Uncertainty Quantification for Reaction Theory

A.E. Lovell

April 21, 2020
Reaction Seminar

LA-UR-20-23038

Outline

- Sources of uncertainty in few-body reactions
- Uncertainty quantification methods
  - χ^2 minimization
  - Bayesian methods
- Results
  - χ^2 minimization – $^{12}C(d,p)$
  - Bayesian methods – $^{48}Ca(d,p)$
- Comparison between methods
- Connections and outlook

- A.E. Lovell, F.M. Nunes, *J. Phys. G* **42**, 034014 (2015)
- A.E. Lovell, F.M. Nunes, J. Sarich, S. M. Wild, *PRC* **95**, 024611 (2017)
- A. E. Lovell, F. M. Nunes, *PRC* **97**, 064162 (2018)
- G. B. King, A. E. Lovell, F. M. Nunes, *PRC* **98**, 044628 (2018)
- G. B. King, A. E. Lovell, L. Neufcourt, F. M. Nunes, *PRL* **122**, 232501 (2019)
- M. Catacora-Rios, G. B. King, A. E. Lovell, F. M. Nunes, *PRC* **100**, 064615 (2019)
- Lovell, Nunes, Catacora-Rios, King, Carriello, *in prep*
- Lovell, Mohan, Talou, *in prep*

Uncertainty quantification in nuclear theory

Enhancing the interaction between nuclear experiment and theory through information and statistics (ISNET)

2015

2015 *J. Phys. G: Nucl. Part. Phys.* 42 Issue 3 **Guest Editors:** David Ireland and Witek Nazarewicz

Focus on further enhancing the interaction between nuclear experiment and theory through information and statistics (ISNET 2.0)

Now

Guest Editors

Dick Furnstahl Ohio State University

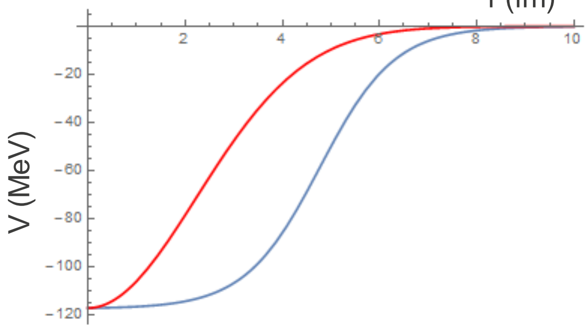
David Ireland University of Glasgow

Daniel Phillips Ohio University

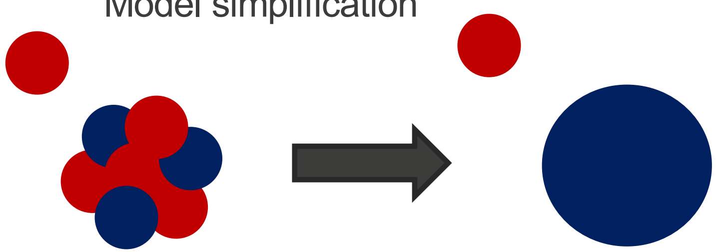
Types of uncertainty in few-body reaction theories

Systematic Uncertainties

Shape of the potential

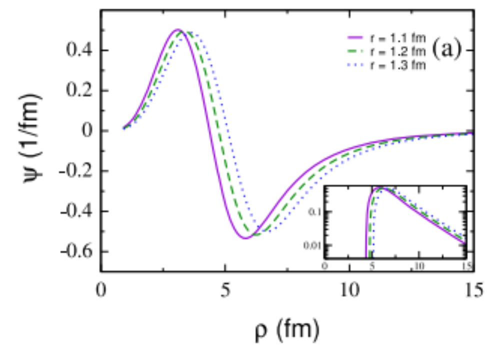


Model simplification



Statistical Uncertainties

Constraints on parameters



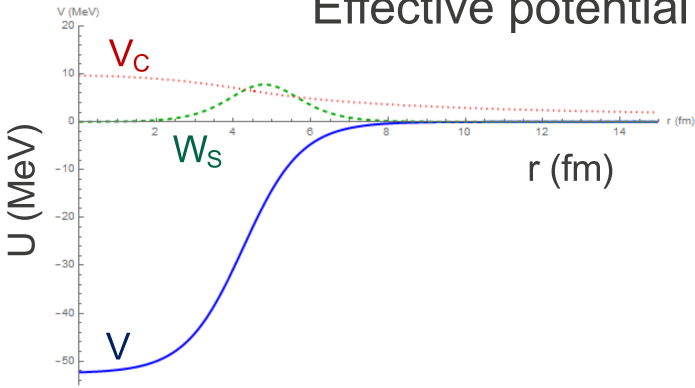
Convergence of functions

$$\sum_{k=1}^{k_{max}} f_k(x) \approx \sum_{k=1}^{\infty} f_k(x)$$

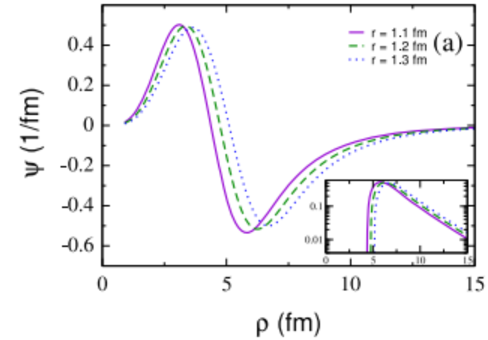
A.E. Lovell and F.M. Nunes J. Phys. G **42** 034014 (2015)

Sources of uncertainty in few-body reaction theories

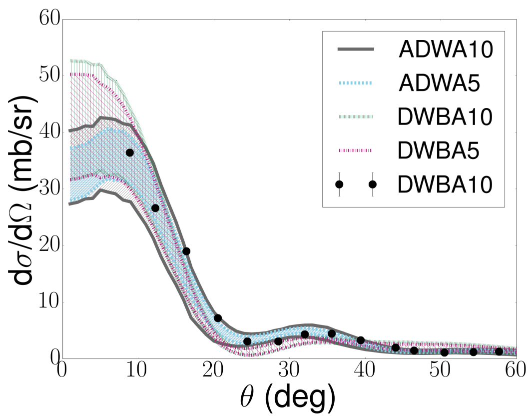
Effective potential



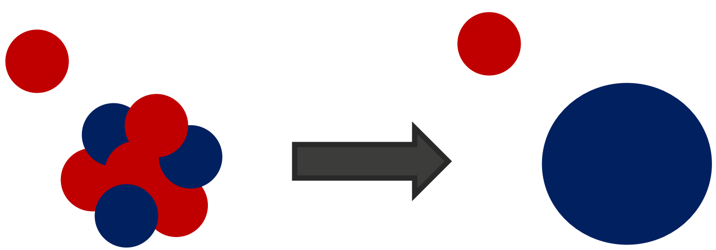
Structure functions



Few-body approximations made



Missing degrees of freedom



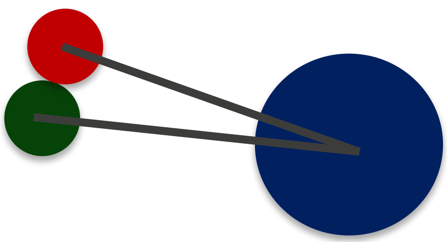
A.E. Lovell and F.M. Nunes J. Phys. G **42** 034014 (2015)

