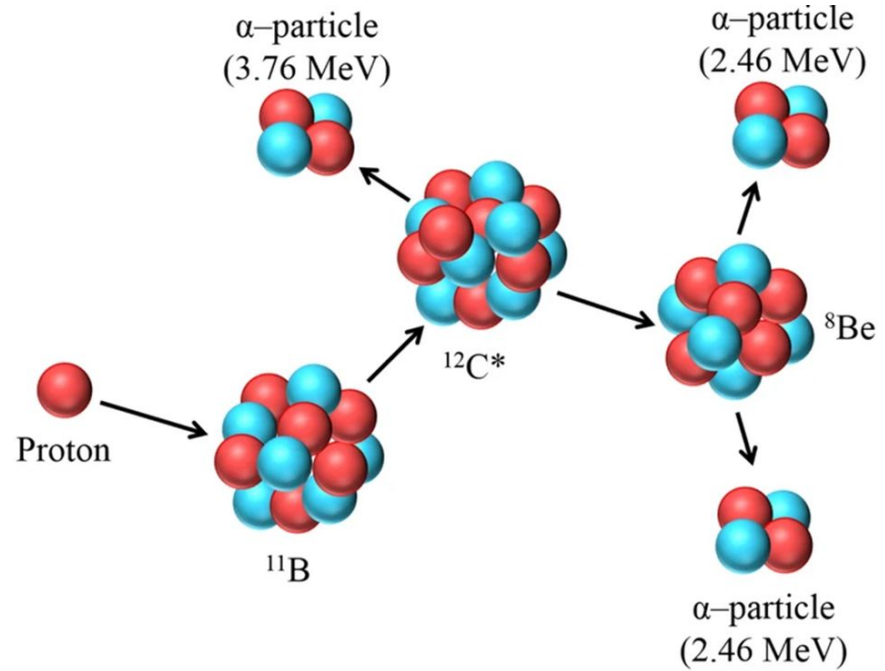


R-Matrix Analysis of Nuclear Reactions with AZURE2

Francisco Gamito and Michael de Sousa
Supervisors: Dr. Elmar Biernat and Prof. Alfred Stadler

Research Motivation

- Proton Boron Capture Therapy (PBCT) cancer treatment
 - Proton Boron fusion reaction
 - Non-invasive radiotherapy
- Thermonuclear fusion energy production
- Current total cross section models are not considered accurate
- We can use AZURE2 to model this nuclear reaction using R-matrix theory and produce a cross section



Credit: Shahmohammadi Beni, M., Islam, M.R., Kim, K.M. et al. On the effectiveness of proton boron fusion therapy (PBFT) at cellular level. Sci Rep 12, 18098 (2022).

<https://doi.org/10.1038/s41598-022-23077-0>

Theory

Nuclear Reactions and Cross Sections

Projectile: proton

Target: Boron-11

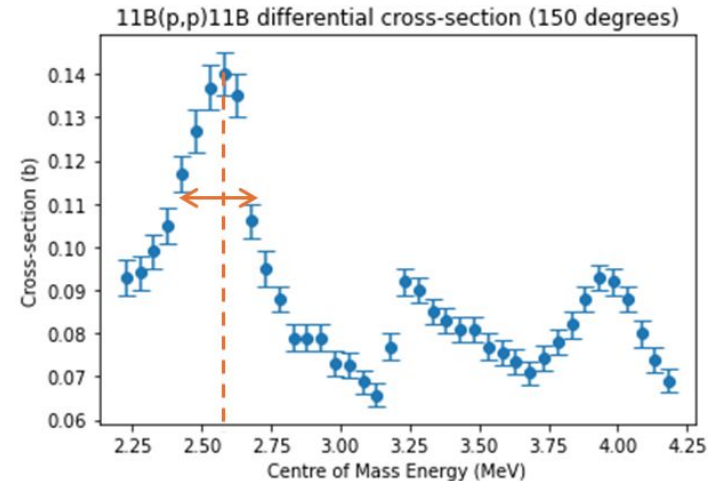
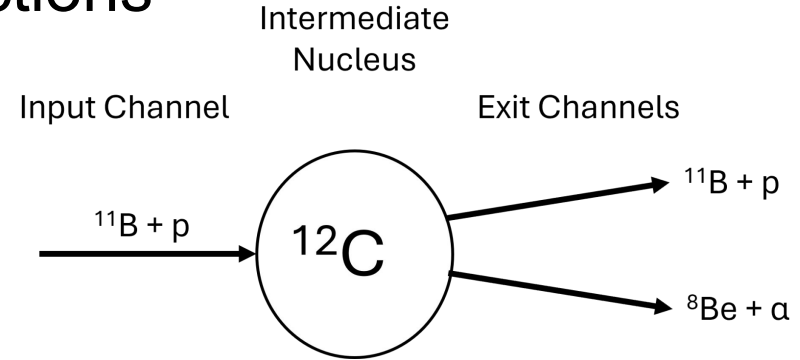
Elastic channel: $^{11}\text{B}(\text{p},\text{p})^{11}\text{B}$

