Uncertainty quantification in nuclear reactions

Filomena Nunes
Michigan State University

In collaboration with:
Amy Lovell, Garrett King, Manuel Rios (MSU)
Stephan Wild and Jason Sarich (ANL)

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DNP 2019

What is the UQ problem:

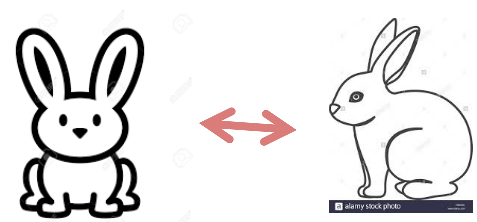
We develop a hypothesis (model)

We confront it with reality (data)

How good is the model?

Is model A better than model B?

How do I mix model A with model B?

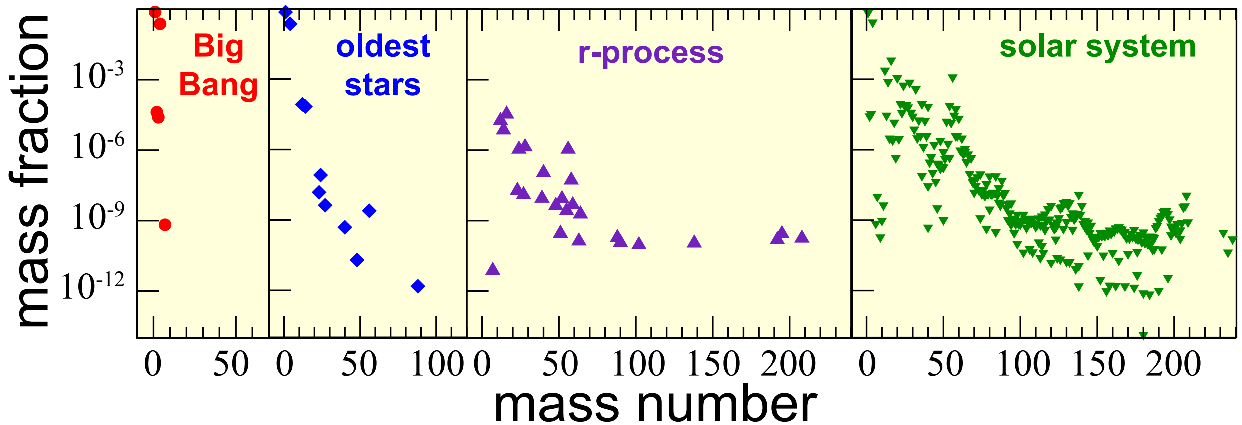


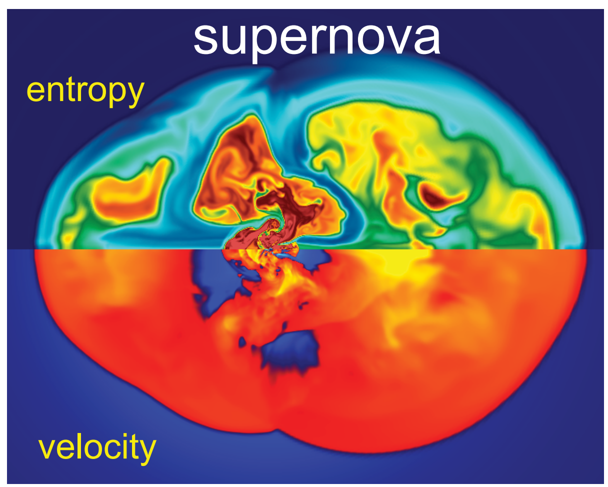
Outline

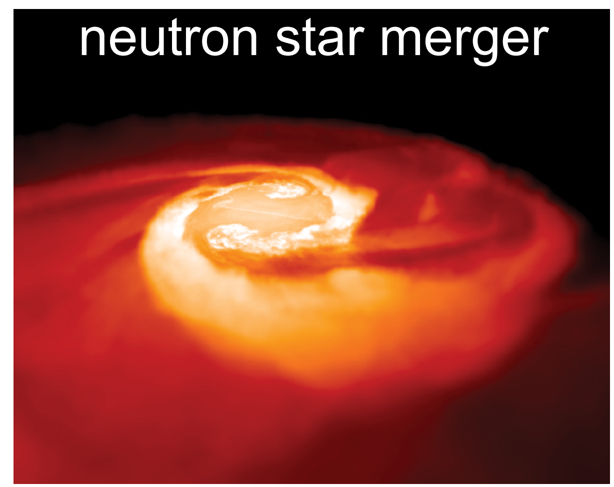
1. What is the nuclear physics problem?
2. What is the UQ problem?
3. UQ with simple frequentist approach
4. Comparison Bayesian and frequentist UQ
5. Exploring experimental conditions with Bayesian UQ
6. Outlook

The nuclear physics context

Where did nuclei come from? How were they produced?