Reactions of interest: A(d,p)B

Few-body models for single-nucleon transfer reactions

$$[T_R + H_{\text{int}}(\vec{r}) + V_{pA} + V_{nA} - E]\Psi^{\text{exact}}(\vec{r}, \vec{R}) = 0 \qquad H_{\text{int}} = T_r + V_{np}(r)$$

Adiabatic Wave Approximation (ADWA)



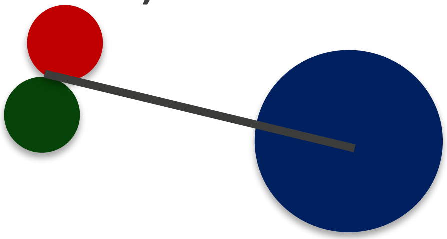
Nucleon-target potentials take into account deuteron break-up

$$[T_R + \epsilon_0 + V_{pA} + V_{nA} - E]\,\Psi^{\text{ad}}(\vec{r}, \vec{R}) = 0.$$

$$\Psi^{\text{ad}}(\vec{r}, \vec{R}) = \phi_0(\vec{r})\chi_0^{\text{ad}}(\vec{R}) + \sum_{i>0} \phi_i(\vec{r})\chi_i^{\text{ad}}(\vec{R})$$

Finite-range, Johnson and Tandy, *Nucl. Phys. A* **235** 56 (1974)

Distorted-Wave Born Approximation (DWBA)



Uses an effective deuteron-target potential

$$\Psi^{\text{exact}}(\vec{r}, \vec{R}) \;\Rightarrow\; \Phi_{I_b I_a}(\vec{r}_i)\chi_i(\vec{R}_i)$$

np bound state

Deuteron scattering state

I.J. Thompson and F.M. Nunes, *Nuclear Reactions for Astrophysics*, (Cambridge University Press, Cambridge, 2009)

Phenomenological optical model potentials

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

Volume Term

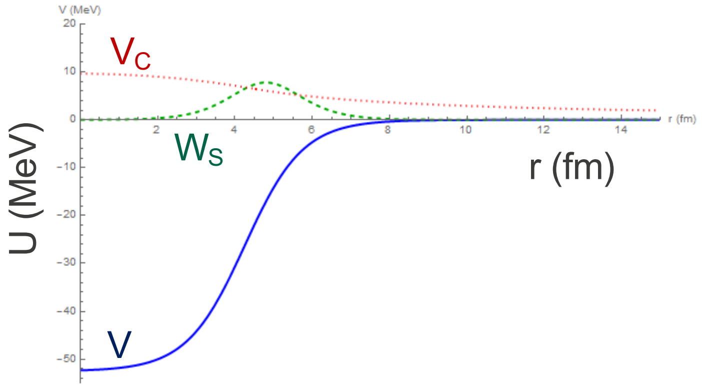
$$V(r) = f(r; V_o, R_o, a_o)$$

Surface and Spin-Orbit Terms

$$V(r) = \frac{d}{dr} f(r; V_o, R_o, a_o)$$

$$f(r; V_o, R_o, a_o) = -\frac{V_o}{1 + e^{(r-R_o)/a_o}}$$

$\approx$ 6-12 free parameters



I.J. Thompson and F.M. Nunes, *Nuclear Reactions for Astrophysics*, (Cambridge University Press, Cambridge, 2009)

χ^2 minimization and covariance propagation

- In fitting the model to the observables, the goal is to minimize the residuals

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

$$[m(\hat{\mathbf{x}};\theta_1) - d_1, \ldots, m(\mathbf{x};\theta_n) - d_n]^T \sim \mathcal{N}(0, \Sigma)$$

$\hat{\mathbf{x}}$ → Best fit set of parameters

- Assume that the parameters are normally distributed around the best-fit set, pull parameter sets and run them through the model

$$\mathcal{N}(\hat{\mathbf{x}}, \mathbb{C}_p) = \frac{1}{\sqrt{2\pi|\mathbb{C}_p|}} e^{-\frac{1}{2}(\mathbf{x}-\hat{\mathbf{x}})^T \mathbb{C}_p^{-1} (\mathbf{x}-\hat{\mathbf{x}})}$$

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

$$\mathbb{C}_p \to s^2 \mathbb{C}_p$$

- 95% confidence intervals are constructed by removing the top 2.5% and bottom 2.5% of the calculations at each angle

Makes use of I. Thompson's fresco/sfresco: www.fresco.org.uk

Bayesian optimization

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

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

Parameter sets are accepted through the Markov Chain Monte Carlo algorithm (MCMC)

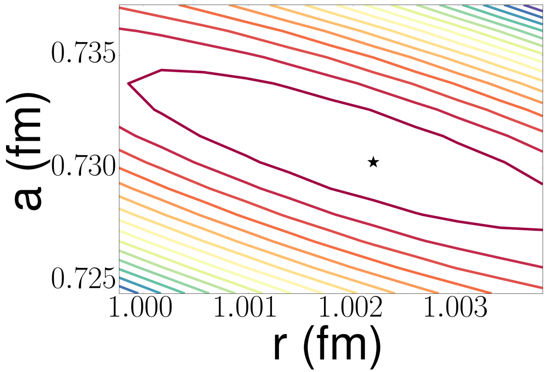
Confidence intervals are defined by the densest region of each parameter distribution or observable calculation

$$p(H) \propto \prod_{i=1}^{N_p} \exp\left[\frac{(x^i - x_0^i)^2}{(x_0^i)^2}\right]$$

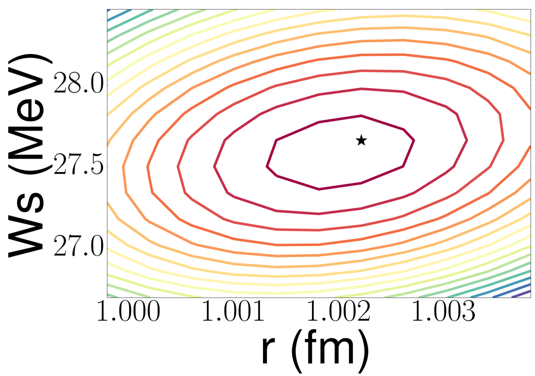
Built on top of I. Thompson's fresco: www.fresco.org.uk

