UNCERTAINTY ESTIMATION FOR GLOBAL *R*-MATRIX ANALYSES

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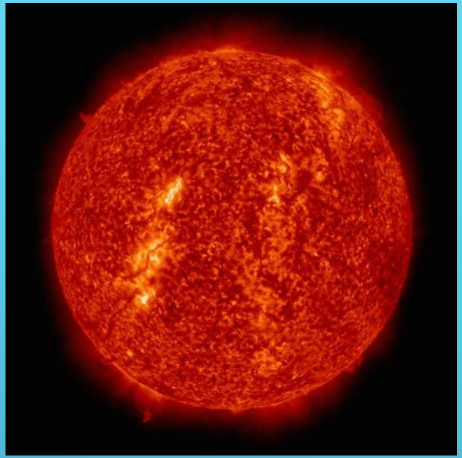
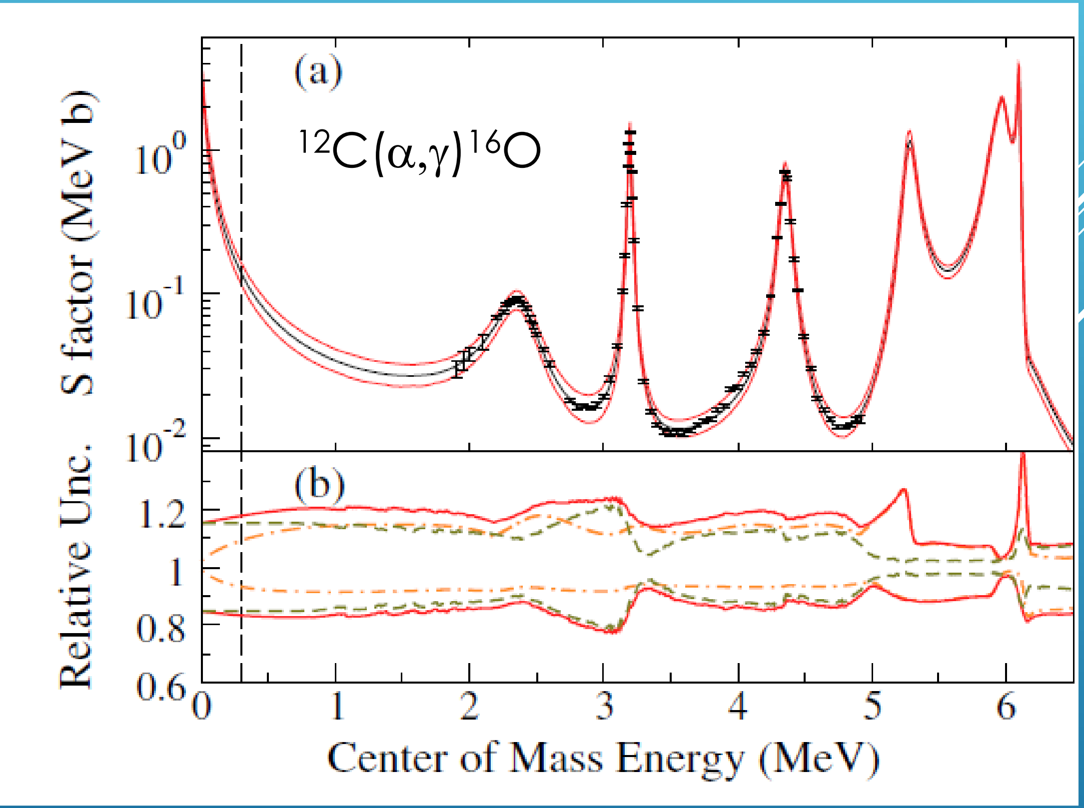
- Modeling the creation of the elements
  - Big Bang
  - Stars
  - Supernovae
- Requires highly precise and accurate determination of several nuclear reactions at low energies
- These energies are often in accessible experimentally
  - Evaluate sets of nuclear data
  - Extrapolate cross section to regions with no data