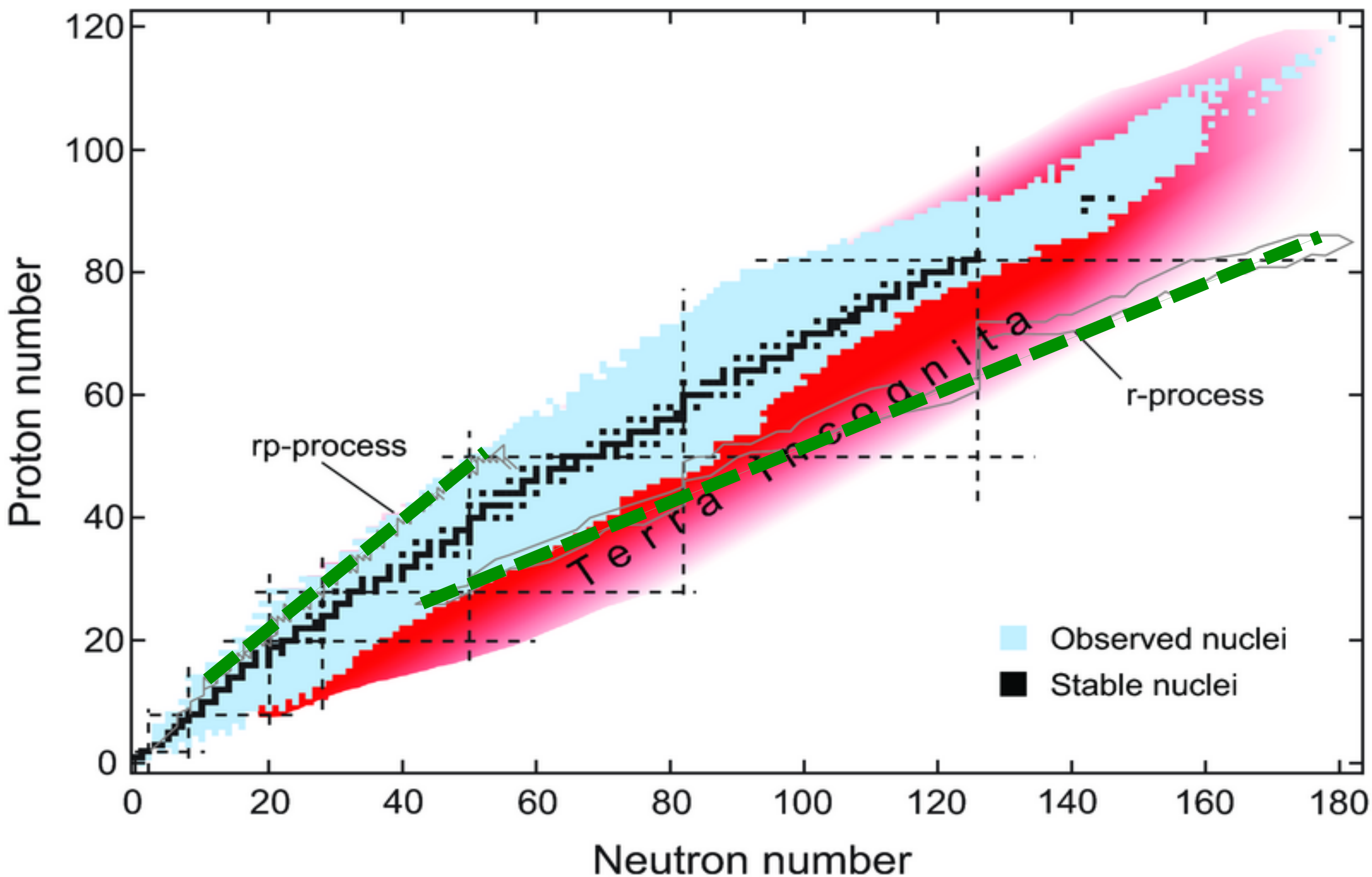






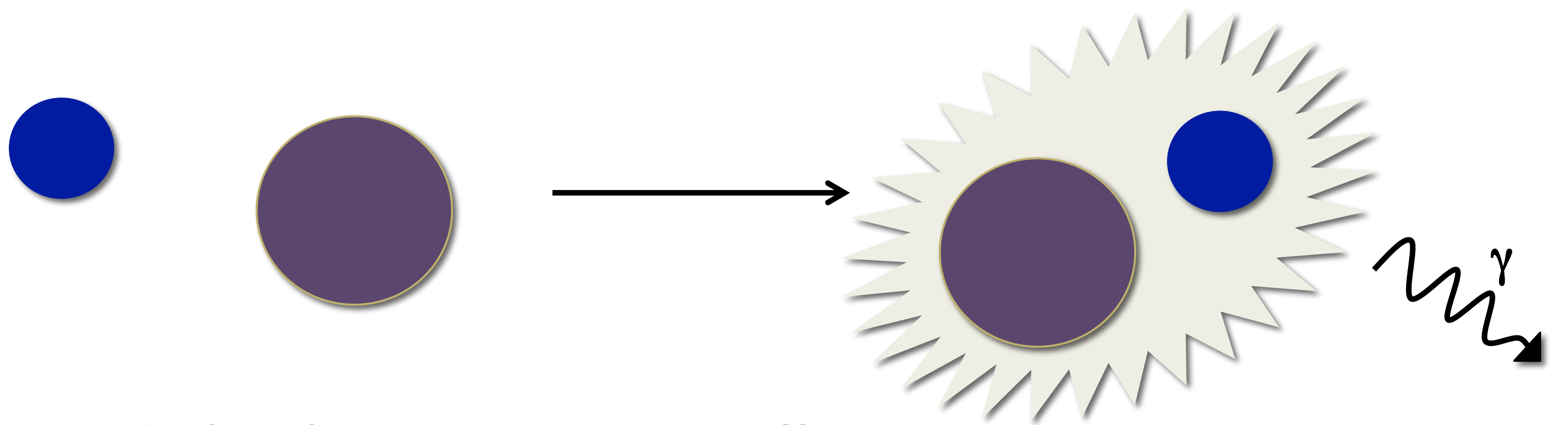
FRIB theory manifesto, Balantekin et al, MPLA 2014 (arXiv:1401.6435)

r-process nucleosynthesis and rare isotopes

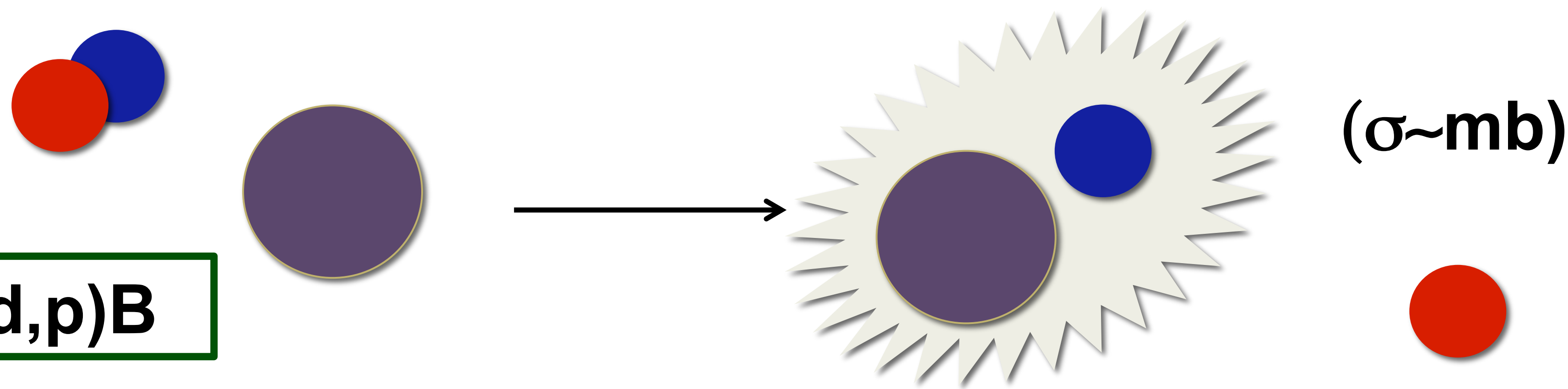


r-process: how do we measure neutron capture on unstable nuclei?

✧ (n,g) cross sections on unstable nuclei: **Currently Impossible**!



✧ (d,p) cross section offers an indirect measurement!

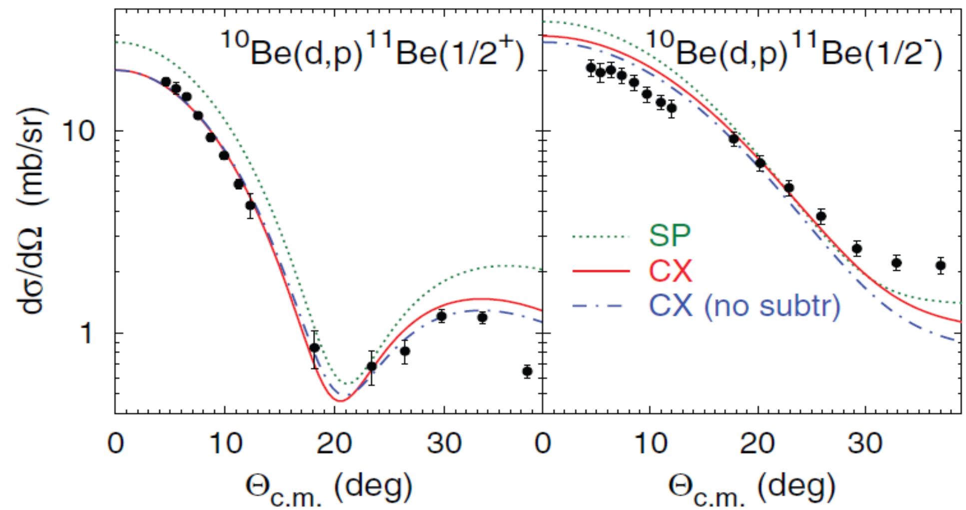


A(d,p)B

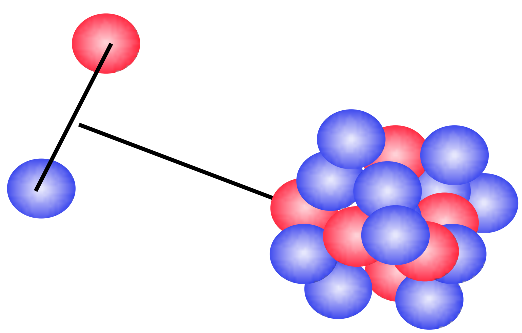
What is the nuclear physics problem: how certain are our reaction predictions?

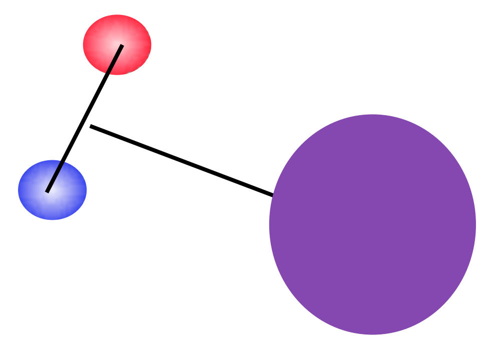
A(d,p)B

Deuteron induced reactions typically treated as a three-body problem

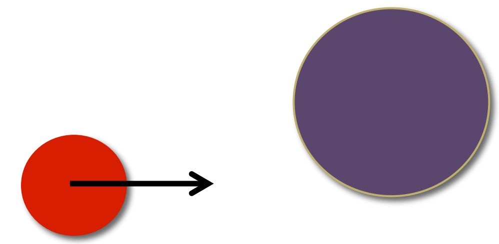


Deltuva, PRC91, 024607 (2015)





What is the UQ problem:



We develop a hypothesis (model)

optical model

[T+U(R)-E]Φ=0

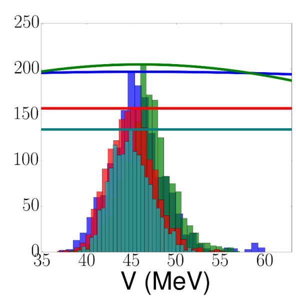
We confront it with reality (data)

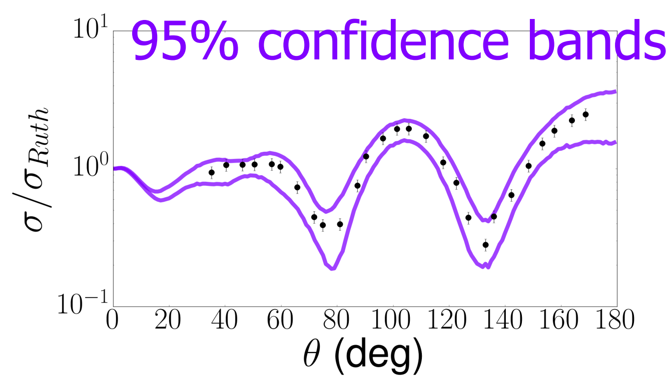
typically elastic scattering angular distributions

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{m(\mathbf{x};\theta_i) - d_i}{\sigma_i} \right)^2$$

How good is the model?