Fitting elastic scattering with χ^2 minimization

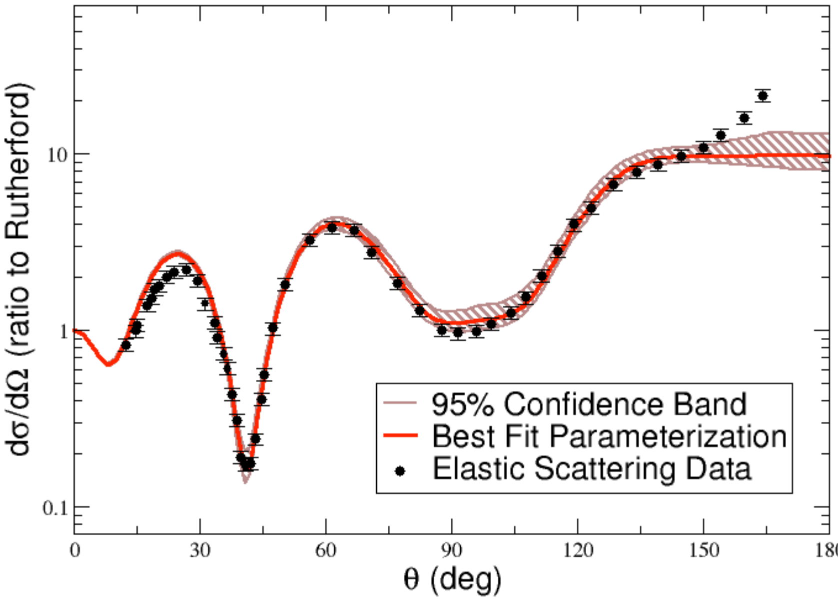
Correlated parameters



Uncorrelated parameters



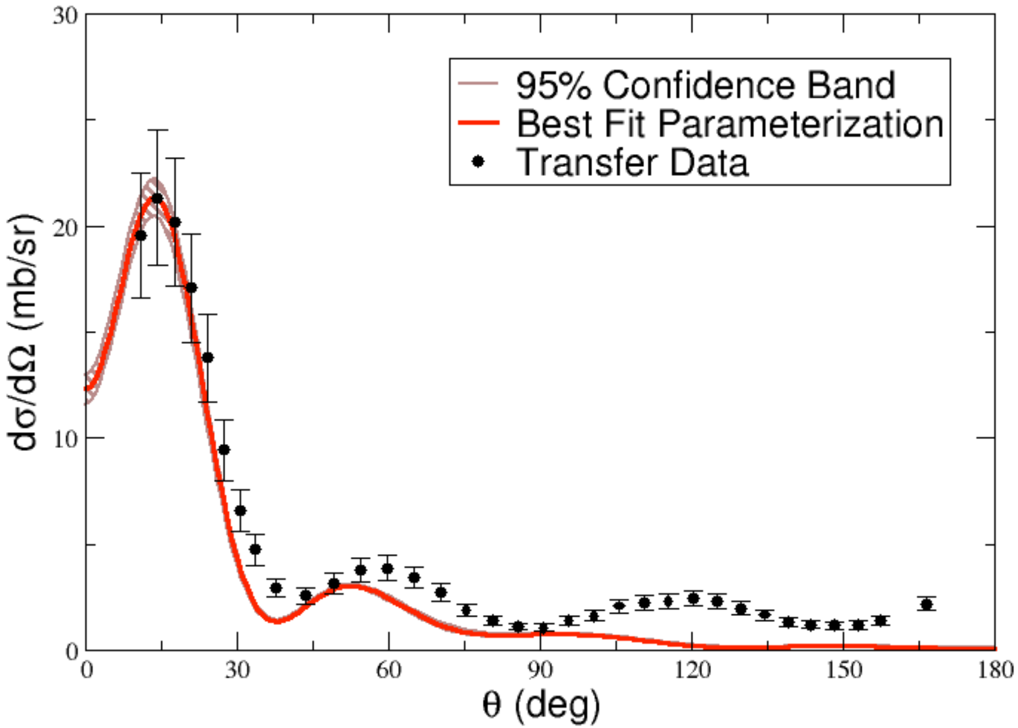
$^{12}C(d,d)$ @ 11.8 MeV



A.E. Lovell, F.M. Nunes, J. Sarich, S. M. Wild, *PRC* **95**, 024611 (2017)

Propagating to the transfer cross section (DWBA)

$^{12}C(d,p)^{13}C$(g.s.) @ 11.8 MeV

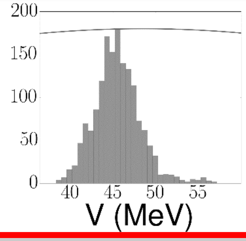


A.E. Lovell, F.M. Nunes, J. Sarich, S. M. Wild, *PRC* **95**, 024611 (2017)

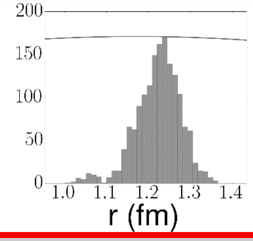
Bayesian posterior distributions

^{48}Ca(n,n) @ 12 MeV

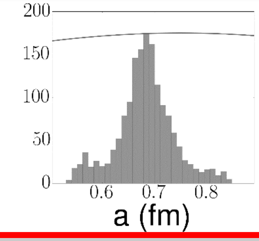
Real Volume



μ=45.51
σ=2.74
(MeV)

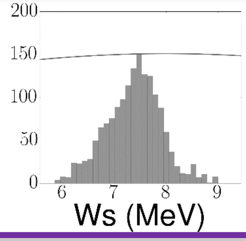


1.22
0.05
(fm)

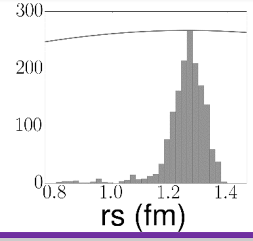


0.68
0.06
(fm)

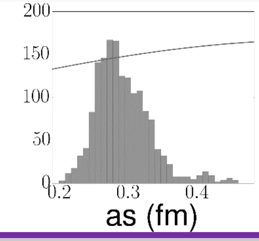
Imaginary Surface



7.38
0.54
(MeV)

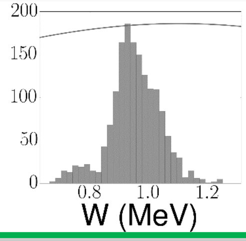


1.25
0.08
(fm)

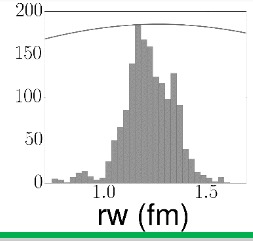


0.29
0.04
(fm)

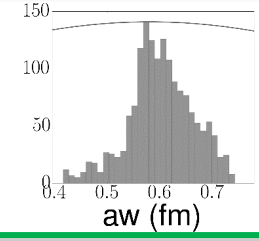
Imaginary Volume



0.95
0.09
(MeV)



1.21
0.12
(fm)

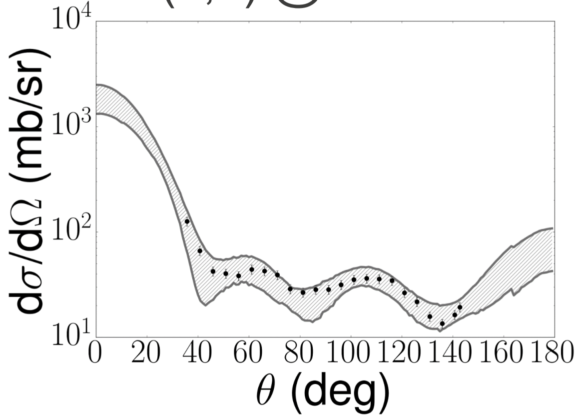


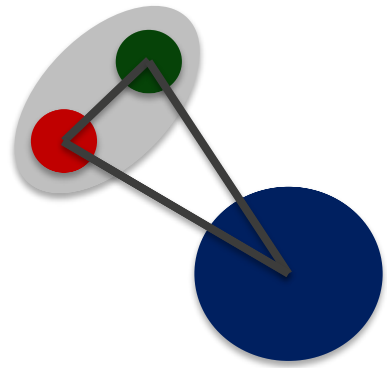
0.60
0.06
(fm)

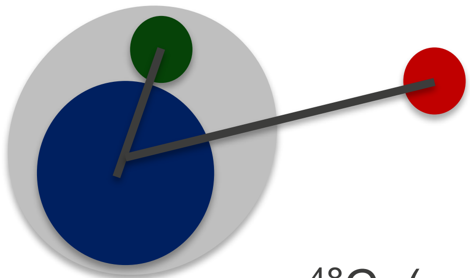
A. E. Lovell, F. M. Nunes, *PRC* **97**, 064162 (2018)