Inelastic channel: $^{11}\text{B}(\text{p},\alpha_1)^8\text{Be}^* // ^{11}\text{B}(\text{p},\alpha_1)2\alpha$

A cross section is a measure of the probability that a nuclear reaction will occur

Integrating differential cross section produces **total cross section**

Peaks in cross-section data are resonances with a certain **partial width** and **energy**



R-Matrix Theory

$$\phi_c = \left(\frac{1}{v_c} \right)^{1/2} (y_c I_c + x_c O_c)$$

- External region
 - Only Coulomb interaction
 - Analytical solution

$$\phi_c = \left(\frac{m_c a_c}{\hbar^2} \right)^{1/2} \sum_{c'} R_{cc'} \left(\frac{\hbar^2}{m_{c'} a_{c'}} \right)^{1/2} [\rho_{c'} \phi'_{c'} - B_{c'} \phi_{c'}]$$

- Internal region
 - Complete set of eigenstates
 - Coulomb and strong forces

- The R-matrix describes all the information about the internal compound system

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E}$$

- Partial widths and energies give analytical boundary condition
 - These are transformed at the start and end of the calculations

AZURE2



Outline of AZURE2

Made by the Joint Institute of Nuclear Astrophysics (JINA)

AZURE2 has 5 tabs that were relevant:

- Particle Pairs
- Levels and channels
- Segments
- Calculate
- Plot

	Light Particle	Light Spin	Heavy Particle	Heavy Spin	Excitation Energy	Separation Energy	Channel Radius
1	<i>p</i>	1/2+	^{11}B	3/2-	0	15.96	4.5
2	α	0+	^8Be	2+	3.03	7.37	5.02

Compound Nucleus Levels

Include?	Fix?	Level Spin	Energy [MeV]
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1-	17.231
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	0+	17.698
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1+	18.2181
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	0-	18.2459
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	3-	18.3346
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2-	18.3493
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	3-	18.5046
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2+	18.9029
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1-	19.5
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	4-	19.5534
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2-	19.5708
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1+	19.6414
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2+	19.9
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	0-	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	0+	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1-	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1+	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2-	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2+	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	3-	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	3+	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	4-	25
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	4+	25

Channels In Selected Level

Fix?	Channel Pair	s	l
<input type="checkbox"/>	$^{11}\text{B}+p$ [0.000 MeV]	1	1
<input type="checkbox"/>	$^{11}\text{B}+p$ [0.000 MeV]	1	3
<input checked="" type="checkbox"/>	$^{11}\text{B}+p$ [0.000 MeV]	2	1
<input type="checkbox"/>	$^{11}\text{B}+p$ [0.000 MeV]	2	3
<input type="checkbox"/>	$^8\text{Be}+\alpha$ [3.030 MeV]	2	0
<input type="checkbox"/>	$^8\text{Be}+\alpha$ [3.030 MeV]	2	2
<input type="checkbox"/>	$^8\text{Be}+\alpha$ [3.030 MeV]	2	4

Channel Configuration

4

Maximum Orbital Momentum

1

Maximum Gamma Multipolarity

1

Maximum Gamma Multipolarities Per Decay

Channel Details (select from list to view):