Constrains on the model





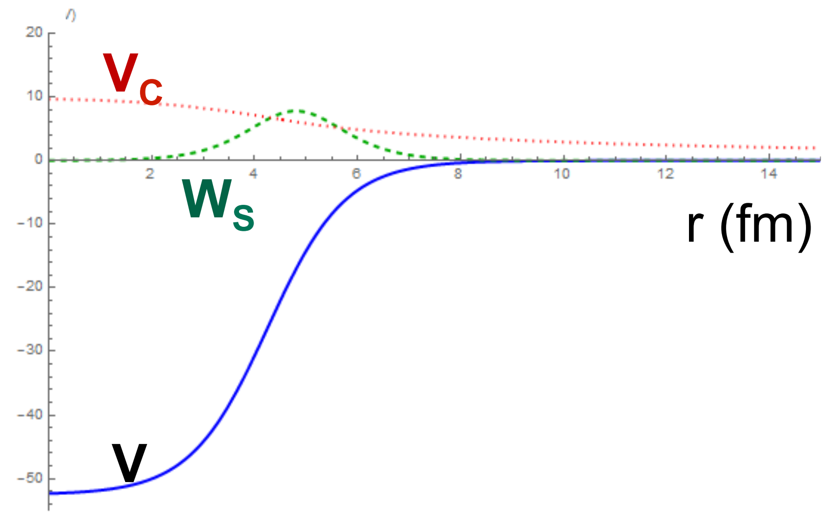
What are the parameters of the model?

Optical potentials (assumed local to reduce computational time)

$$U(r) = V(r) + iW(r) + (V_{so}(r) + iW_{so}(r))(\mathbf{l} \cdot \mathbf{s}) + V_C(r)$$

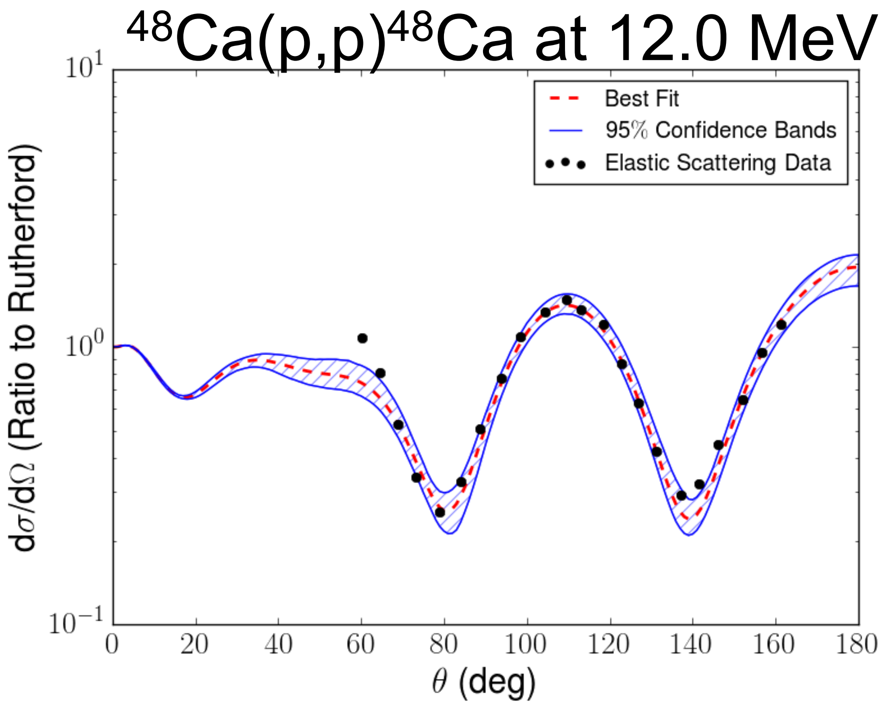
Parameters:

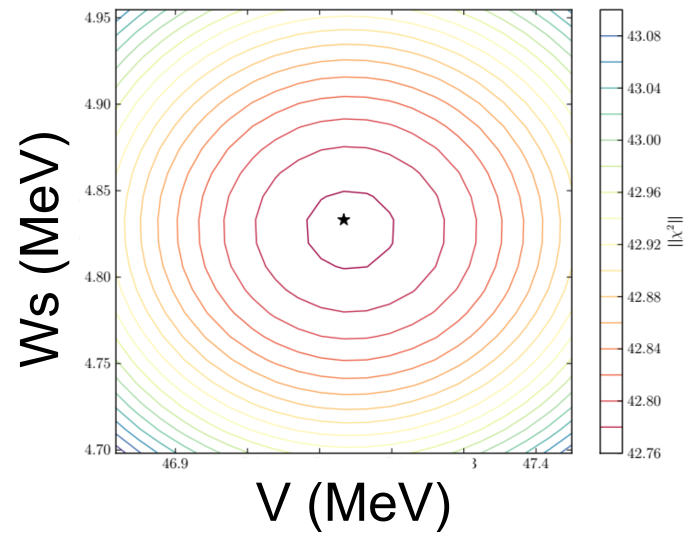
- Volume real V r a
- Volume imaginary W r_W a_W
- Surface imaginary V_s r_s a_s
- Spin-orbit real V_s r_s a_s
- ~~Spin-orbit imaginary V_s r_s a_s~~
- Coulomb r_c

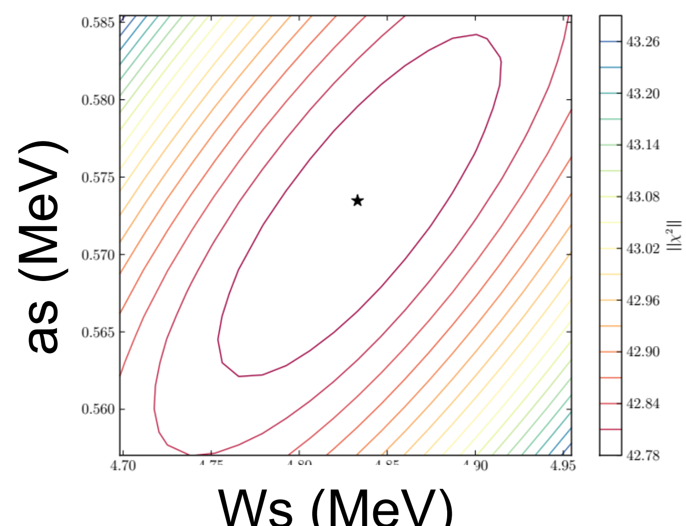


Standard Chi2 minimization

- Pull 200 sets from Chi2 distribution
- Create 95% confidence intervals by removing 2.5% top and 2.5% bottom of the predicted observables







Lovell, Nunes, Sarich, Wild, PRC 95,024611 (2017)

Chi2 minimization and correlations

Previously: Uncorrelated Model

- Data and residuals are normally distributed

$$[d_1, ..., d_p]^T \sim \mathcal{N}(\mu, \Sigma)$$

$$[m(\mathbf{x};\theta_1) - d_1, ..., m(\mathbf{x};\theta_p) - d_p]^T \sim \mathcal{N}(0, \Sigma)$$

- With covariance matrix

$$\Sigma_{ii} = \sigma_i^2$$

- Leads to the minimization function

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{m(\mathbf{x};\theta_i) - d_i}{\sigma_i} \right)^2$$

Instead: For a Correlated Model

- Model is also normally distributed

$$[m(\mathbf{x};\theta_1), ..., m(\mathbf{x};\theta_p)]^T \sim \mathcal{N}(\mu, \mathbb{C}_m)$$

- Residuals then have the distribution

$$[m(\mathbf{x};\theta_1) - d_1, ..., m(\mathbf{x};\theta_p) - d_p]^T \sim \mathcal{N}(0, \mathbb{C}_m + \Sigma)$$