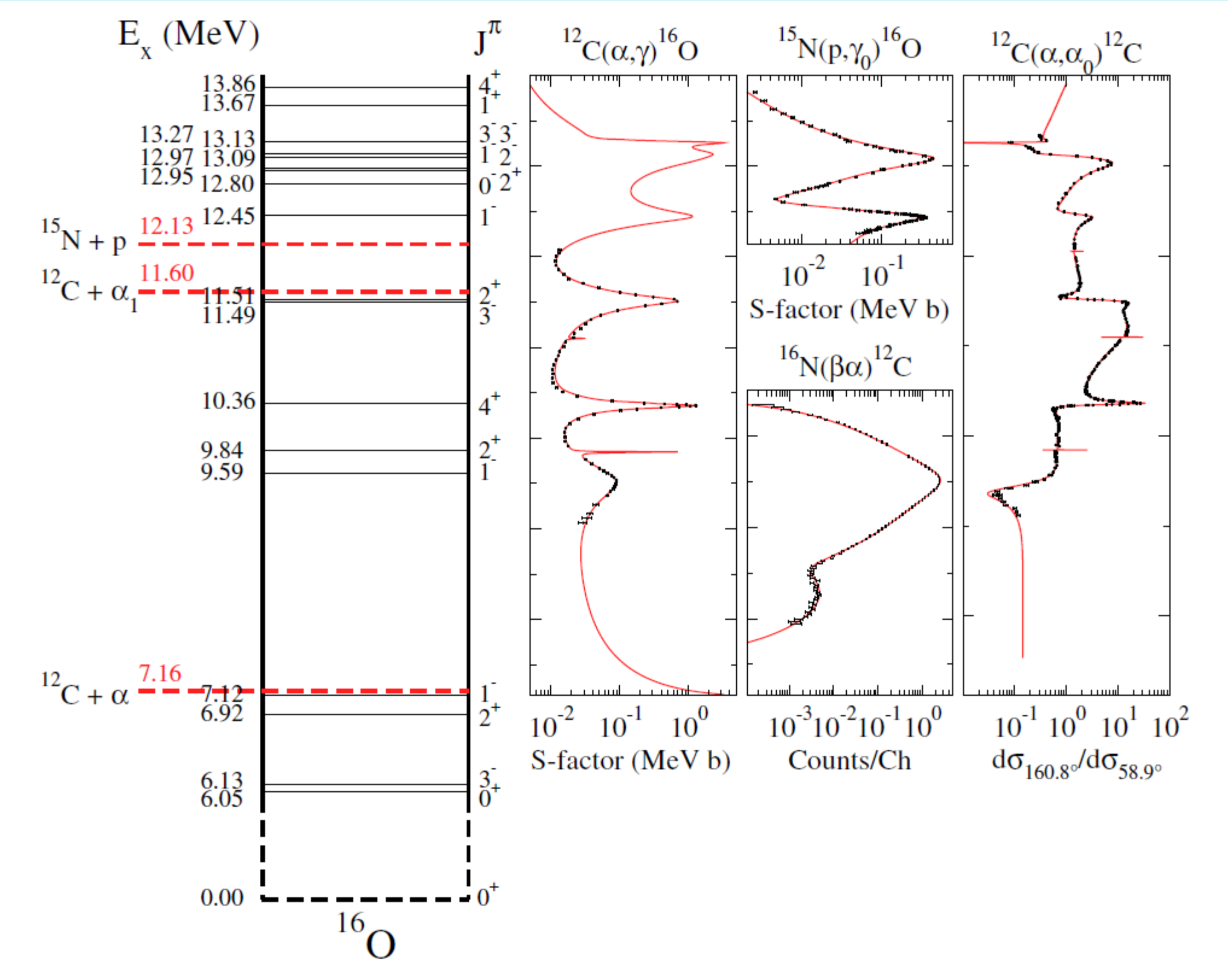
Red Giant,
Helium Burning





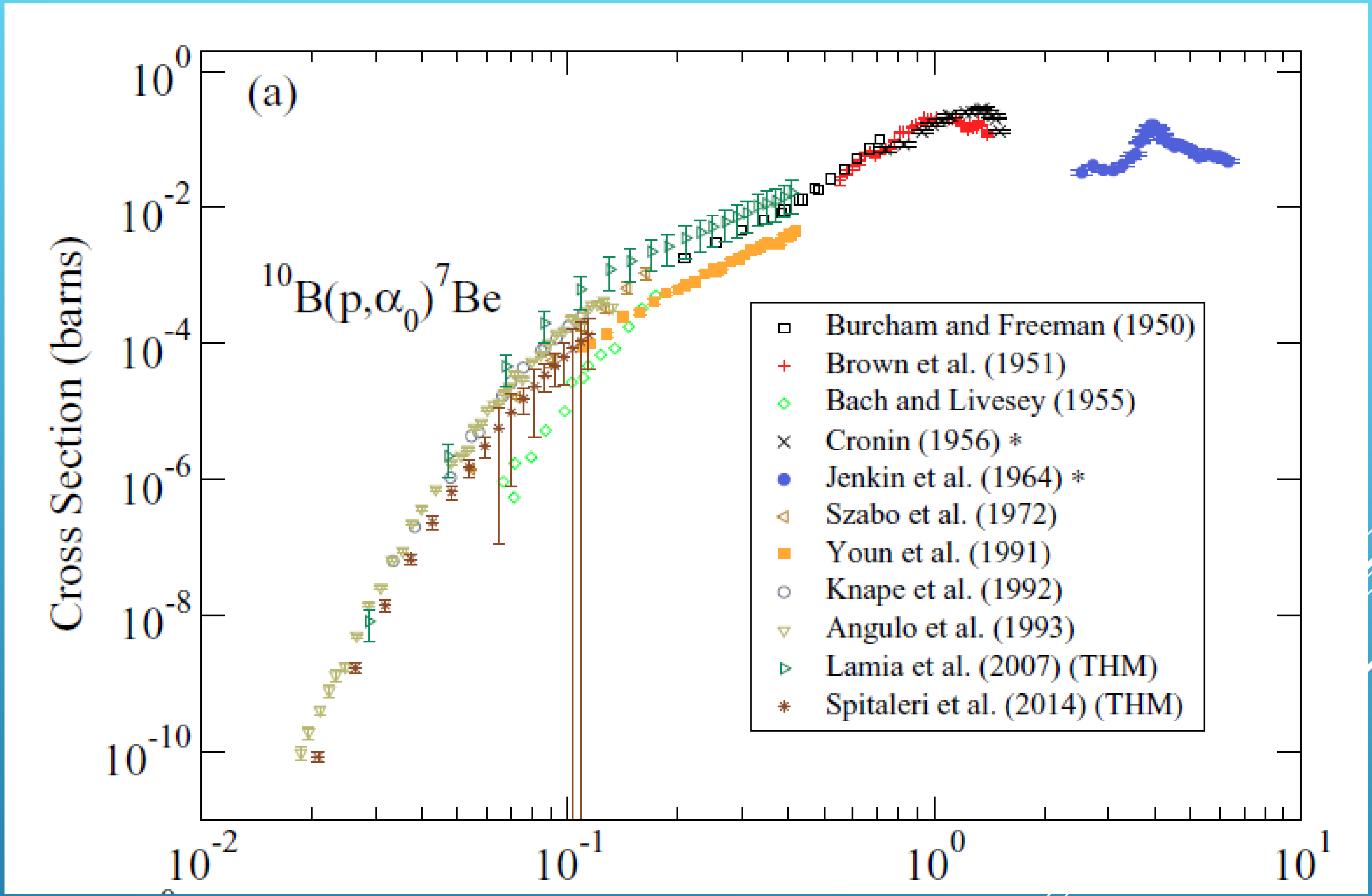
NUCLEAR ASTROPHYSICS

- Nuclear reactions populate a shared compound system
- Can make a mathematical model that links these reactions
- This provides many additional physics constraints through the model and provides the constraint of many addition data sets of different types
- Need to assess the data using the model as an intermediary to gauge the level of consistency and propagate this to a level of uncertainty



MORE COMPLICATED THAN JUST A SINGLE DATA SET OR EVEN A SINGLE REACTION

- Data sets measured over many years
- using many different techniques
- sometimes with different definitions of uncertainties