Bayesian elastic scattering confidence intervals

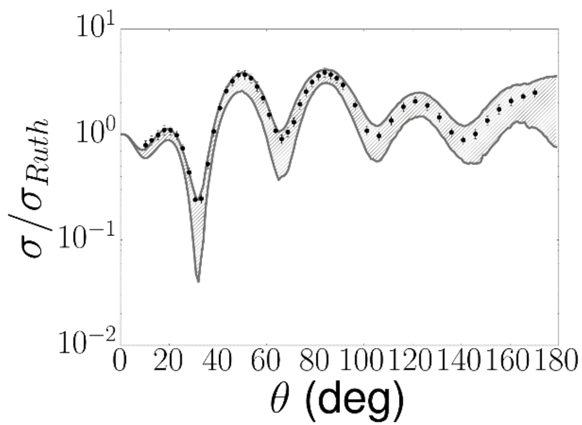
^{48}Ca(n,n) @ 12.0 MeV





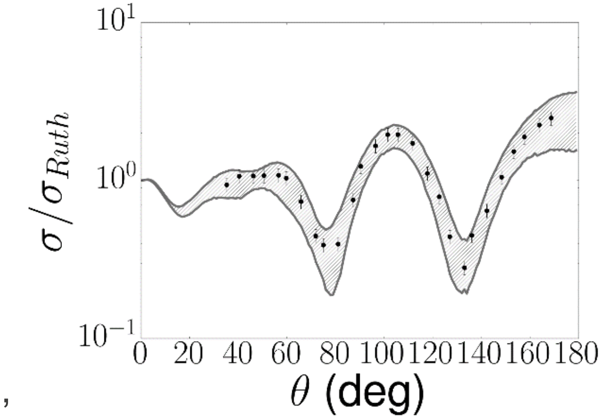


^{48}Ca(p,p) @ 25.0 MeV



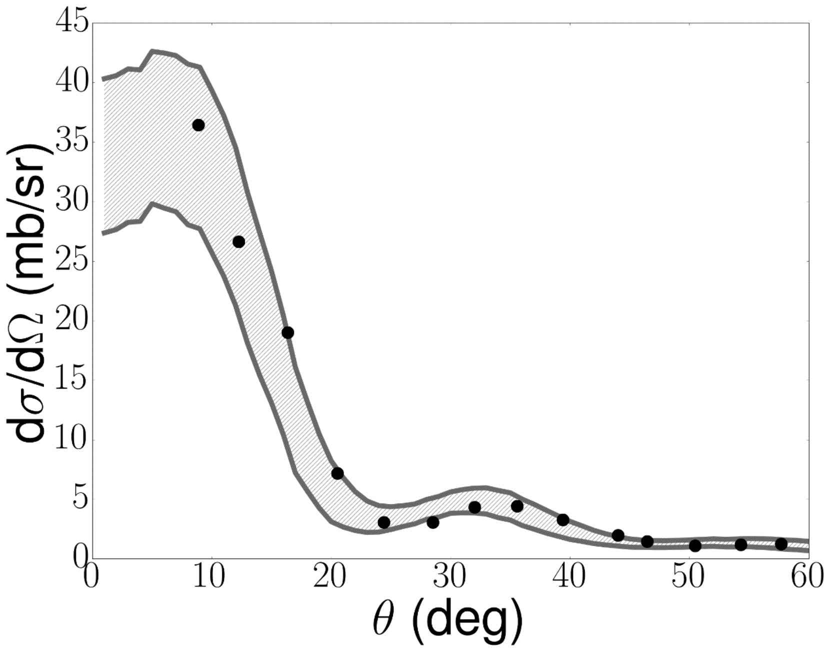
^{48}Ca(p,p) @ 14.03 MeV

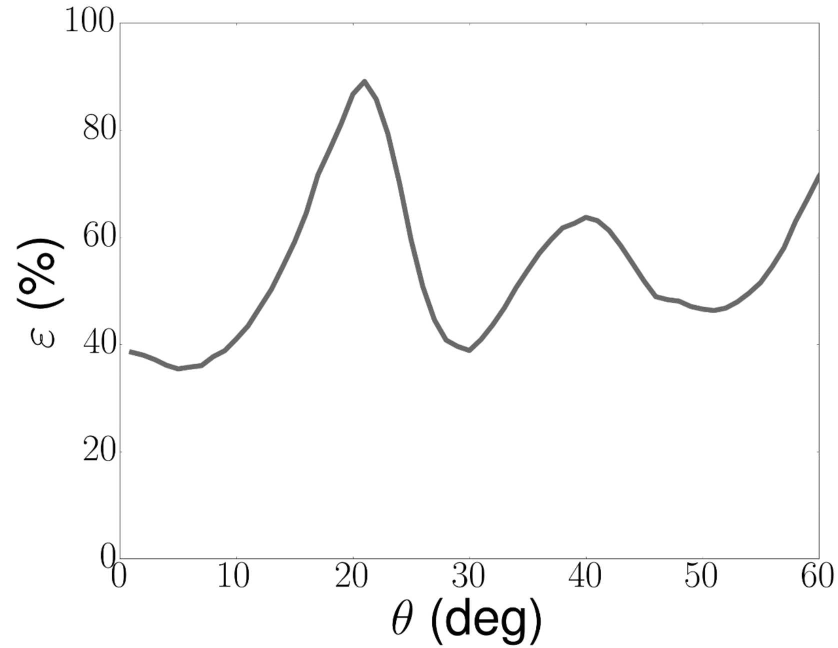
A. E. Lovell, F. M. Nunes, *PRC* **97**, 064162 (2018)



Propagation to the transfer cross section (ADWA)