- With covariance matrix

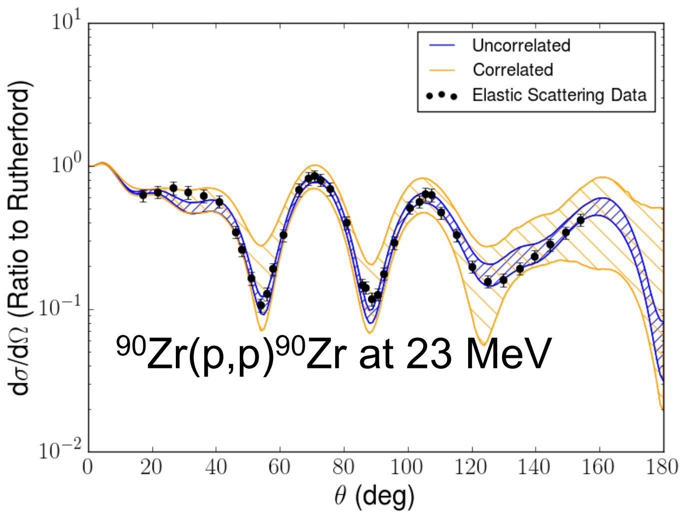
$$\mathbb{C}_m + \Sigma$$

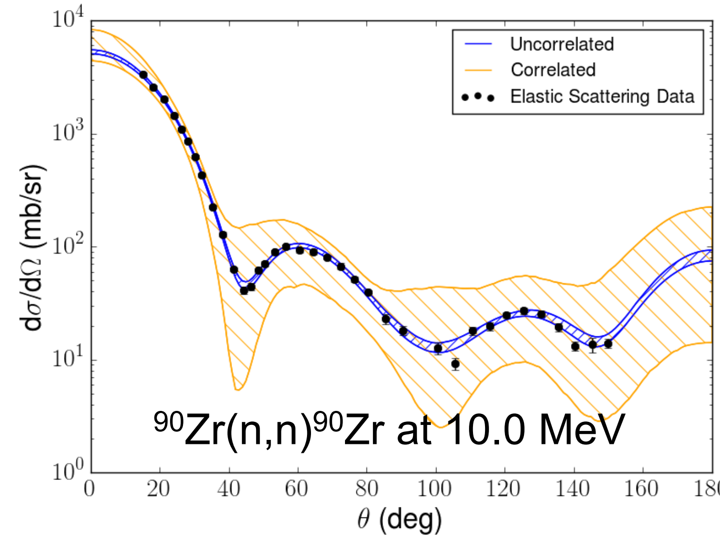
- Leads to the minimization function

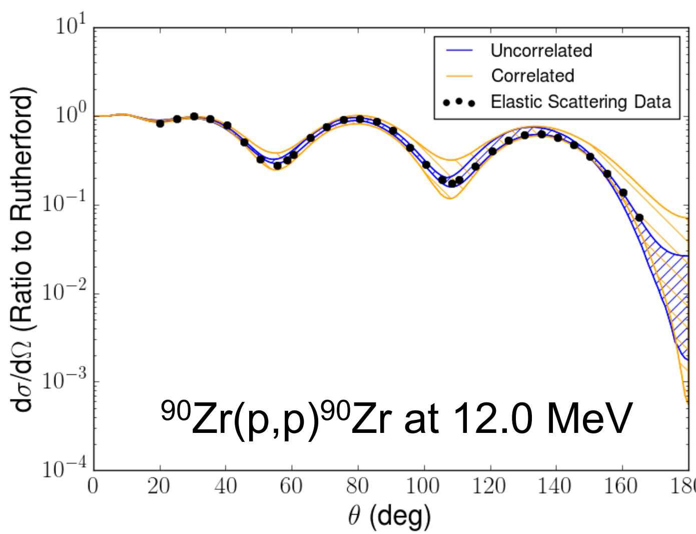
$$\chi^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (m(\mathbf{x};\theta_i) - d_i)(m(\mathbf{x};\theta_j) - d_j)$$

$$W = (\mathbb{C}_m + \Sigma)^{-1}$$

Chi2 minimization and correlations







Correlated Chi2 produces **wider** confidence intervals

Lovell, Nunes, Sarich, Wild, PRC 95,024611 (2017)

What is the model for (d,p) reactions?

DWBA: distorted wave Born approximation

Exact T-matrix for A(d,p)B in POST from:

$$T_{post} =< \phi_{nA}\, \chi^{(-)}_{pB} \mid \Delta V_f \mid \Psi^{(+)}_1(\vec{r}_1, \vec{R}_1) >$$

deuteron elastic component

Take first term of Born series: $\Psi^{(+)}_1(\vec{r}_1, \vec{R}_1) \rightarrow \phi_{np}\, \chi_{dA}$

$$T^{DWBA}_{post} =< \phi_{nA}\, \chi^{(-)}_{pB} \mid \Delta V_f \mid \phi_{np}\, \chi_{dA} >$$

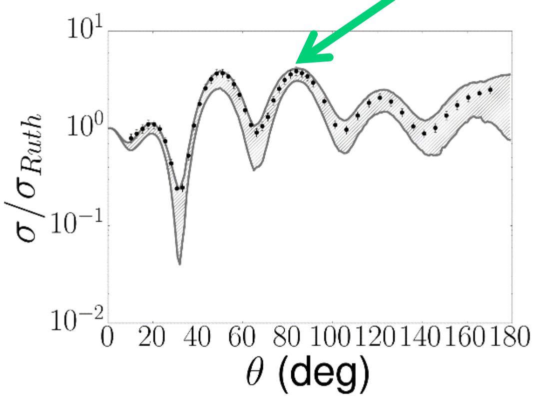
What is the model for (d,p) reactions?

DWBA: distorted wave Born approximation

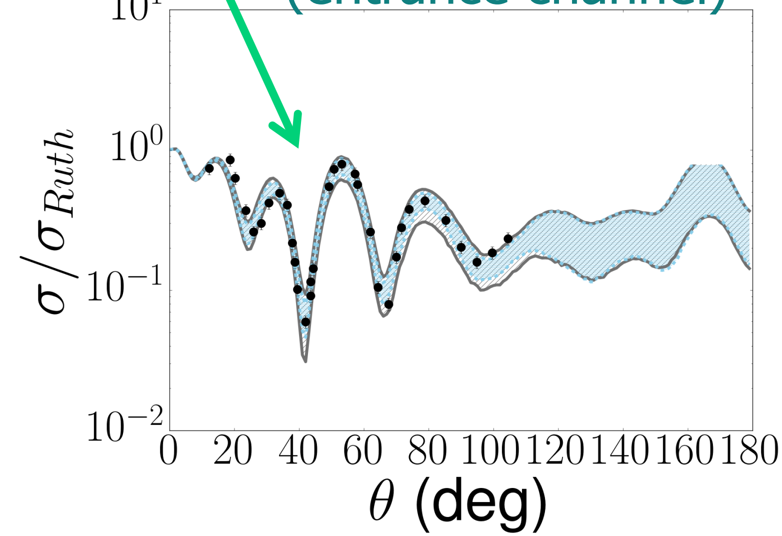
$$\Psi_1^{(+)}(\vec{r}_1, \vec{R}_1) \rightarrow \phi_{np}\, \chi_{dA}$$

$$T_{post}^{DWBA} = < \phi_{nA}\, \chi_{pB}^{(-)} \mid \Delta V_f \mid \phi_{np}\, \chi_{dA} >$$

proton elastic data
(exit channel)



deuteron elastic data
(entrance channel)



What is the model for (d,p) reactions?

ADWA: Adiabatic wave approximation

Exact T-matrix for A(d,p)B in POST from:

Johnson and Tandy, NPA1974

$$T_{post} = < \phi_{nA}\, \chi_{pB}^{(-)} \mid \Delta V_f \mid \Psi_1^{(+)}(\vec{r}_1, \vec{R}_1) >$$

finite range adiabatic approximation

Adiabatic wave approximation:

3B wave function expanded in Weinberg states

$$\Psi^{\text{exact}} = \sum_{i=0}^{\infty} \phi_i(\vec{r})\chi_i(\vec{R})$$

$$(T + \lambda_i V_{np} - \epsilon_d)\phi_i = 0$$

$$U_{ij}(\vec{R}) = -\langle \phi_i | V_{np}(U_{nA} + U_{pA}) | \phi_j \rangle$$

Typically, only keep the first Weinberg State

$$\Psi^{ad} \approx \phi_0(\vec{r})\chi_0(\vec{R})$$

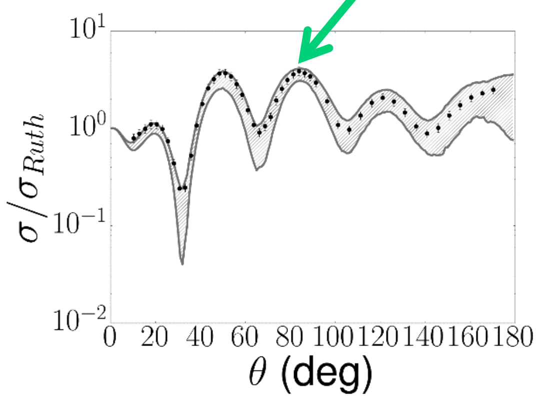
What is the model for (d,p) reactions?