18.9029 MeV level with spin 2+ transitioning via pair key #1
Channel configuration is
s = 2, l = 1

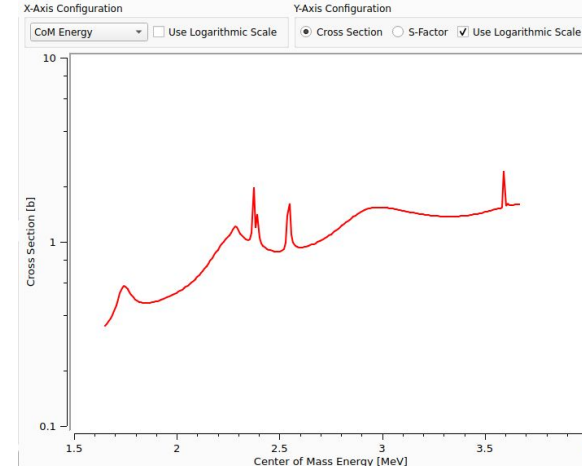
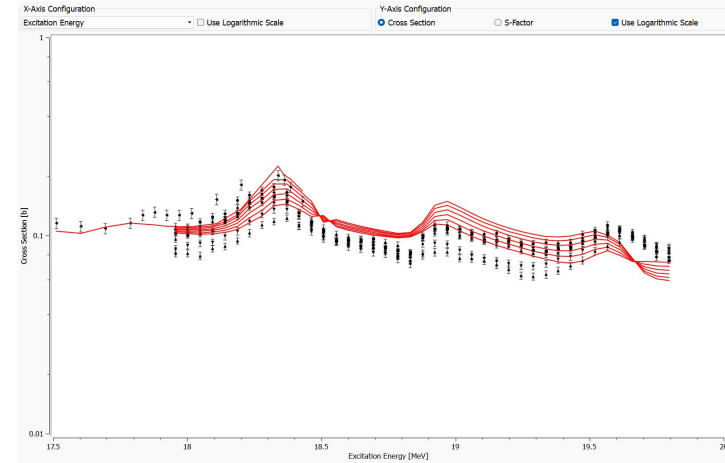
Light Particle Spin: 1/2+
Light Particle Z: 1
Light Particle M: 1
Light Particle G: 0
Heavy Particle Spin: 3/2-
Heavy Particle Z: 5
Heavy Particle M: 11
Heavy Particle G: 0
Excitation Energy: 0
Separation Energy: 15.96
Channel Radius: 4.5

Partial Width: eV

Performing Calculations in AZURE2

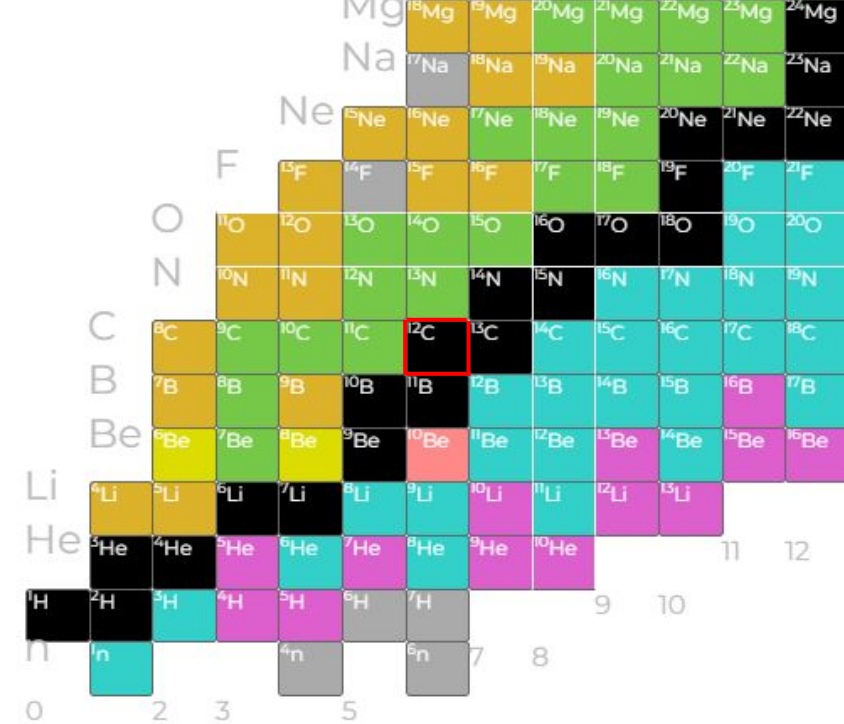
We performed two different types of calculations:

- Fit Segments From Data
 - Outputs fitted partial widths and energies for each level with chi-square values
- Calculate Segments Without Data
 - Uses fitted parameters to predict the cross-section at energies or angles we do not have data for



Our Strategy

- Input data from IBANDL database
- Input accepted energy levels and partial widths of the ^{12}C nucleus from LiveChart
- Use Fit Segments From Data and update input parameters with output
- Repeat until we get a good fit