- **Data evaluation**



DATA ARE OFTEN DISCREPANT

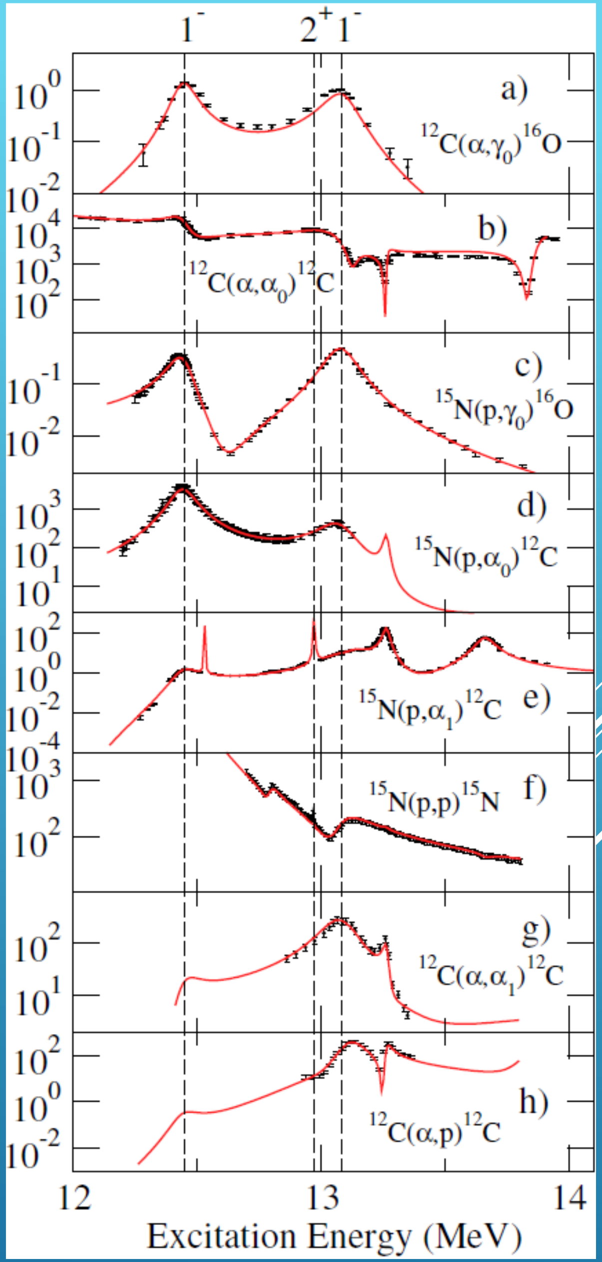
THE *R*-MATRIX APPROACH

- Phenomenological *R*-matrix is a reaction framework that has adjustable parameters that can be varied in order to match the theory with experimental nuclear cross section data
  - χ^2 fitting usually
- The nuclear level formulation results in many fit parameters
  - energy, partial widths for each level
  - normalization factors for each experimental data set
- many parameter (often >100) fitting problem to a large amount of experimental data (1000's of points) from different sources
- **Some underlying function whose parameters are adjusted to describe some experimental data**
  - **many parameters**
  - **imperfect data**