ADWA: Adiabatic wave approximation

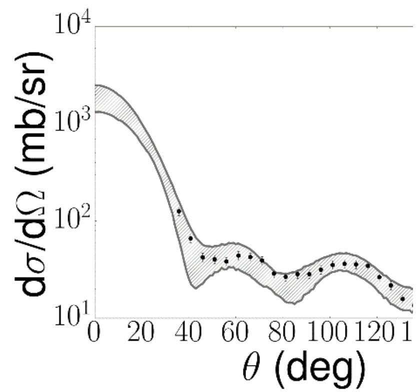
$$T^{(d,p)} = \langle \phi_{An} \chi_p | V_{np} | \phi_d \chi_d^{ad} \rangle$$

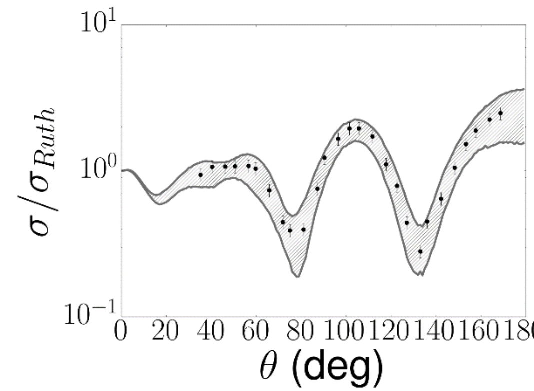
$$U_{ij}(\vec{R}) = -\langle \phi_i | V_{np}(U_{nA} + U_{pA}) | \phi_j \rangle$$

proton elastic data
(exit channel)



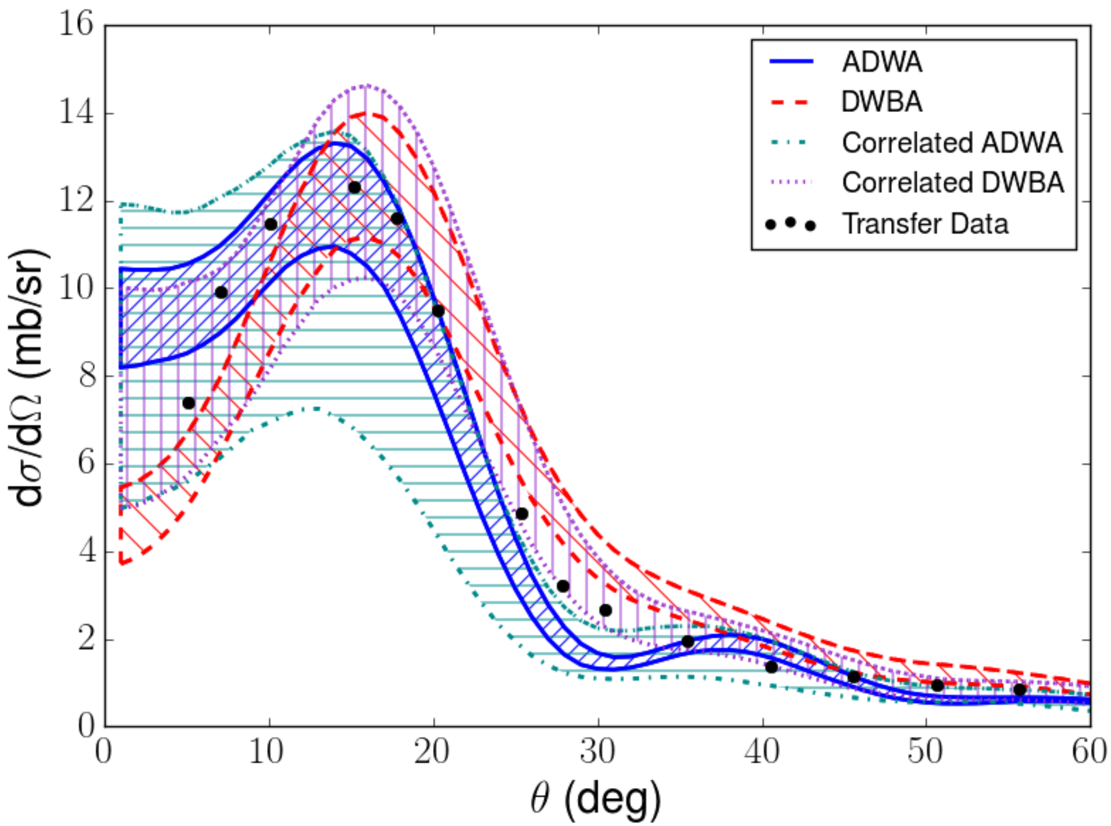
neutron and proton elastic data
(entrance channel)





Chi2 minimization: transfer predictions

^{90}Zr(d,p)^{90}Zr at 23 MeV



Uncorrelated: which model is better? data looks like a mix of ADWA and DWBA…

Correlated: Uncertainties are too large to discriminate between models

King, Lovell, Nunes, PRC 98, 044623 (2018)

Limitations of the frequentist approach

Philosophical aspects:

- Probability as frequency: number of events over a total number of trails
- A 95% confidence band means that when repeating the measurement many times, 95% of the times the data should fall within the band.
- There is no way to include UQ on events that cannot be repeated (e.g. how likely is it that the power will fail during this talk?).

Practical aspects:

- Problem with local minima versus the global minimum
- Inclusion of prior knowledge comes through ranges allowed for parameters – potential for introducing biases
- What is the correct Chi2 function that includes the correct correlations in the theoretical model?

Bayes' theorem

P(green,red)= 5/9 x 4/9

P(red,green)= 4/9 x 5/9

P(green,red)=P(red,green)

Bayesian statistics

Thomas Bayes (1701–1761)

Bayes’ Theorem

$$P(\mathcal{H}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{H})P(\mathcal{H})}{P(\mathcal{D})}$$

Posterior – probability that the model/parameters are correct after seeing the data

Prior – what is known about the model/parameters before seeing the data

Likelihood – how well the model/parameters describe the data $p(D|H) = e^{-\chi^2/2}$

Evidence – marginal distribution of the data given the likelihood and the prior

Markov Chain Monte Carlo (MCMC)

$$p(H_i)p(D|H_i)$$

Randomly choose new parameters

$$p(H_f)p(D|H_f)$$

$$R < \frac{p(H_f)p(D|H_f)}{p(H_i)p(D|H_i)}$$

Comparing frequentist and Bayesian

- Probability as frequency
- A 95% confidence band means that when repeating the measurement many times, 95% of the times the data should fall within the band.

Practical aspects:

- local minima
- ranges allowed for parameters – potential for introducing biases
- correlations in the theoretical model?

- Probability as degree of belief
  - Posterior distribution updates our degree of belief on the model, in light of the data
- A 95% confidence interval means, given the data, what are the parameter ranges of the model for a 95% degree of belief.

