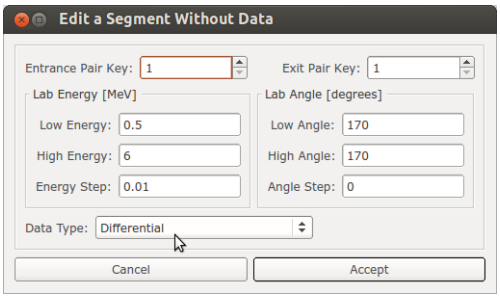

Figure 15: Adding a segment for extrapolation.

reactions, perhaps we need the cross section at a specific angle for which we have no data. AZURE allows us to make these calculations by creating extrapolation segments.

> **Task 14**: *Add an extrapolation segment to calculate the scattering cross section at 170 degrees between 0.5 and 6 MeV.*

These work in essentially the same way as data segments. Click the plus button in the bottom left hand corner of the lower part of the segments tab. A pop-up window should appear, similar to Fig. 15. Here you can specify the entrance and exit channel particle pairs, The minimum, maximum laboratory energies and the energy step, and the minimum and maximum laboratory angles with an angle step. Fill these in now - the angle step for this single-angle segment can be set to zero.

To run the extrapolation, switch to the Calculate tab and switch the calculation type using the drop-down list to Calculate segments without data. Then click Save and Run. The results can be viewed just like the data segments in the Plot tab.

3 ^{12}C$(\alpha,\alpha)^{12}$C - Extending to higher energies

Here we can build on the first example to extend the fit to higher energies. Initially, we try to correct the (minor) deviations seen at higher energies for some angles.

> **Task 15**: *By looking at the literature levels, try and identify if particular broad resonances could cause the deviations seen at higher energies. Add an appropriate background pole and see if the fit improves.*

There are several possible candidate states listed on the NNDC website, including a (possible) state at 11.260 MeV (0^+, width 2500 keV) and a promising 800 keV wide 3^- state at 11.600 MeV. Add this second resonance and perform a fit. Do things improve at higher energy?

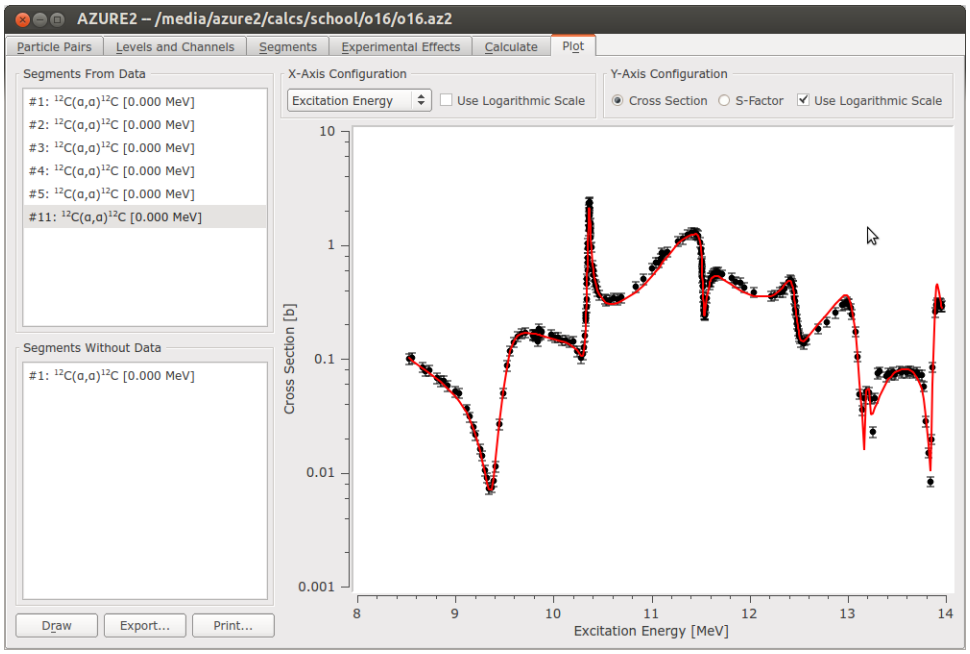

Figure 16: Results with higher energy data and background poles.

The fit however, is free to move the 3^- state as it sees fit. If we look at the output parameters, this resonance has been moved down in energy and become significantly narrower. This might provide a better fit to the data we have, but it's rather unsatisfying. The background contributions in this case comes from a specific state. Why should we include a generic background contribution when we can measure the cross section at higher energies and determine the background at lower energies more precisely?