- Standard χ^2 fitting with additional terms for systematic uncertainties
- Systematic uncertainty is common for entire data set
  - Approximation, but works well for many experiments and can be practically implemented
  - What is the underlying PDF? (I'm assuming Gaussian)
- MINUIT2 (root fitter) is used to minimize χ^2
  - Gradient methods
  - Multi processing

$$\chi^2 = \sum_i \left(\sum_j R_{ij}^2 + \frac{(n_i - 1)^2}{\sigma_{\mathrm{syst},i}^2} \right),$$

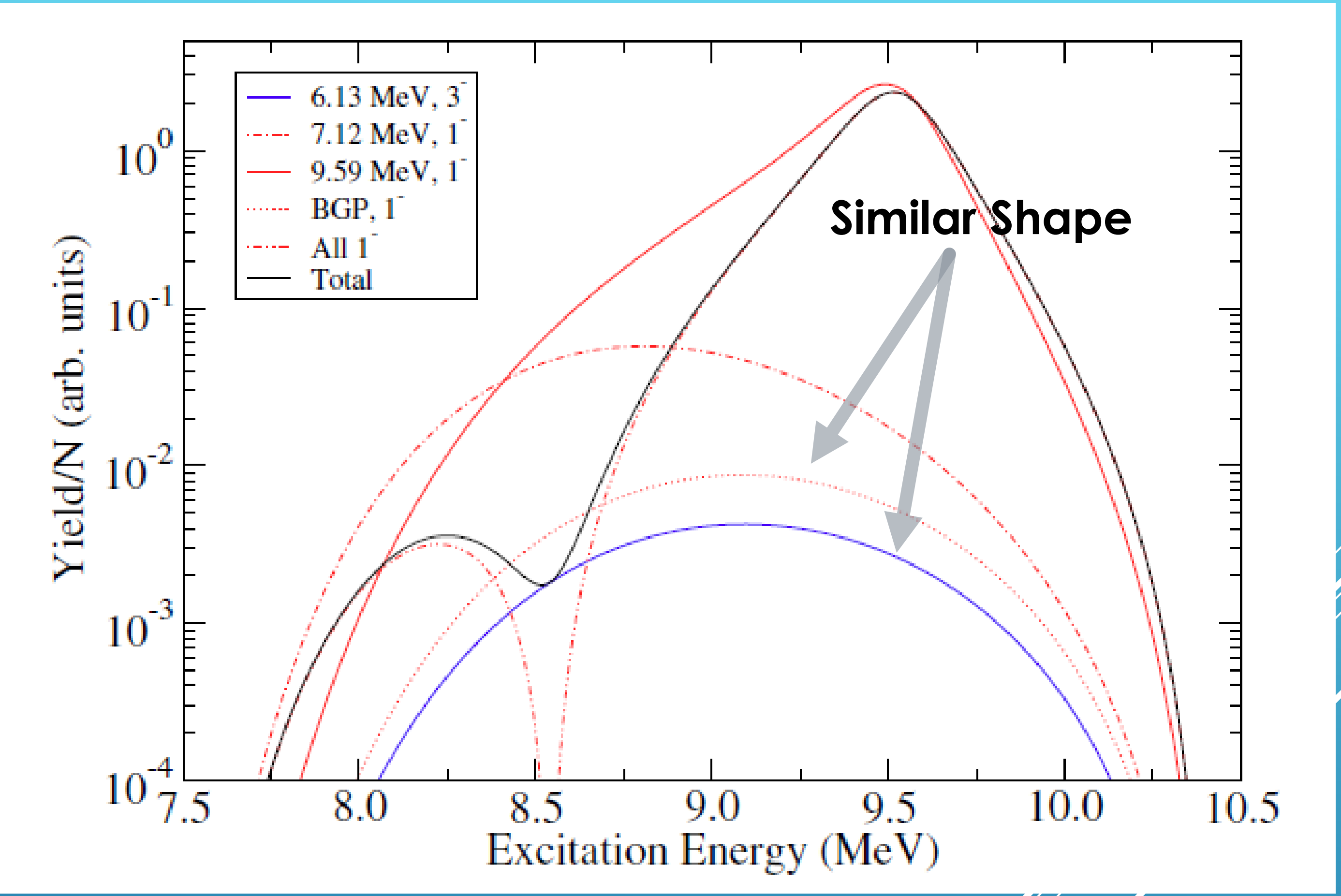
$$R_{ij} = \frac{f(x_{i,j}) - n_i y_{i,j}}{n_i \sigma_{i,j}},$$