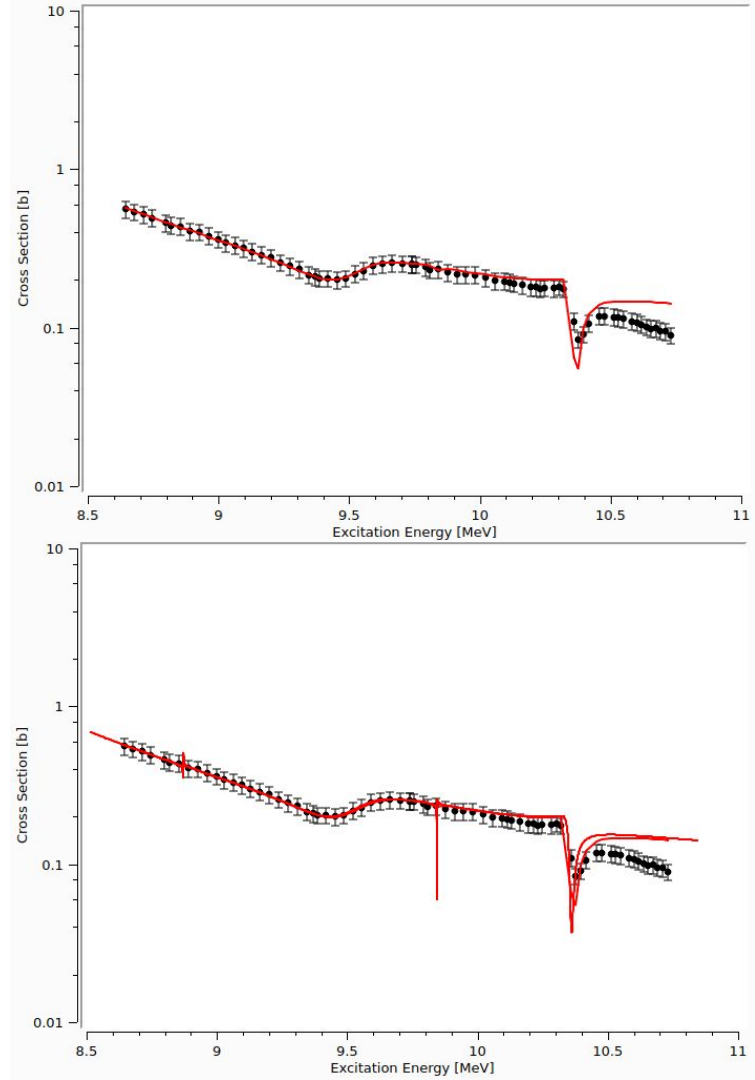


Source:

<https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html>

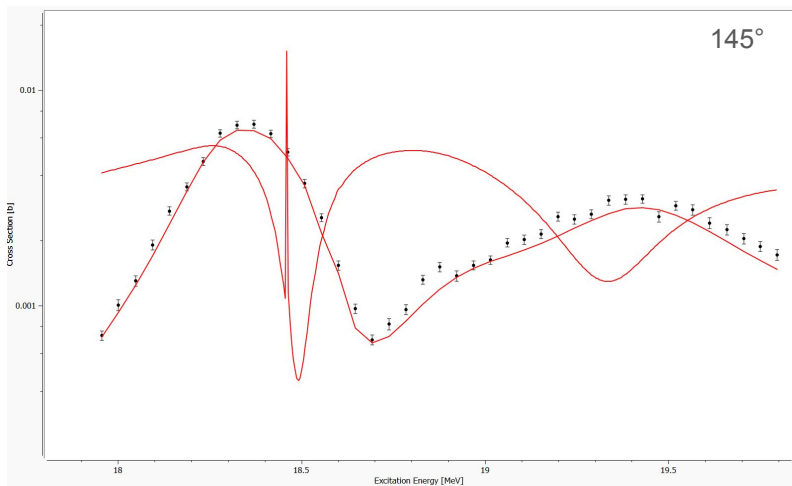
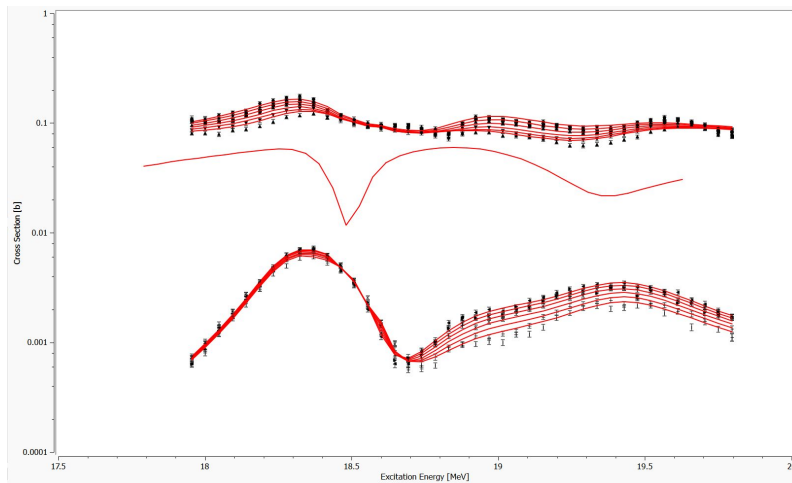
What makes a fit good?

