R-Matrix Analysis of Nuclear Reactions with AZURE2

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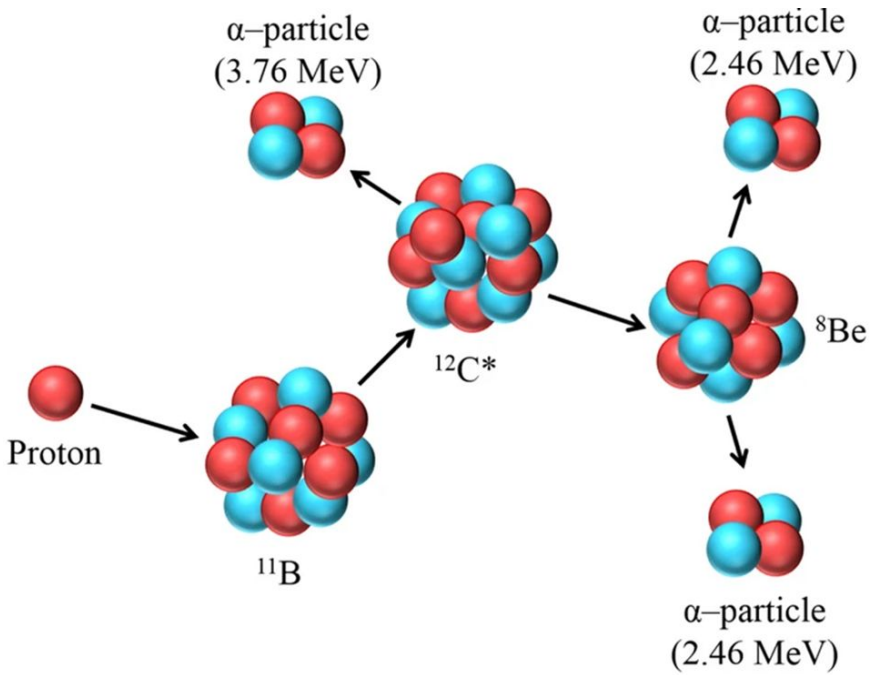
Research Motivation

- 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

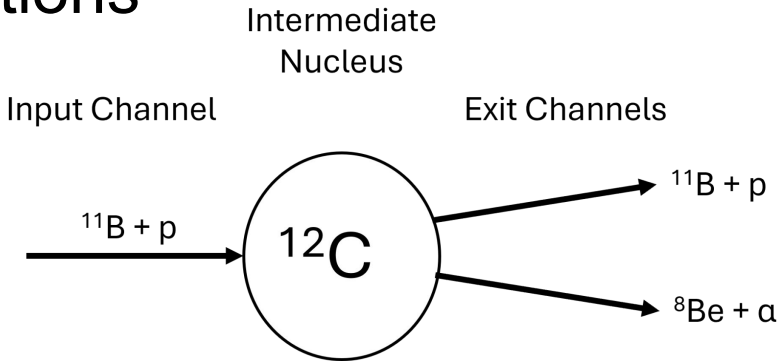
Nuclear Reactions and Cross Sections

Projectile: proton

Target: Boron-11

Elastic channel: **11B(p,p)11B**

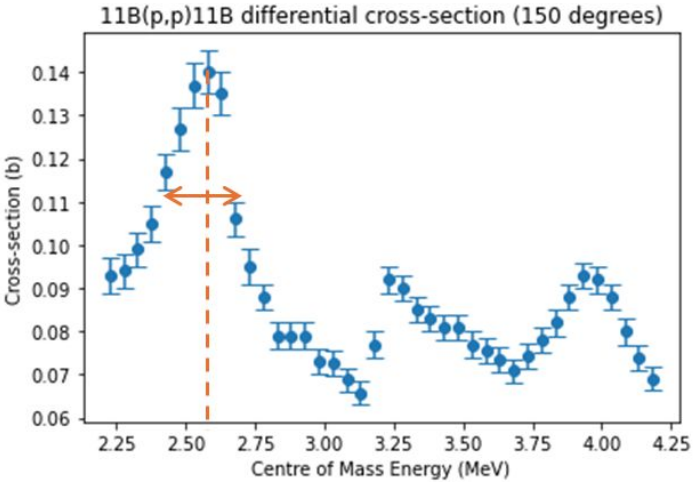
Inelastic channel: **11B(p,α_1)8Be* // 11B(p,α_1)2α**