> **Task 16**: *Extend the calculations to higher energies using the data of Feng* et al*[6].*

This data set covers a wide energy range, from 2.0-9.0 MeV α-particle energies at a single laboratory angle 165 degrees. Guidance on the resonance parameters can be found in the literature and in a previous analysis of this reaction [7]. You will need to allow background resonances for natural parity states from 0^+ to 4^+ to obtain a good fit. This is reasonable, given the large number of broad states at these energies, and will produce a fit like that shown in Fig. 16.

Be careful when fitting narrow resonances. They tend to be sensitive to the quality of the data and different sources might disagree significantly. Whilst these states might only impact a narrow energy range, their sharp nature can play havok with the χ^2 fitting procedure, with a few points contributing a significant fraction of the total χ^2. If these narrow resonances are genuinely unimportant to the broader fit, it is often best to exclude them from the χ^2 fitting and fix the relevant resonance parameters. Also, be careful when comparing the widths

of narrow resonances; target effects can play a significant role in apparently broadening the width of resonances.

A reasonable fit can be obtained with this single-channel calculation, but in fact, the proton-channel opens at $S_p = 12.127$ MeV and some of the resonances present in this calculation are known to have significant proton branches. To constrain this, data on ^{15}N(p,p)^{15}N could be added e.g. from Ref. [8], or reaction data on ^{15}N(p,α)^{12}C or the inverse ^{12}C(α,p)^{15}N. Additionally, just below the proton threshold α-decays to excited states in ^{12}C open up - the first 2^+ state in ^{12}C is at 4.439 MeV. Some states observable in ^{15}N+p scattering have significant α_1 widths (see e.g. analysis of Ref. [9]).

4 ^{13}C(p,p)^{13}C

Task 17: *Set up and analyse data on proton-scattering from ^{13}C.*

For this example we need to start afresh. You should find the directories already setup: `azure2/n14/`. The data used here is from Refs. [10] and [11] (though there are many other sets available). The added complication compared to the previous example is that now multiple channels may populate each resonance, since the channel spin $\vec{I}_p + \vec{I}_{^{13}\mathrm{C}}$ now need not be zero. In most cases it is best to assume that the lowest-ℓ channel will have the largest width. The analysis proceeds as before:

(a) Open AZURE2 and configure directory settings

(b) Add ^{13}C+p to the compound nucleus

(c) Add a background level for each allowed J^π

(d) Add segments for `milne_1954.dat` and `hebbard_1960.dat` - these are both (p,p) data sets. Look inside to see what data is available and see Appendix A for data file format.

(e) Run the first calculation

(f) Starting from low energy, identify each resonance. Add them to the compound nucleus and vary their $J^\pi$to find the most likely candidate spin-parity.

(g) With all narrow states identified, perform a fit to the data

(h) Verify the results against literature values

You should be able to obtain a fit similar to that shown in Fig. 17.

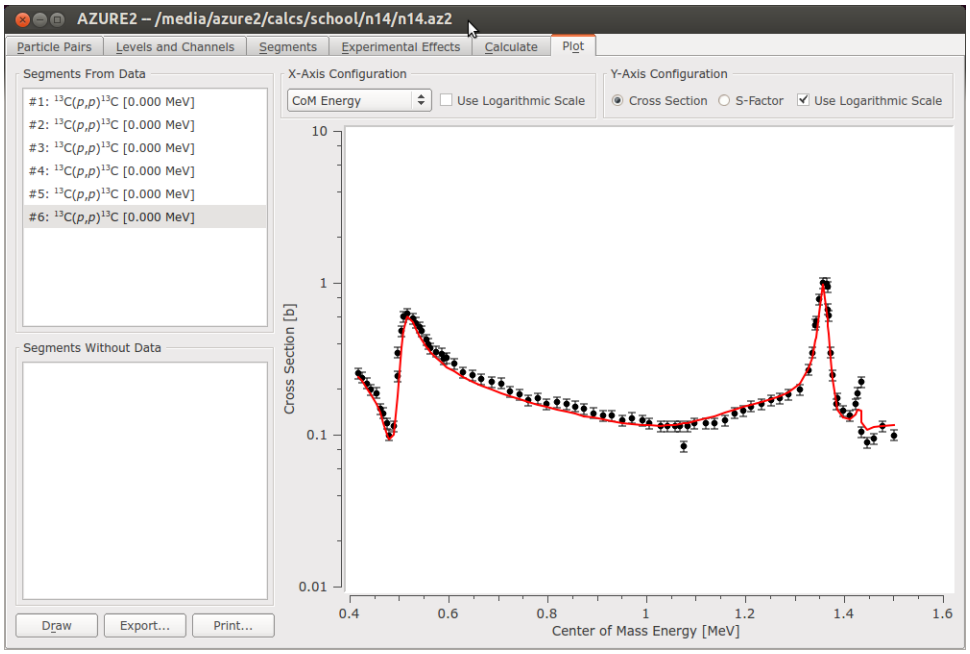

Figure 17: Results for proton scattering on ^{13}C.