FITTING TECHNIQUE

PARAMETER CORRELATIONS

- Strong parameter correlations
- MINUIT2 looses its mind



$^{16}N(\beta\alpha)^{12}C$

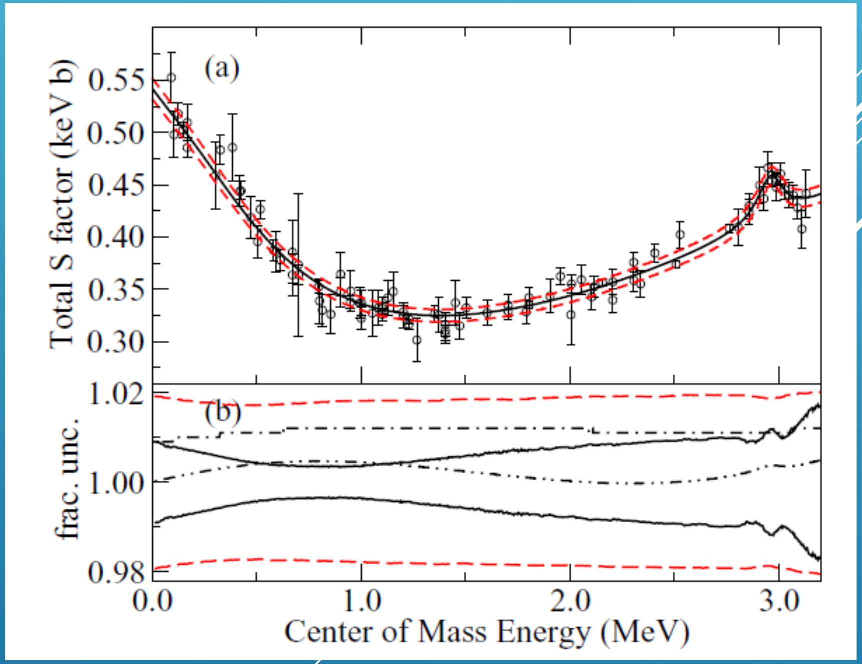
- Try to get a good fit to the experimental data (MINUIT2)
  - Need good starting parameters for the fit
  - MINUIT2 often gets **stuck in local χ^2 minima**
  - Fix/free normalization fit parameters
- Try to calculate covariance and correlation matrices with MINOS
  - MINOS crashes because parameters are too correlated
  - Fix/unfix parameters and repeat until highly correlated parameters are found and fixed or removed
  - Free normalization parameters results in more local minima, often have to get very good values for other parameters, then let these fit

HOW DOES THIS GO IN PRACTICE

PROPAGATING THE UNCERTAINTY TO THE CROSS SECTIONS

- Don't really care about parameter uncertainties
- Want cross section uncertainties
- Don't know how to get this from the parameter covariance matrix
- Frequentist Monte Carlo on the data using the uncertainties of the data (assuming they represent 1σ uncertainties) and the systematic uncertainties

$$\sigma_{cc'} = \frac{\pi}{k^2}\frac{\Gamma_c\Gamma_{c'}}{(E - E_\lambda) + \Gamma_{total}^2/4}$$