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

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

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

- 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

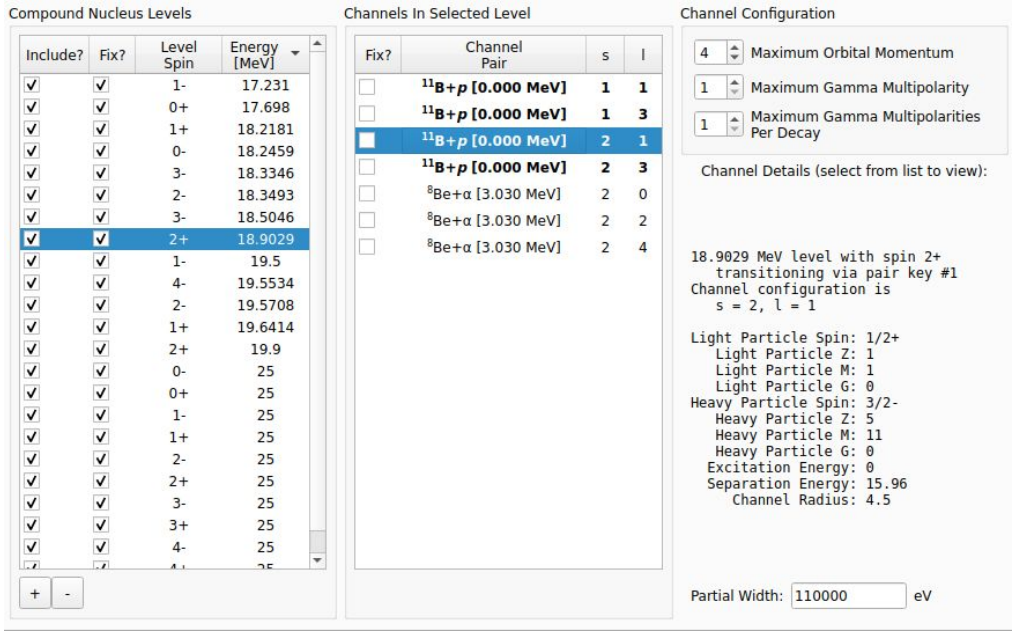
Outline of AZURE2

Made by the Joint Institute of Nuclear Astrophysics (JINA)

AZURE2 has 5 tabs that were relevant:

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

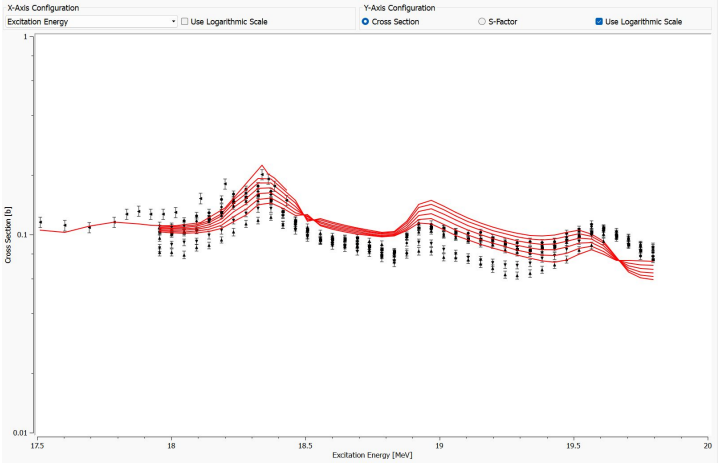
	Light Particle	Light Spin	Heavy Particle	Heavy Spin	Excitation Energy	Separation Energy	Channel Radius
1	*p*	1/2+	^{11}B	3/2-	0	15.96	4.5
2	α	0+	^{8}Be	2+	3.03	7.37	5.02