Practical aspects:

- Markov Chain Monte Carlo (MCMC) spans full space and is fully automated
- Inclusion of prior (reduction of biases)
- Correlations automatically included
- Computationally more expensive

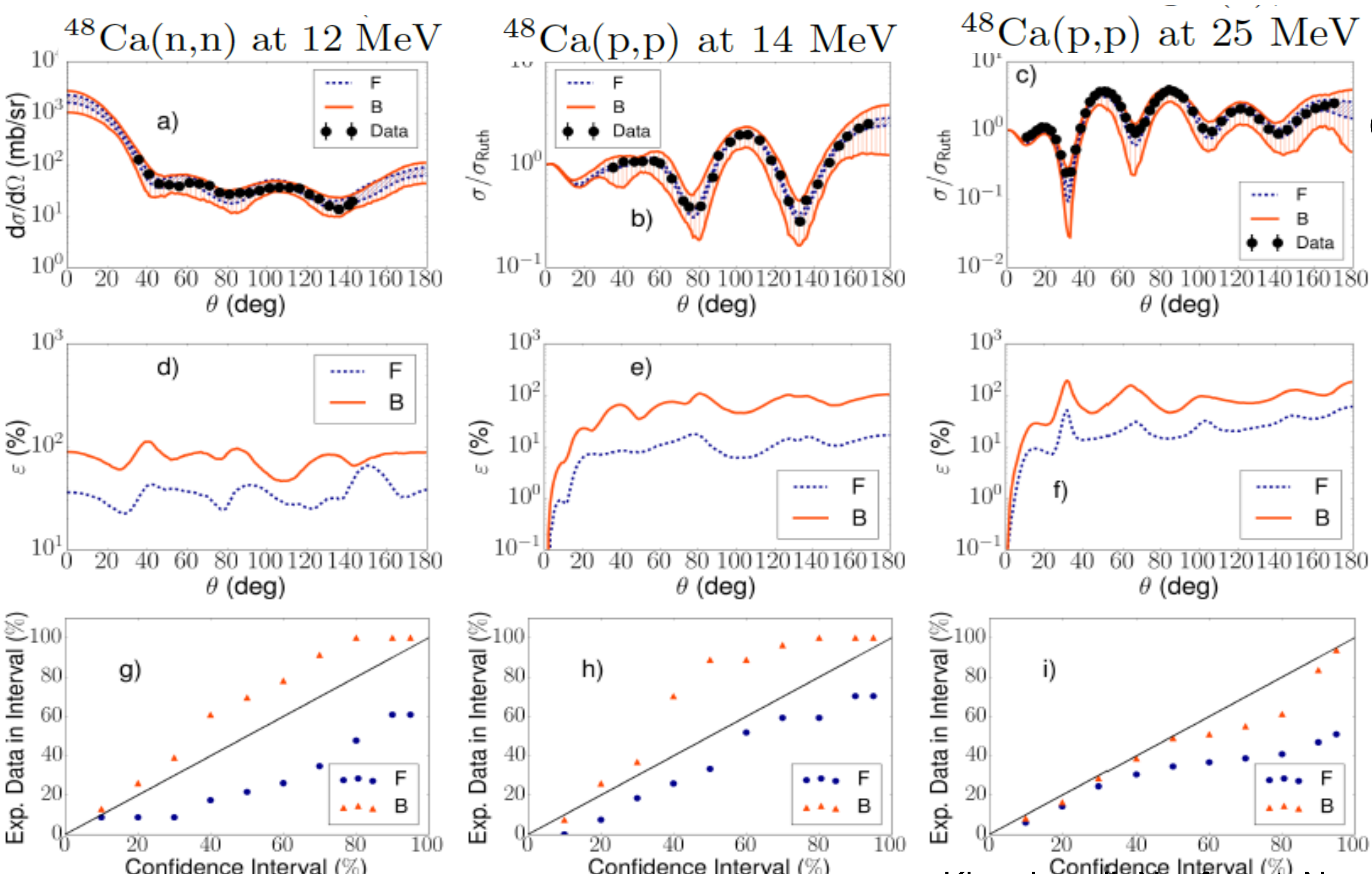
The Bayesian Conspiracy: "What matters is that Bayes is cool, and if you don't know Bayes, you aren't cool."

Yudkowsky offers to decode the secret:

> *Maybe you see the theorem, and you understand the theorem, and you can use the theorem, but you can't understand why your friends and/or research colleagues seem to think it's the secret of the universe. Maybe your friends are all wearing Bayes' Theorem T-shirts, and you're feeling left out. Maybe you're a girl looking for a boyfriend, but the boy you're interested in refuses to date anyone who "isn't Bayesian". What matters is that Bayes is cool, and if you don't know Bayes, you aren't cool.*

http://www.anotherpanacea.com/2012/10/the-bayesian-conspiracy-what-matters-is-that-bayes-is-cool-and-if-you-dont-know-bayes-you-arent-cool/

Optical model uncertainties: comparing frequentist and Bayesian



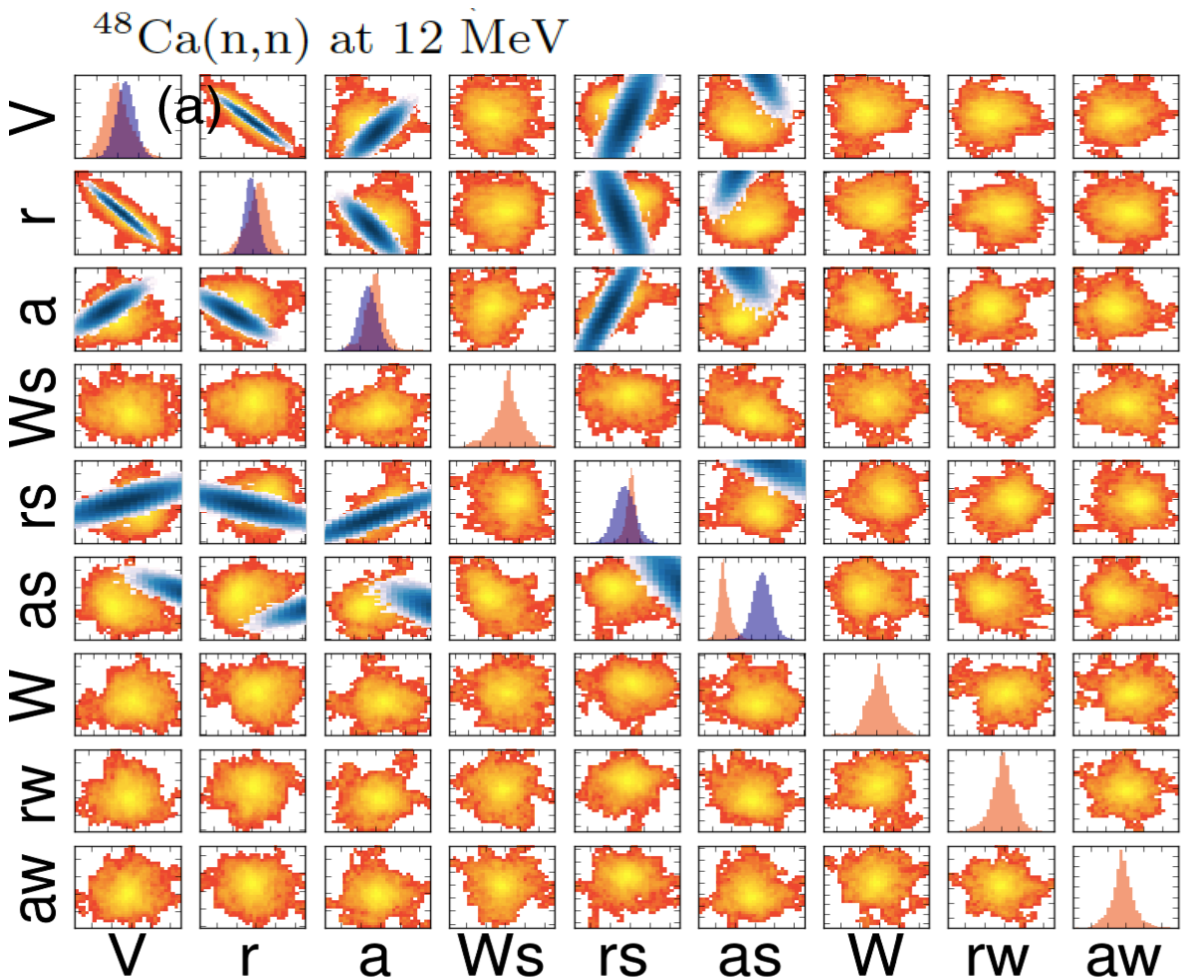
Cross section angular distributions

Percentage uncertainty width

Empirical coverage

King, Lovell, Neufcourt, Nunes PRL (2019)