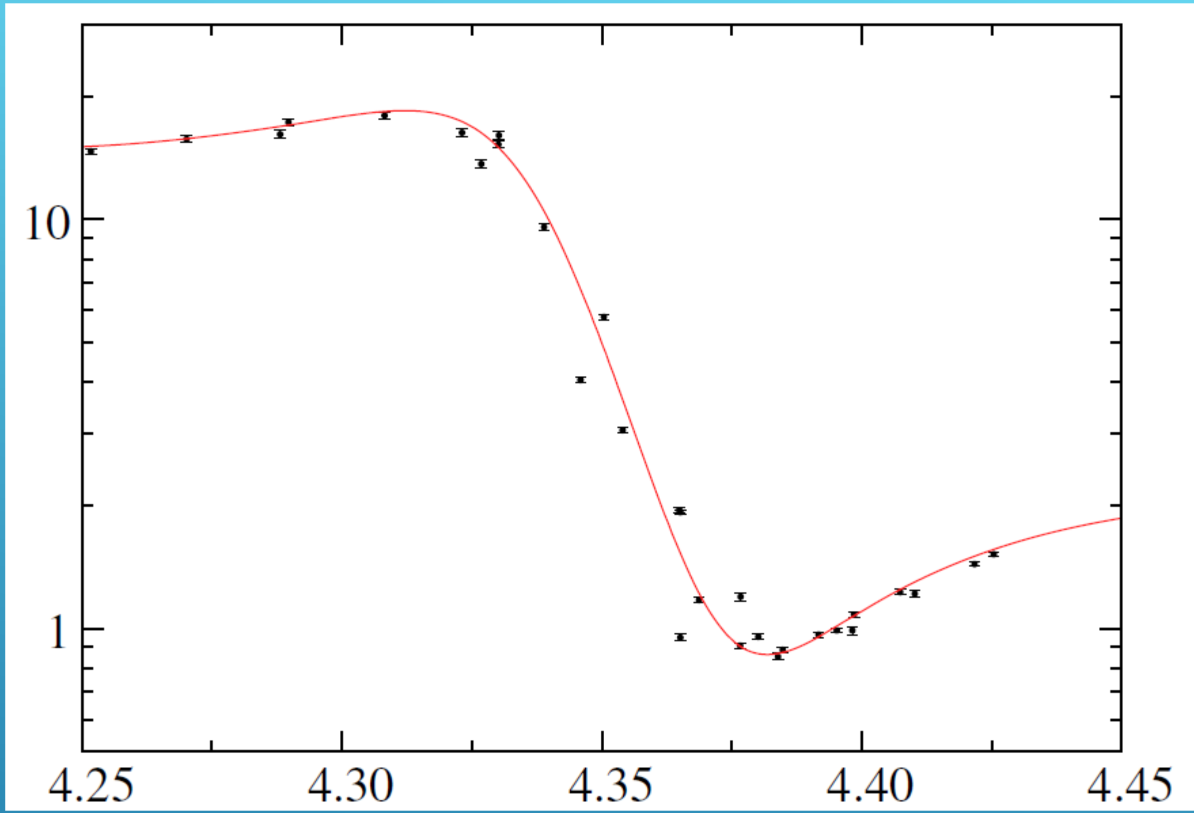


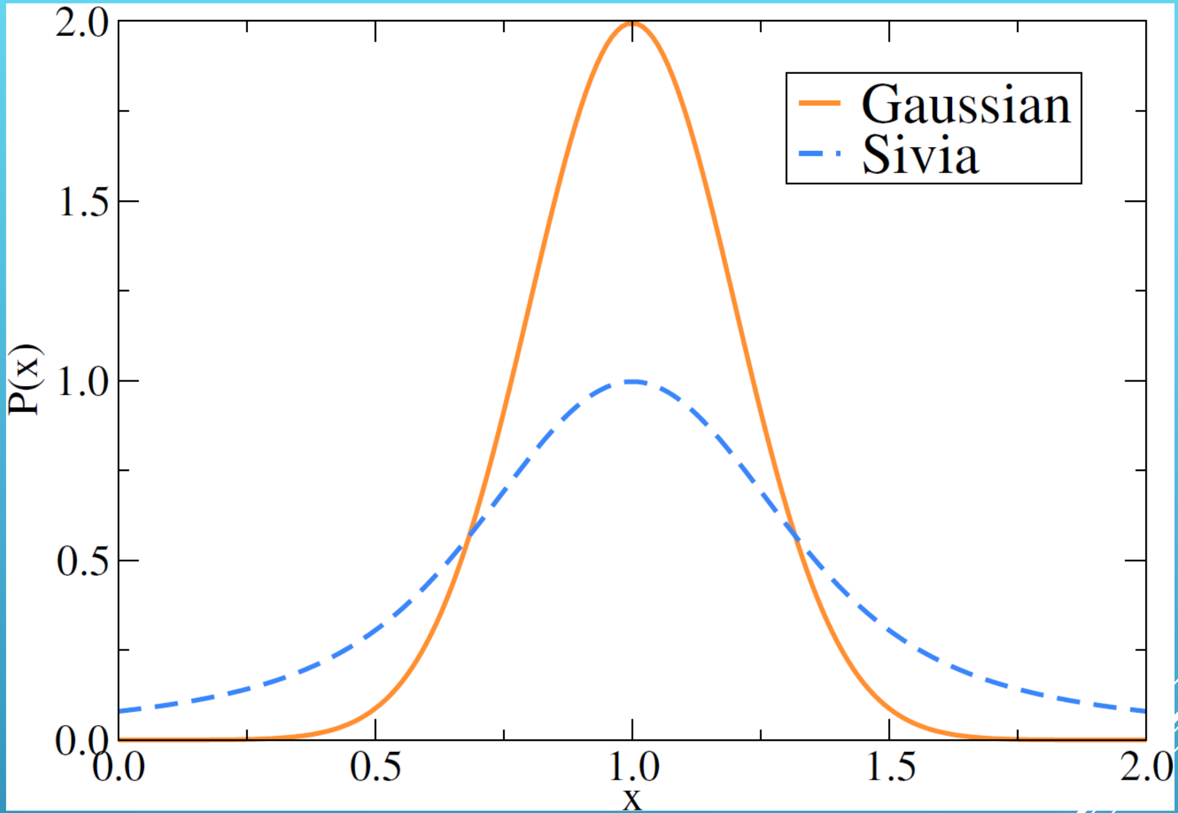
- Some people minimize to χ^2/(number of data points – number of fit parameters) of each data set
- Often does lead to a solution that seems more physically reasonable
- Removes the weight from data sets with large numbers of data with small uncertainties
- Assuming both types of uncertainties are Normally distributed

$$\chi^2 = \sum_i \left(\frac{\sum_j R_{ij}^2}{N_i - \nu} \right) + \frac{(n_i - 1)^2}{\sigma_{\mathrm{syst},i}^2},$$

$$R_{ij} = \frac{f(x_{i,j}) - n_i y_{i,j}}{n_i \sigma_{i,j}},$$

REDUCED χ^2 FITTING?