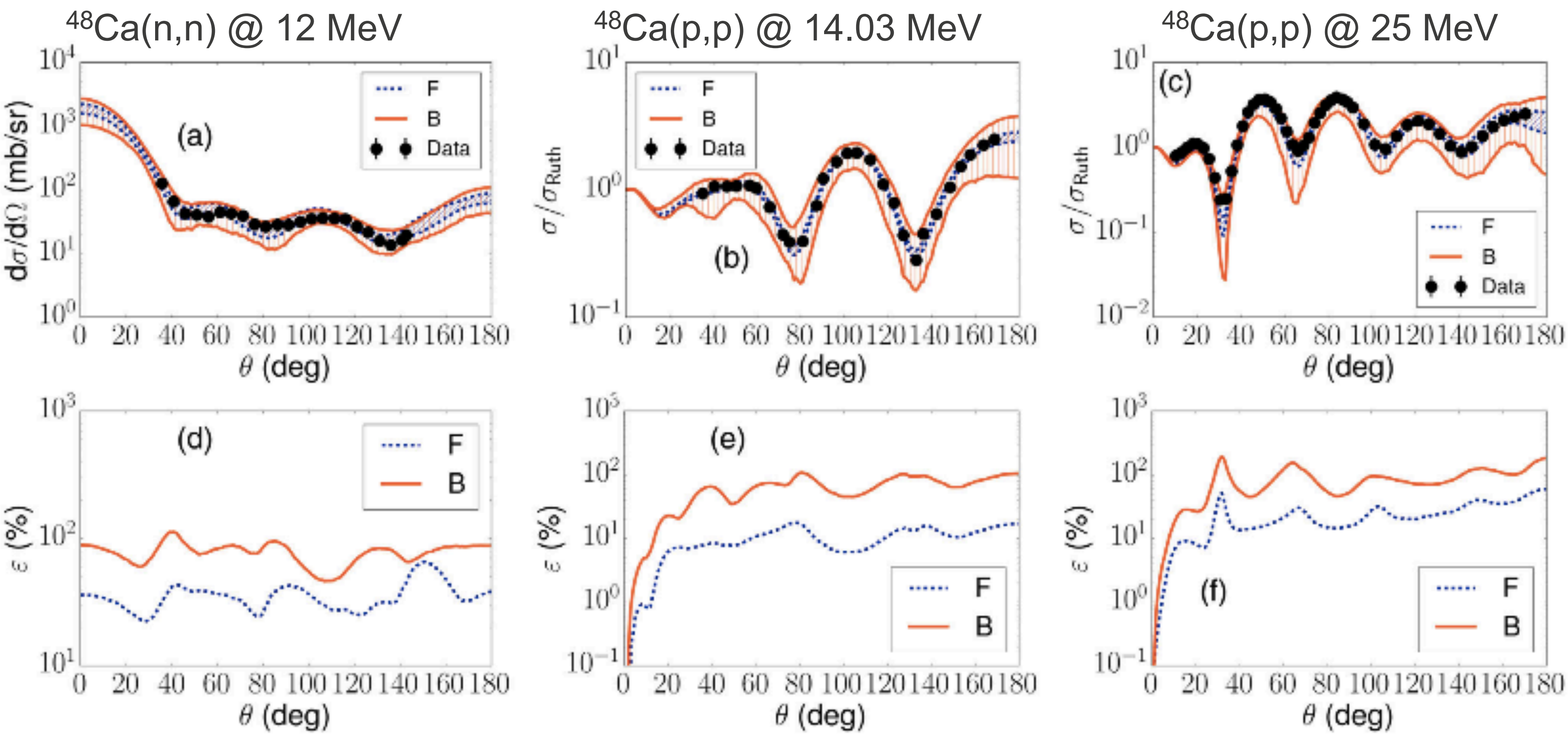
^{48}Ca(d,p)^{49}Ca(g.s.) @ 24 MeV





A. E. Lovell, F. M. Nunes, *PRC* **97**, 064162 (2018)

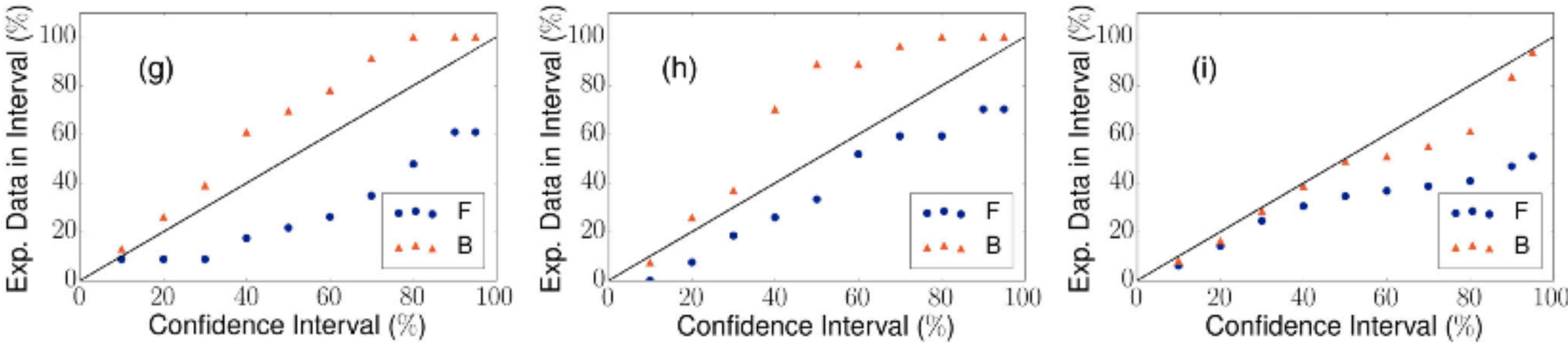
Direct comparison between χ^2 and Bayesian: cross section uncertainties



G.B. King, A.E. Lovell, L. Neufcourt, F.M. Nunes, *PRL* **122**, 232502 (2019)

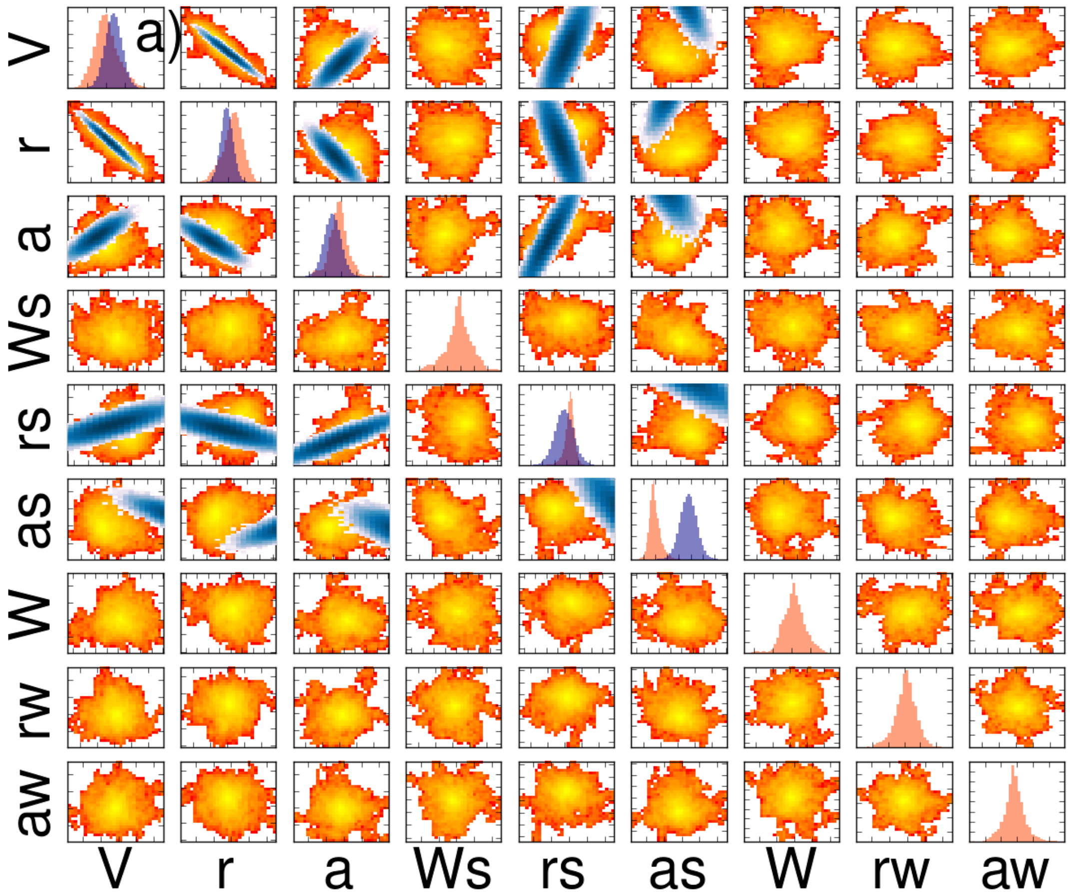
Direct comparison between χ^2 and Bayesian: confidence in uncertainties