Optical model uncertainties: comparing frequentist and Bayesian

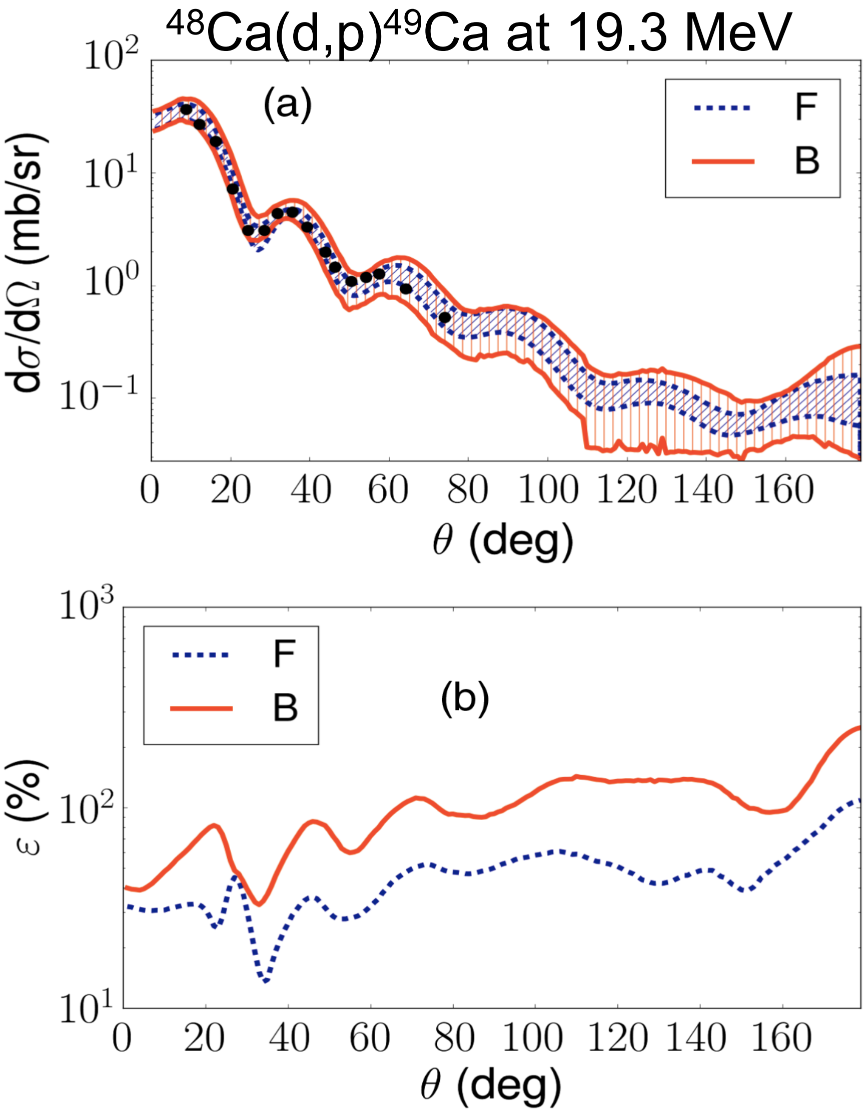


parameter correlations in Bayesian look very different than in the frequentist approach

blue (frequentist)
orange (Bayesian)

King, Lovell, Neufcourt, Nunes PRL (2019)

Propagating optical model uncertainties to (d,p) comparing frequentist and Bayesian



Uncertainties are larger than previously thought

Need to explore ways to reduce optical potential uncertainties

King, Lovell, Neufcourt, Nunes PRL (2019)

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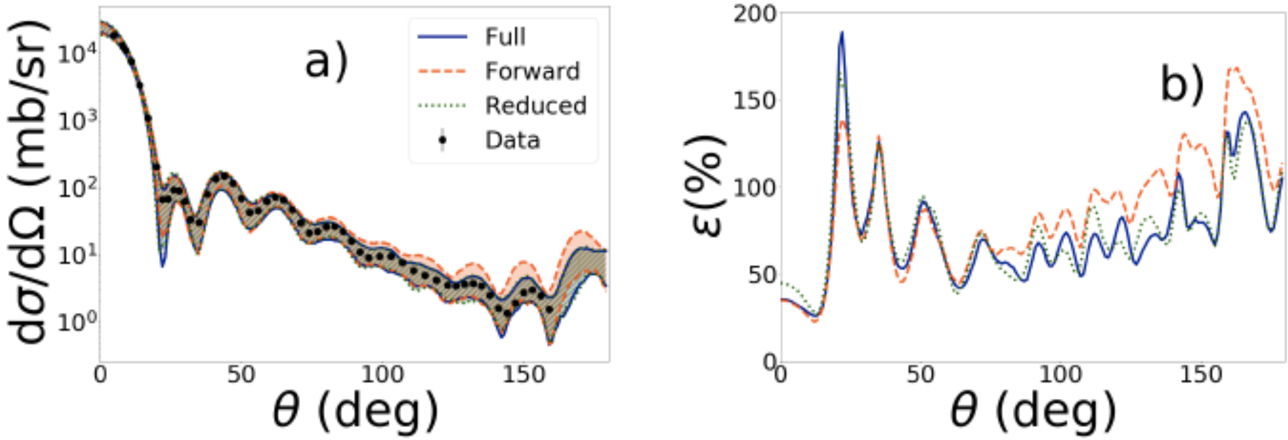
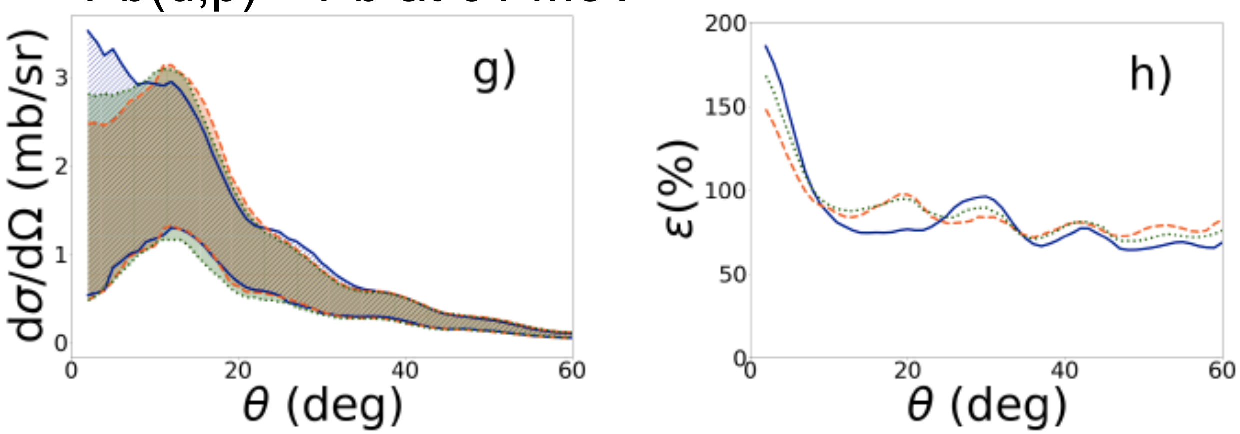
Exploring experimental conditions: Angular information