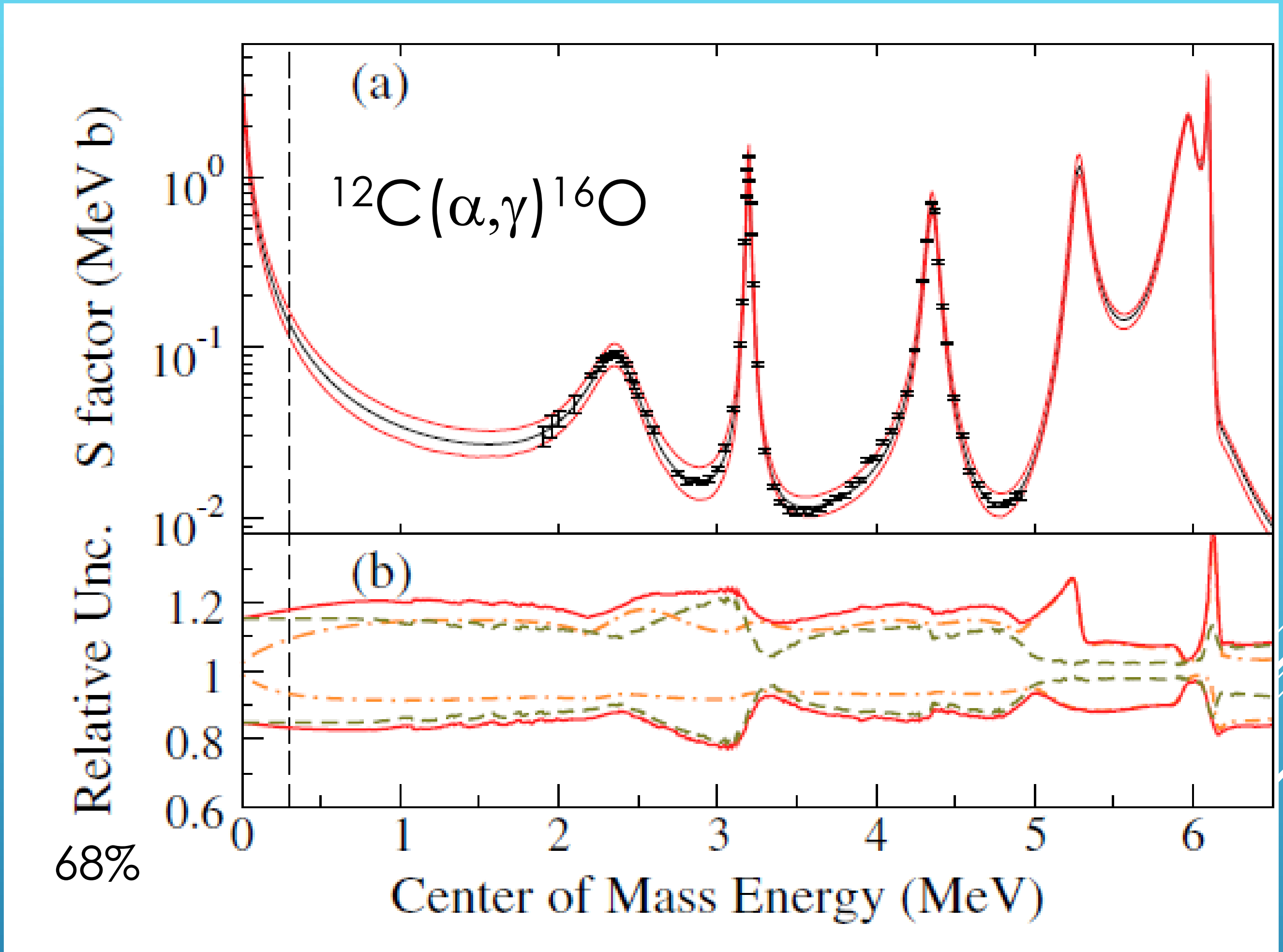
- Uncertainties are obviously underestimated
- Error bar inflation? Which ones?
- Alternate interpretation of experimental uncertainties

$$L = \sum_j \log\left[\frac{1 - e^{-R_{ij}^2/2}}{R_{ij}^2}\right]$$

Sivia and Skilling (2006)