^{48}Ca(n,n) @ 12 MeV ^{48}Ca(p,p) @ 14.03 MeV ^{48}Ca(p,p) @ 25 MeV



G.B. King, A.E. Lovell, L. Neufcourt, F.M. Nunes, *PRL* **122**, 232502 (2019)

Direct comparison between χ^2 and Bayesian: parameter correlations



$^{48}Ca(n,n)^{48}Ca$ @ 12 MeV

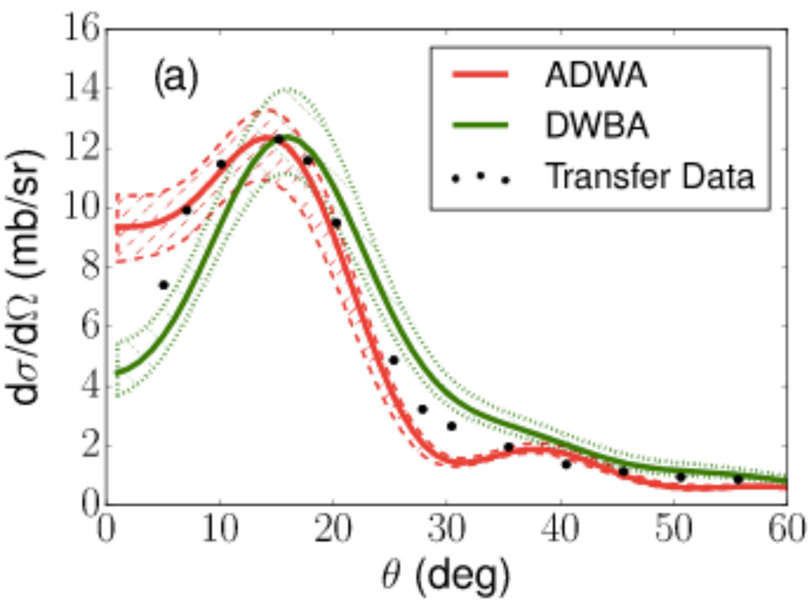
χ^2 minimization

Bayesian

G.B. King, A.E. Lovell, L. Neufcourt, F.M. Nunes, *PRL* **122**, 232502 (2019)

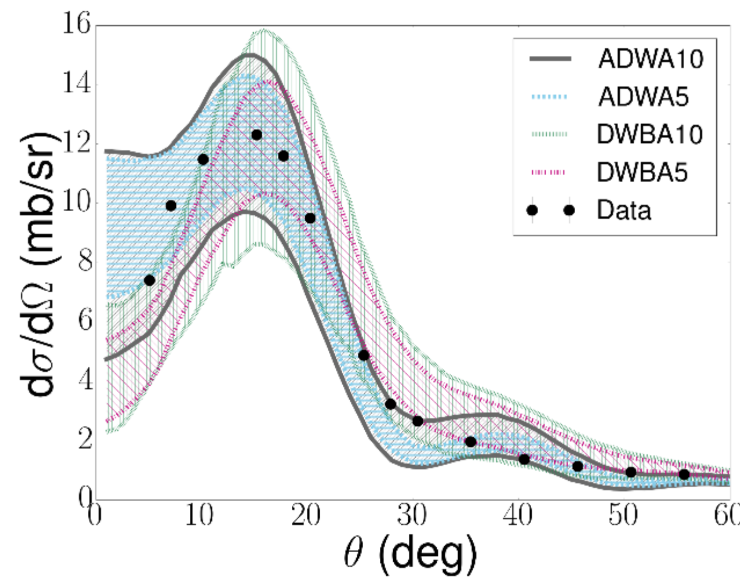
Other sources of uncertainty: few-body approximations

^{90}Zr(d,p)^{91}Zr(g.s) @ 22.7 MeV
χ^2 minimization



G.B. King, A.E. Lovell, F.M. Nunes, *PRC* **98**, 044623 (2018)

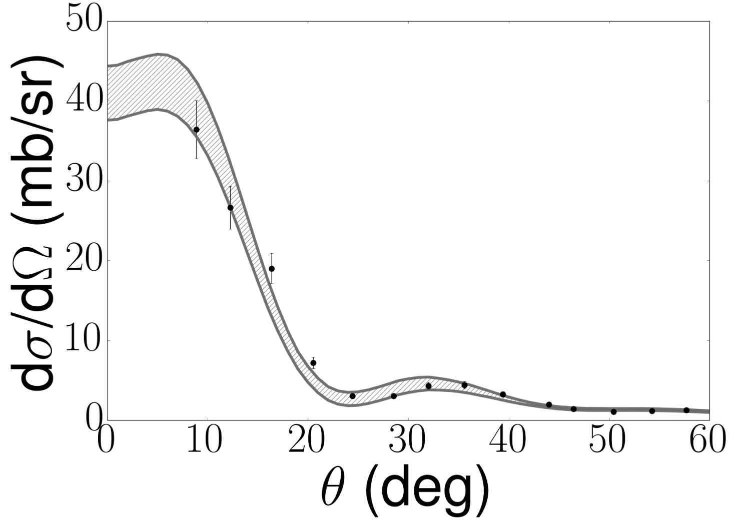
^{90}Zr(d,p)^{91}Zr(g.s) @ 22.0 MeV
Bayesian

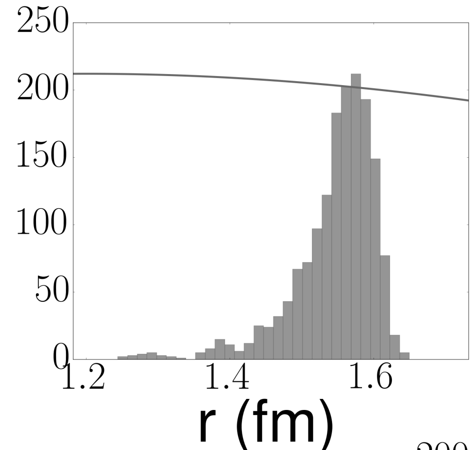


A.E. Lovell, MSU/NSCL Thesis (2018)

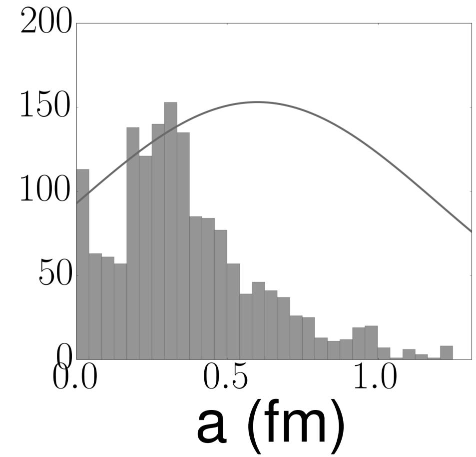
Other sources of uncertainty: structure functions

$^{48}Ca(d,p)^{49}Ca(g.s.)$ @ 19.3 MeV





Preliminary work to constrain the single-particle geometry

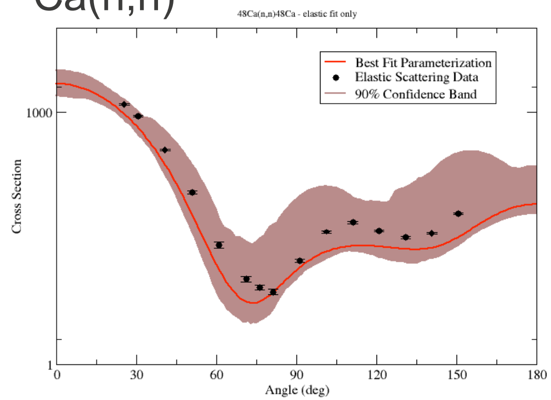


Much better to use an independent constraint, such as the asymptotic normalization coefficient (ANC)