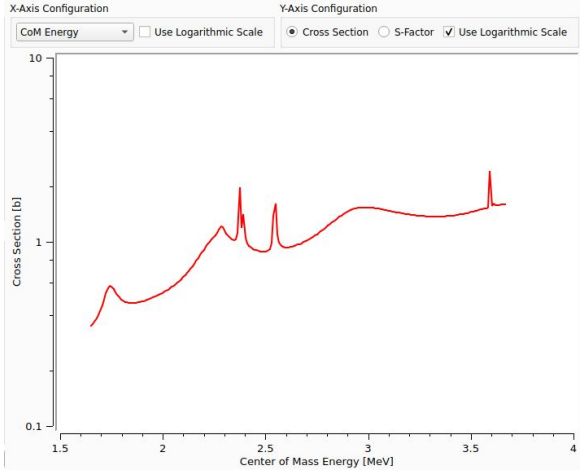


Performing Calculations in AZURE2

We performed two different types of calculations:

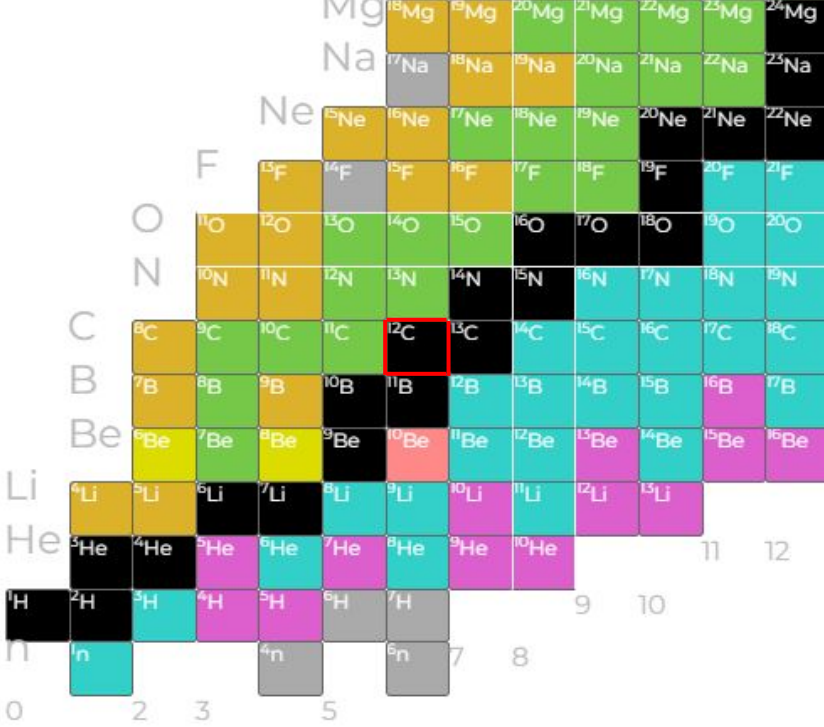
- Fit Segments From Data
  - Outputs fitted partial widths and energies for each level with chi-square values
- Calculate Segments Without Data
  - Uses fitted parameters to predict the cross-section at energies or angles we do not have data for





Our Strategy

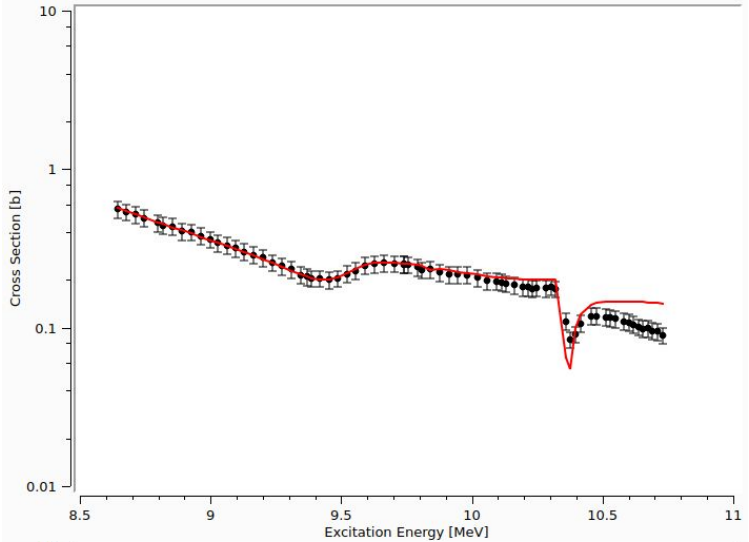
- Input data from IBANDL database
- Input accepted energy levels and partial widths of the 12C nucleus from LiveChart
- Use Fit Segments From Data and update input parameters with output
- Repeat until we get a good fit