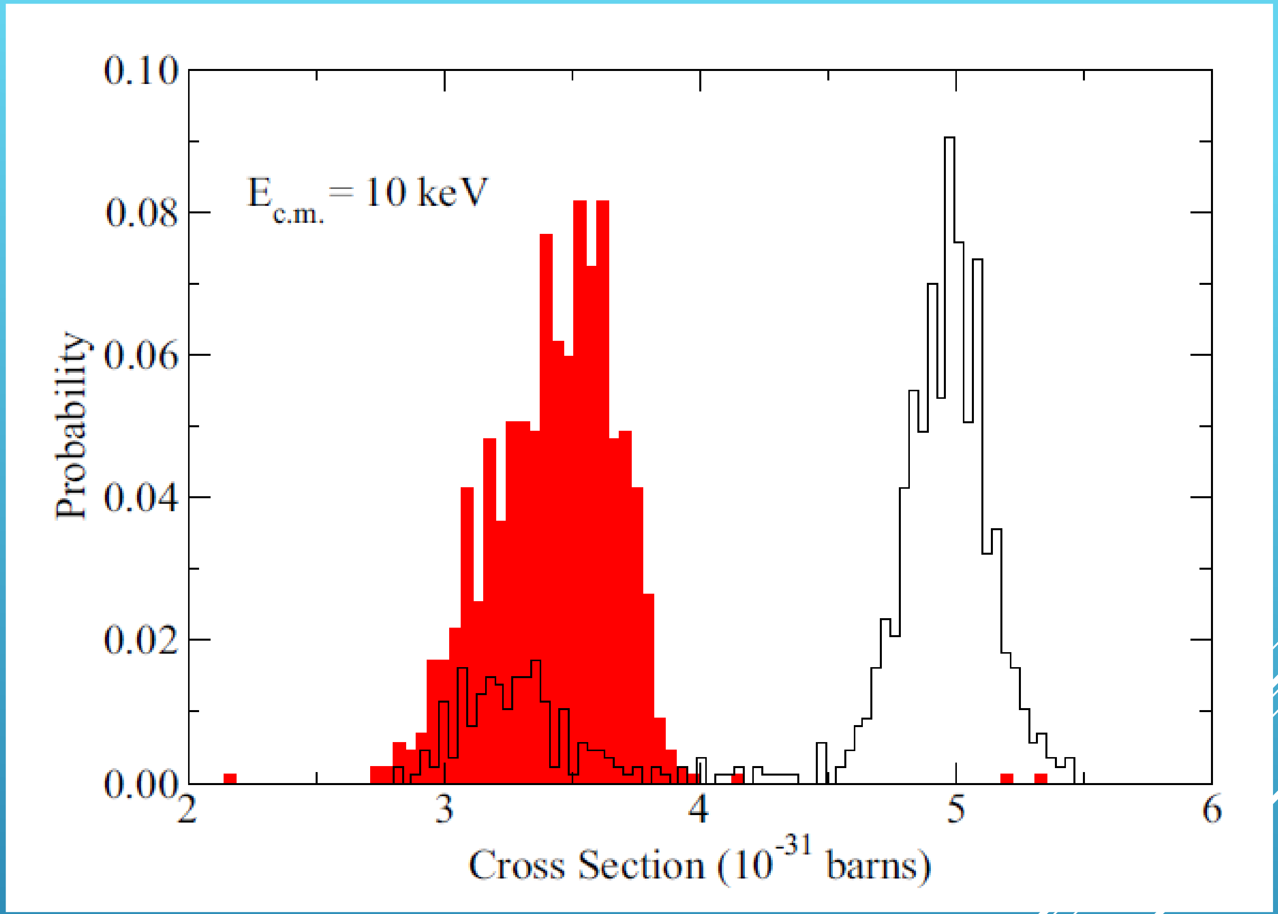
NOT FULLY CHARACTERIZED UNCERTAINTIES

- Usually a mixture of
  - experimental
    - Statistical
    - Systematic
  - and Model Uncertainties



FINAL UNCERTAINTY ANALYSIS

- Detailed pdfs of uncertainties are interesting
- End user wants (needs) something simple to they can use (Gaussian)



PDFS OF THE UNCERTAINTIES

- Techniques to identify and deal with outlier data?
- Are there minimization algorithms that are optimized for my type of problem?
  - Many fit parameters, many local minima
- Are there tools/techniques to calculate covariance matrix and propagation of uncertainty to quantities other than the fit parameters?
  - Other codes besides MINUIT2 (C++)
- Should I switch to a Bayesian uncertainty method? Is this going to actually give me better uncertainty estimates and be more practical to implement?

MY QUESTIONS / FUTURE GOALS

- Phenomenological fitting is an approach that is often necessary in nuclear physics where an observable can not be calculated to the desired accuracy from fundamental theory
- Phenomenological framework results in many fit parameters that make large analyses practically difficult
- Experimental data is often distorted from the theoretical value by experimental effects (targets, detector geometry, graduate students, etc.)
- Ideally we can refine the data, by making further corrections or by re-evaluating the uncertainties, in order be able to really compare it with the theoretical calculations in a more statistically meaningful way.
- In practice methods are needed to try to estimate the additional uncertainty resulting from the inconsistency of theory with data.

SUMMARY

IAEA

International Atomic Energy Agency

Atoms for Peace

Consultants' Meeting on

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

- Data evaluations are used as inputs for simulation codes for detector development, nuclear energy, nuclear astrophysics, etc.

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