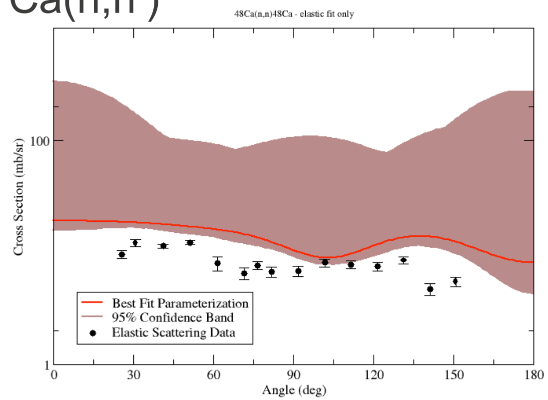
A.E. Lovell, unpublished
In progress work of N. Carriello

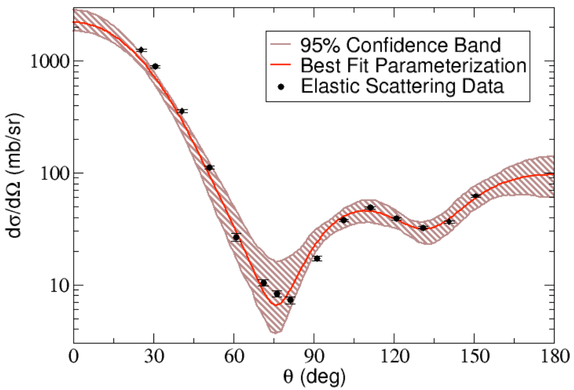
Other sources of uncertainty: degrees of freedom left out of the model

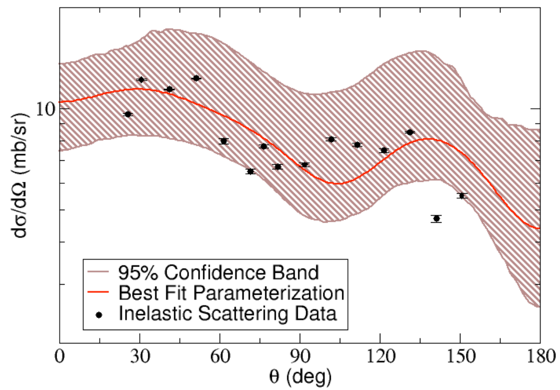
^{48}Ca(n,n)



^{48}Ca(n,n')







Unpublished work in conjunction with: A.E. Lovell, F.M. Nunes, J. Sarich, S. M. Wild, *PRC* **95**, 024611 (2017)

χ^2 minimization

Only elastic scattering fitted

Elastic and inelastic fitted with coupled channel calculation

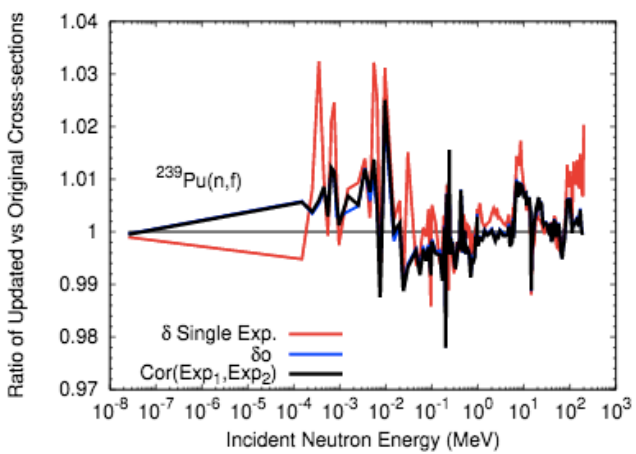
Nuclear data evaluations at LANL

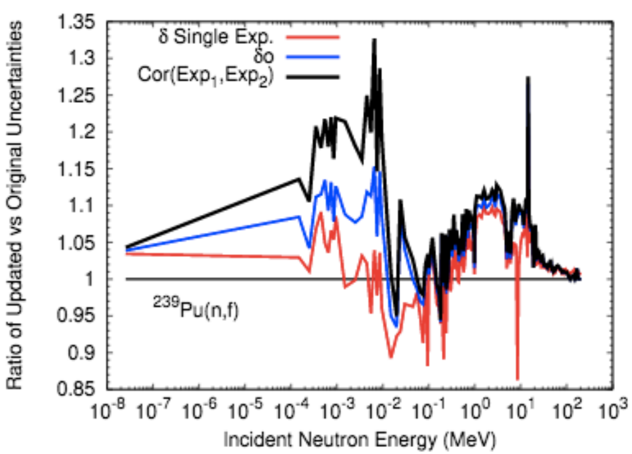
ENDF/B-VIII.0 released February 2, 2018

ENDF/B-VIII.0 fully incorporates the new Neutron Data Standards, includes imp
neutron scattering data and uses new evaluated data from the Coordinated I
Evaluation Library Organization (CIELO) pilot project for neutron reactions on ¹
^{235}U, ^{238}U and ^{239}Pu. Notable advances include updated evaluated data for
structural materials, actinides, fission energy release, prompt fission neutron an
spectra, thermal neutron scattering data, and charged-particle reactic

D.A. Brown, *et al.*, *NDS* **148**, 1 (2018)

Unc. source	Typical range	Cor(Exp$_i$,Exp$_i$)	Cor(Exp$_i$, Exp$_j$) $i \neq j$
$\delta N_{(a)}$	> 1%	Full	$\neq 0$ if same technique/sample
$\delta N_{(b\&c)}$	0-0.5% (Vapor-deposited target)	Full	$\neq 0$ if same technique/sample
	1% (Painted/electro-plated target)	Full	$\neq 0$ if same technique/sample
δc	Eqs. (3) and (5)	Diagonal	0
$\delta\beta$ & δm; δm	0.02–2%	Gaussian [20]	0.5–0.75
$\delta\beta$ & δm; $\delta\beta$	0.2–1%	Gaussian	0.5–0.75
$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1-4%	Close to full	0.5–1
$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Gaussian	0.75–1.0
δb	0.2–>10%	Gaussian	Possible
δE	1%, 1–3 ns (TOF, for given TOF length)	From conversion	Technique-dependent
$\delta\phi$	0%, >1%	0.5–Full	Technique-dependent
$\delta\zeta$	See Table III	0.9–1	0.5–0.75
δd	>0.1%	Full	0