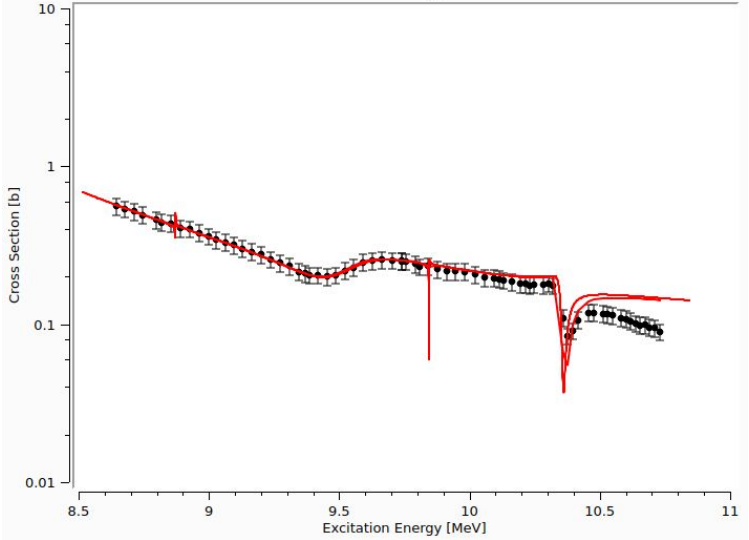


Source: https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html

What makes a fit good?

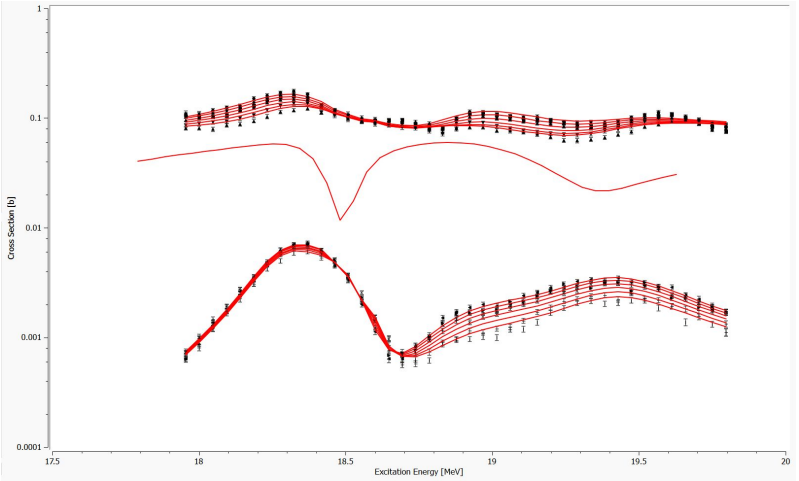
- Chi-square of segments
  - 0.5 - 2 optimal
- Order of energy levels
- Compatible between different data sources
- Predictions match data not included
- End goal is to compare model total cross-section with pre-existing models