^{208}Pb(n,n)^{208}Pb at 30 MeV



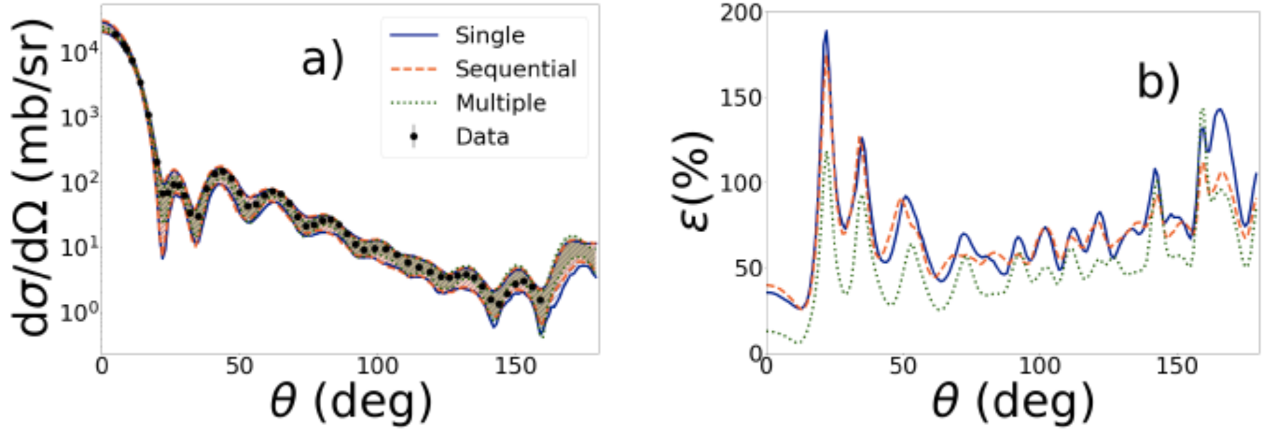
^{208}Pb(d,p)^{209}Pb at 61 MeV



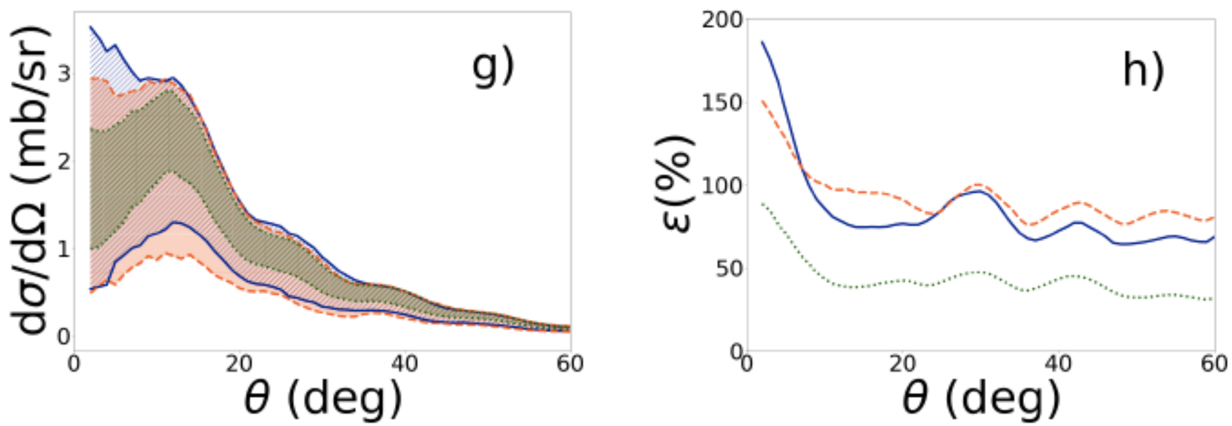
Catacora-Rios, King, Lovell, Nunes; PRC submitted

Exploring experimental conditions: beam energy

$^{208}Pb(n,n)^{208}Pb$ at 30 MeV



$^{208}Pb(d,p)^{209}Pb$ at 61 MeV



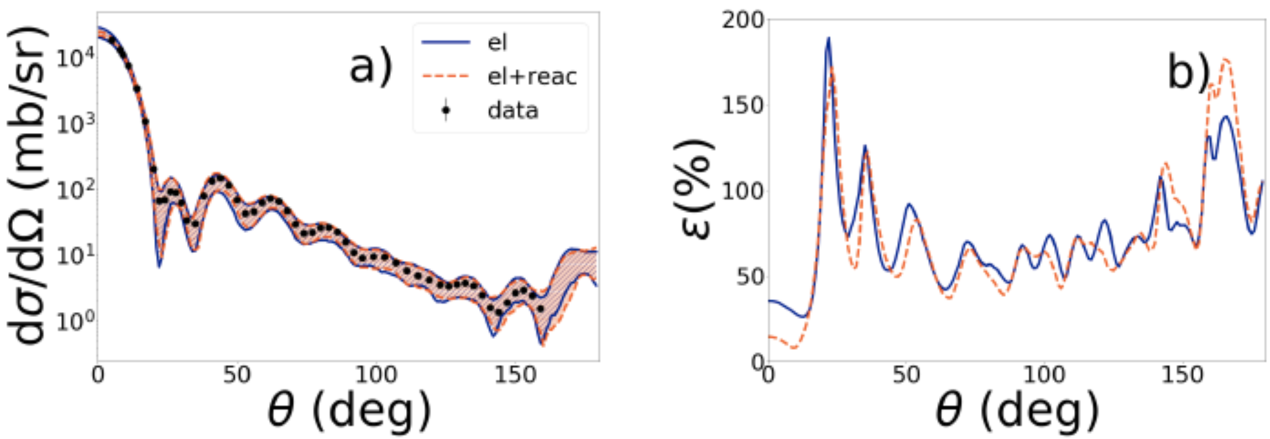
Catacora-Rios, King, Lovell, Nunes; PRC submitted

Exploring experimental conditions: exp error bar

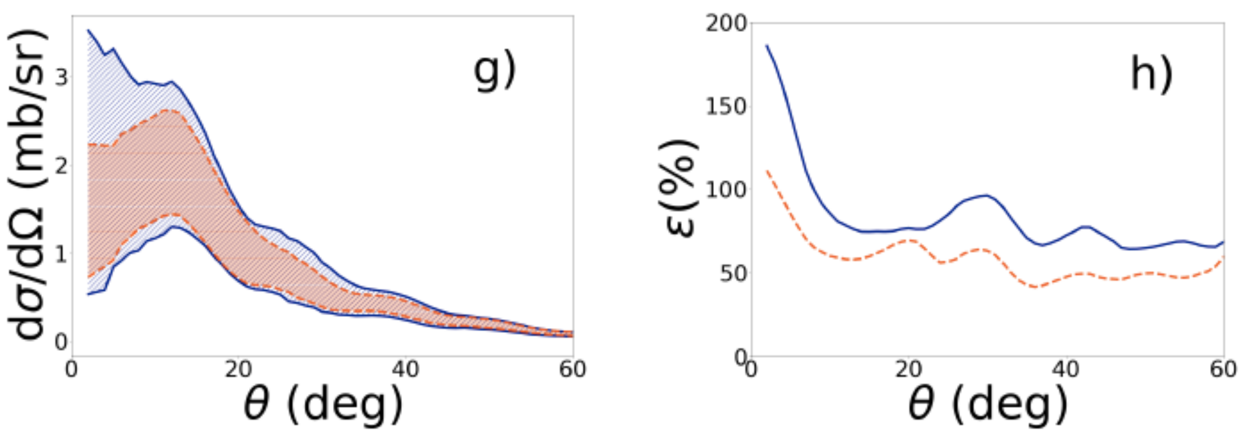
Reaction	$\Delta\varepsilon_{20/10}$	$\Delta\varepsilon_{10/5}$
^{48}Ca(n,n) at 12 MeV	1.53	1.94
^{48}Ca(p,p) at 12 MeV	1.68	1.71
^{48}Ca(p,p) at 21 MeV	1.55	1.74
^{48}Ca(d,p) at 21 MeV	1.68	1.52
^{208}Pb(n,n) at 30 MeV	1.62	1.79
^{208}Pb(p,p) at 30 MeV	1.39	1.61
^{208}Pb(p,p) at 61 MeV	1.99	1.74
^{208}Pb(d,p) at 61 MeV	1.41	1.58

Catacora-Rios, King, Lovell, Nunes; PRC submitted

Exploring experimental conditions: adding total (reaction) cross section



^{208}Pb(n,n)^{208}Pb at 30 MeV



^{08}Pb(d,p)^{209}Pb at 61 MeV

Catacora-Rios, King, Lovell, Nunes; PRC submitted

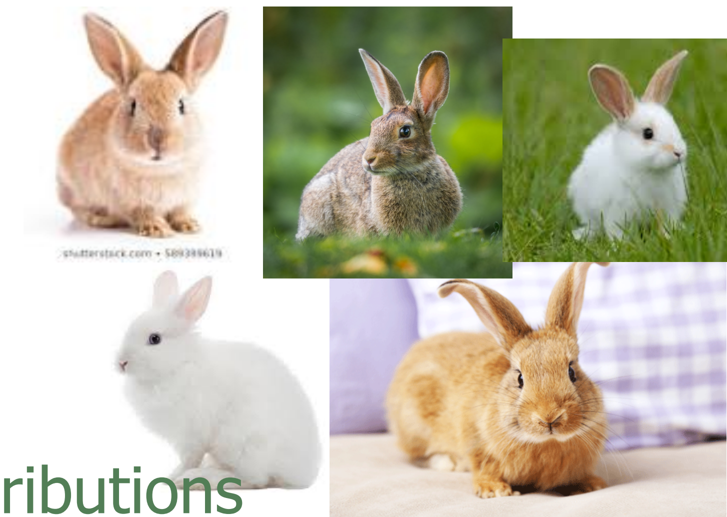
Conclusions

- Frequentist approach is not reliable: high confidence intervals to strongly overestimate the level of confidence on should have in the predictions

- Bayesian approach shows large uncertainties, larger than originally thought.
- Also reveals different picture for parameter correlations

- Still hard to discern between models so exploring ways to decrease uncertainty:
  - Using additional data at nearby energies
  - Using total/reaction cross sections in addition to elastic

Outlook



Diversify the data to reduce uncertainties:

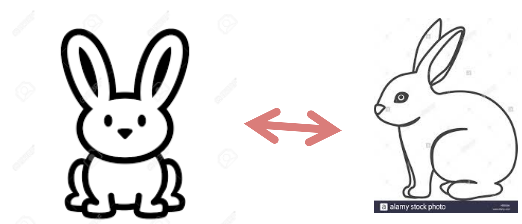
- Including polarization data
- Including charge exchange angular distributions

Model comparison, model mixing and model error?

How good is the model?

Is model A better than model B?

How do I mix model A with model B?



Thank you for your attention!

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