- Chi-square of segments
 - 0.5 - 2 optimal
- Order of energy levels
- Compatible between different data sources
- Predictions match data not included
- End goal is to compare model total cross-section with pre-existing models

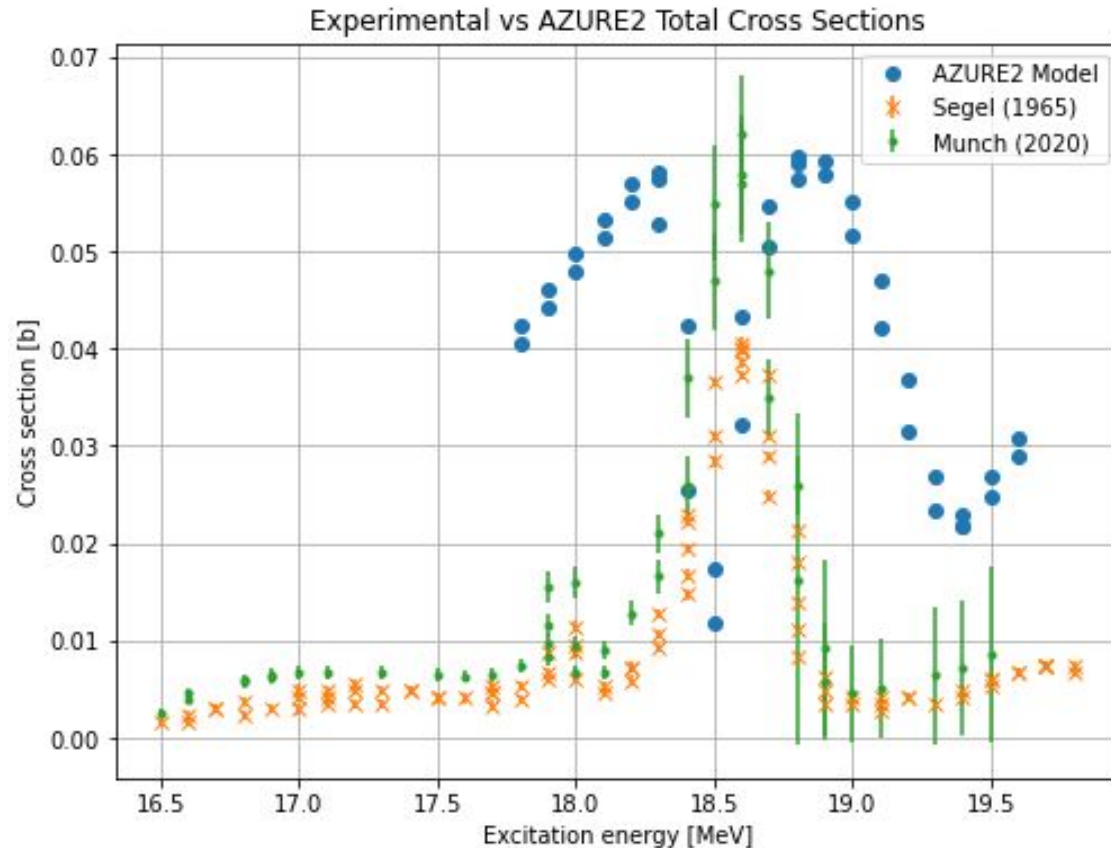


Results so far

- Our best fit to inelastic data
 - Some energy levels excluded
 - One energy level in wrong order
 - All reduced chi-squares from 0.5 - 4
- Model cannot reproduce shape of data
- Challenges:
 - 76 parameters!
 - ~2 hours per fit
- Error analysis coming soon



Total Cross-Section Data vs Model



In future, we expect that this will be able to be automated using a reinforcement learning algorithm. (Depending on computational resources!)

Any questions?