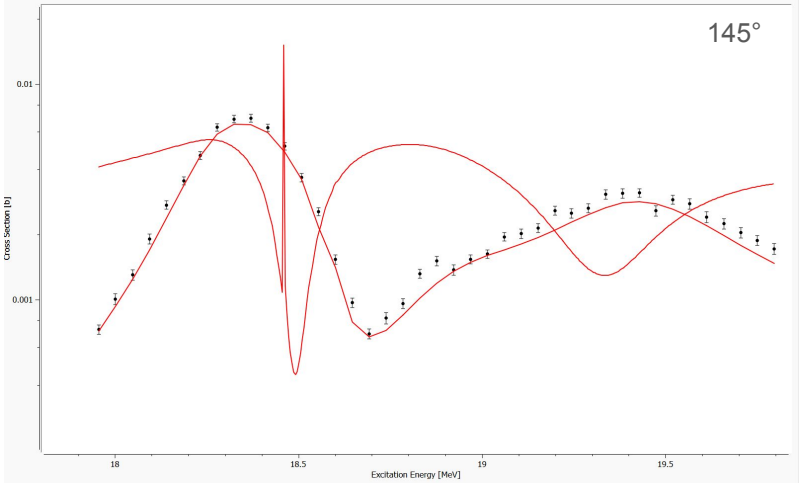




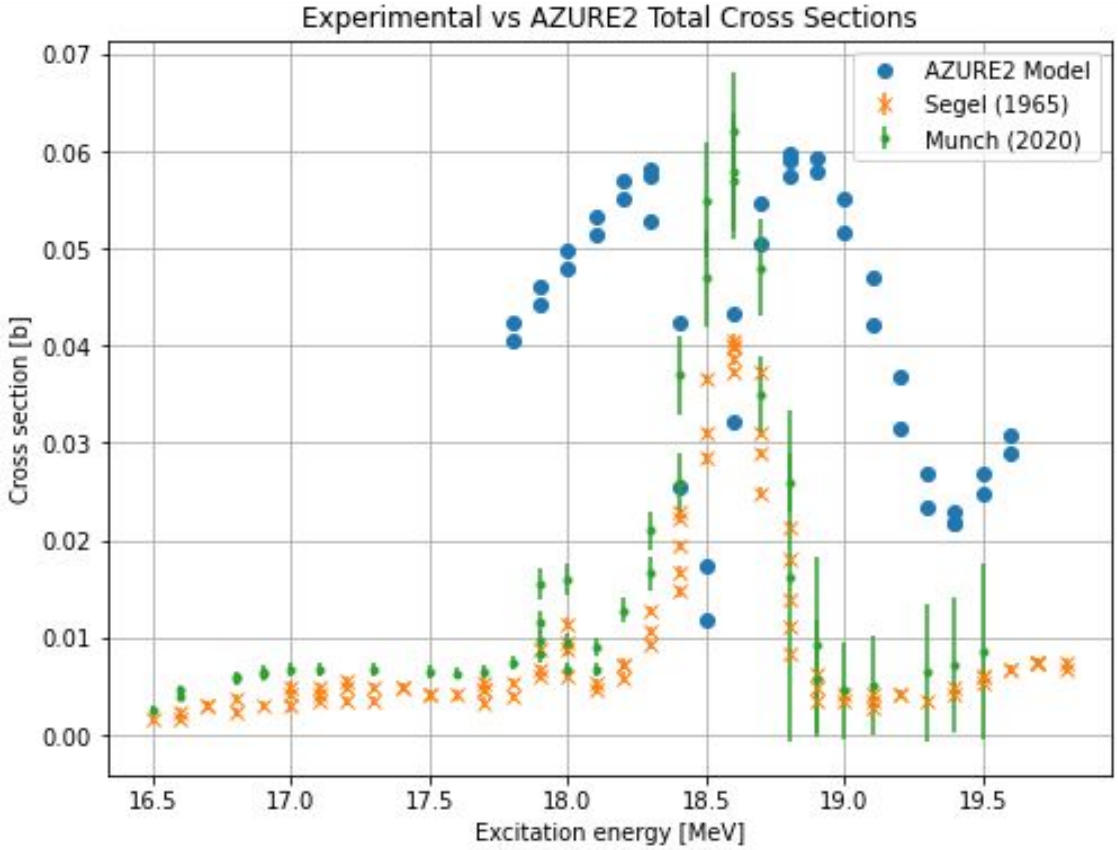
Results so far

- 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?