5 ^{21}Na(p,p)^{21}Na

Task 18: *Perform an analysis of* ^{21}*Na(p,p)*^{21}*Na.*

This final example is on elastic scattering of protons from ^{21}Na (see Ref. [12]). In this case the reaction was used to populate resonances in ^{22}Mg, which has a key role in determining the production of ^{22}Na in explosive stellar scenarios. The relevant directories and files should have been copied over earlier. The data is `azure2/mg22/data/ruiz_2005.dat`. In this case, the spins and parities of the states are not known - or at least, they've not made it into large databases yet. The original paper (see references) can provide a guide to the analysis though. Further, the data is not normalised, and a variable normalisation parameter should be used. This can be added when you create (or edit) a data segment. For the present data file, an initial normalisation of about 0.55 is appropriate. Once you've fit, you should obtain something like Fig. 18.

Appendix A: Data file format

Data files used by AZURE2 must be in a particular format. They consist of four columns, E_{lab}, θ_{lab}, σ_{lab} and $\Delta\sigma_{lab}$. The program assumes regular kinematics, where the light particle is incident on the heavy particle. E_{lab} is the incident light-particle energy in the laboratory frame and θ_{lab} is the angle of the exit light particle in the laboratory frame. The cross section

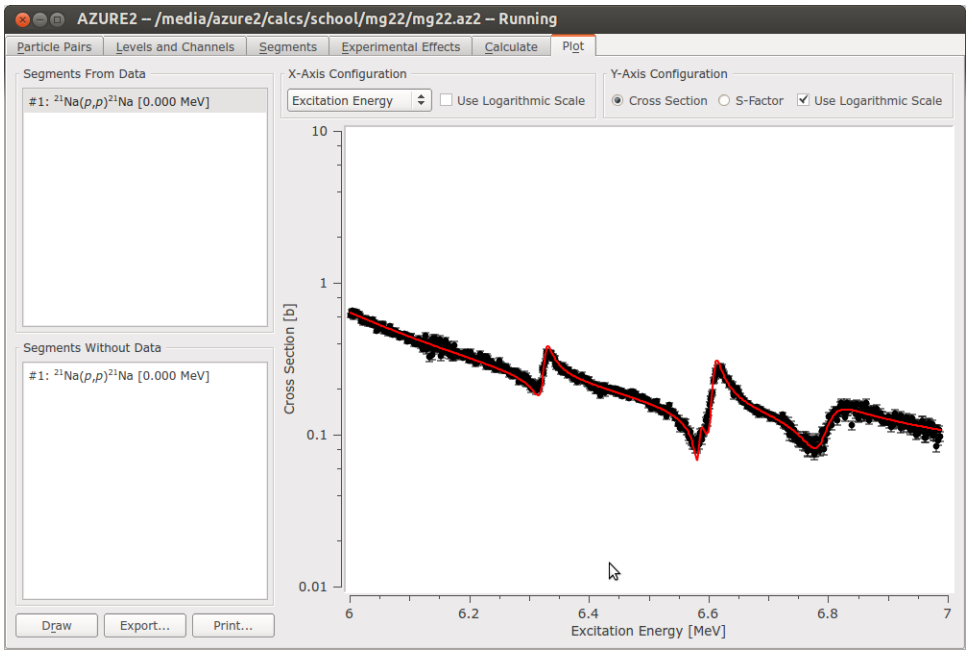

Figure 18: Results for proton scattering on ^{21}Na. Note the normalisation of the data points is fit.

σ_{lab} and error $\Delta\sigma_{lab}$ must be in the laboratory frame.

If the data is angle-integrated, then a dummy angle must be entered for θ_{lab}, which will be ignored by AZURE2. Be warned, the format of data in online libraries varies greatly. EXFOR in particular sticks to the original paper, so each data set requires careful and potential conversion to be properly used. IBANDL has the advantage that the data is consistently presented in the laboratory frame as required by AZURE, though the coverage is perhaps less comprehensive than EXFOR.

Appendix B: Output data format

Output files are written to the directory specified. Unlike input segments all output is given in the centre-of-mass system. The output files are named differently for data calculations (ending in `.out`) and extrapolations (ending in `.extrap`). The columns are shown in Table 2.

References

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Table 3: Column numbers for output files ending in `.out` and `.extrap`.

`.out`	`.extrap`	Quantity
1	1	Centre of mass energy (MeV)
2	2	Excitation energy in compound nucleus (MeV)
3	3	Centre of mass angle (degrees)
4	4	R-matrix cross section (b)
5	5	R-matrix S-factor (MeV.b)
6	-	Data cross section (b)
7	-	Data cross section error (b)
8	-	Data S-factor (MeV.b)
9	-	Data S-factor error (MeV.b)

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