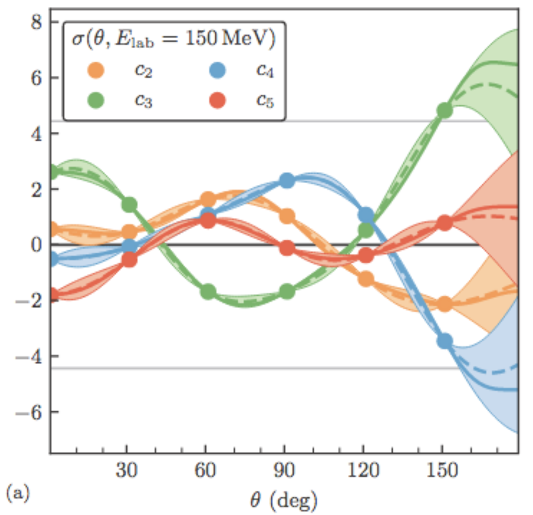




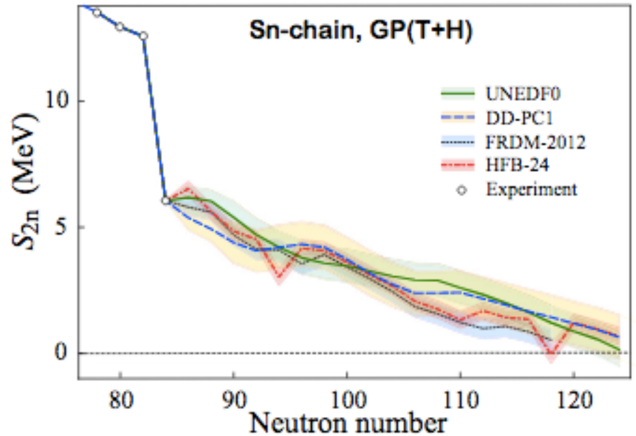
D. Neudecker, *et al.*, *NDS* **163**, 228 (2020)

Many groups are exploring machine learning as a method for uncertainty quantification

Gaussian Processes



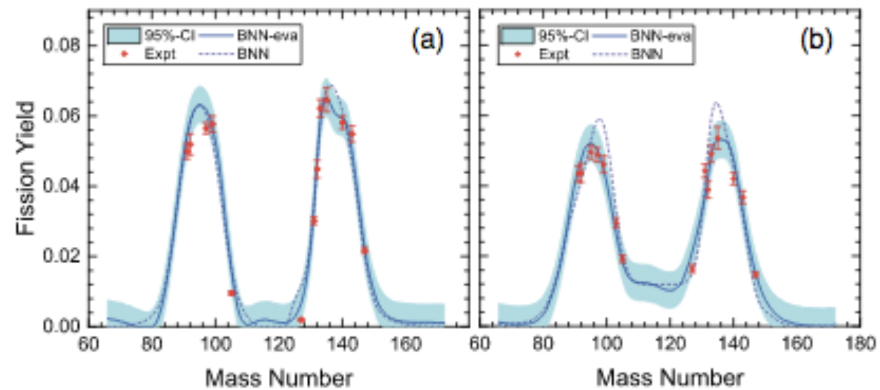
J.A. Melendez, *et al.*, *PRC* **100**, 044001 (2019)



L. Neufcourt, *et al.*, *PRC* **98**, 034318 (2018)

Bayesian Neural Networks

Zi-Ao Wang, *et al.*, *PRL* **123**, 122501 (2019)



Mixture density networks: probabilistic ML algorithm

Input → output

$$y = f(x)$$

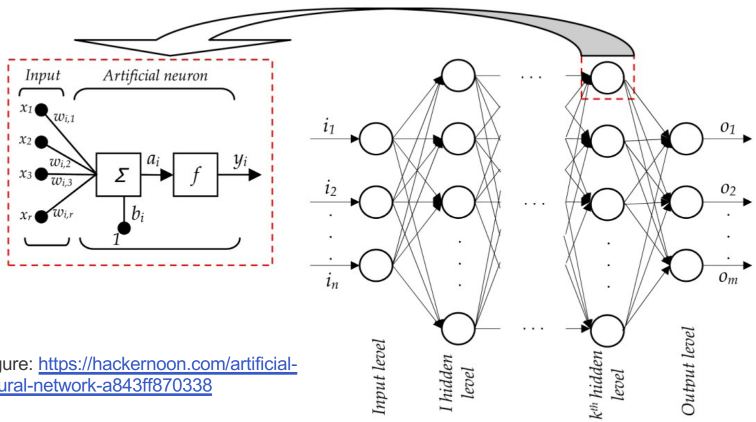
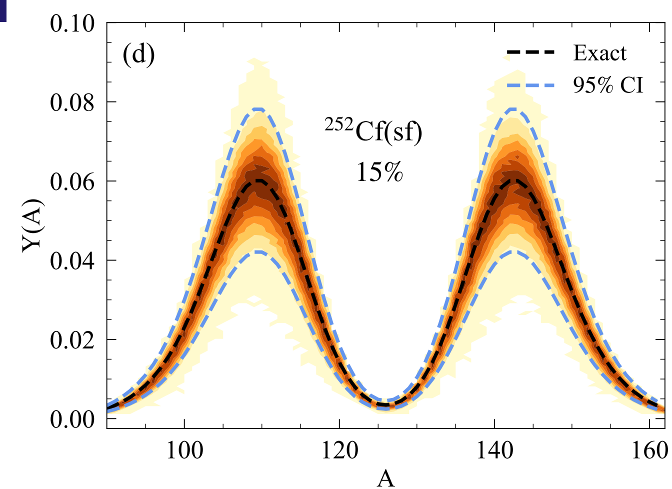
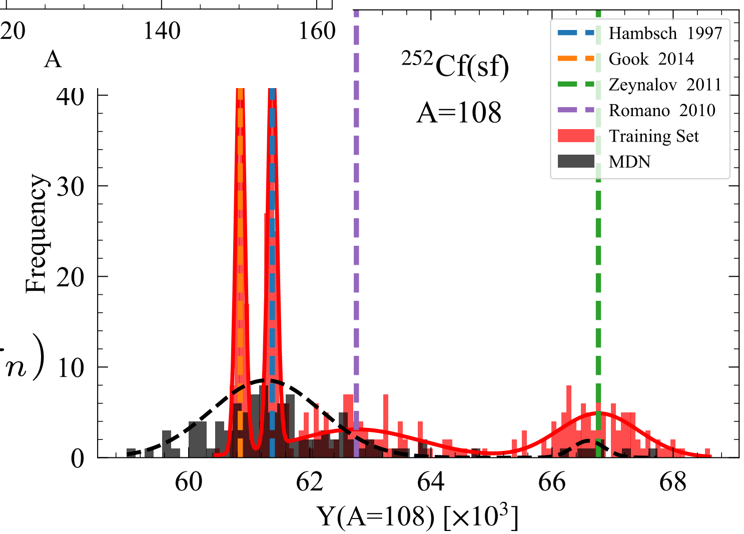


Figure: https://hackernoon.com/artificial-neural-network-a843ff870338



A.E. Lovell, A.T. Mohan, P. Talou, *in prep*



$$f(\mathbf{x}) = \alpha_1 \mathcal{N}(\mu_1, \sigma_1) + \alpha_2 \mathcal{N}(\mu_2, \sigma_2) + \ldots + \alpha_n \mathcal{N}(\mu_n, \sigma_n)$$

C.M. Bishop, Neural Computing Research Group Report NCRG/94/004 (1994)

Summary

- Uncertainty quantification is gaining more prominence in nuclear theory
- Methods have moved from χ^2 minimization and covariance propagation to Bayesian methods (and are now including machine learning methods as well)
- We have studied both χ^2 minimization and Bayesian methods to constrain uncertainties in the optical potential and found significant differences between the two, particularly in the robustness of the uncertainties and correlations between optical model parameters
- Ongoing studies are beginning to quantify uncertainties from other pieces of the few-body problem

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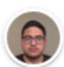
April 23

Day 8	TBD
9_{00} 10_{00}	Exploring experimental conditions to reduce uncertainties in the optical potential EN  Manuel Catacora-Rios Michigan State University