Los Alamos NATIONAL LABORATORY

Model Uncertainty Quantification

A.E. Lovell, LANL T-2
Mini-CSEWG

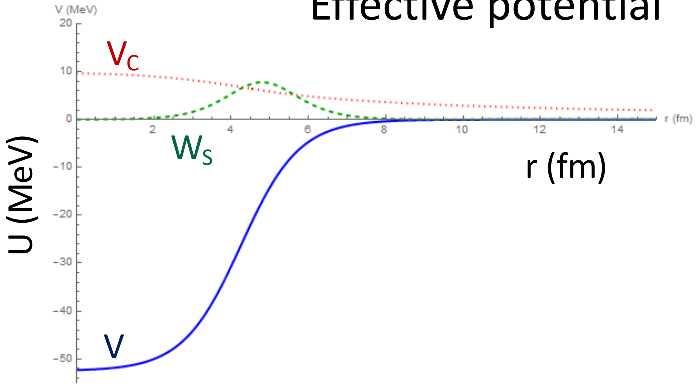
August 15, 2024

LA-UR-24-28652

Theory uncertainties largely divide into parametric uncertainties and model uncertainties*

Parametric uncertainties

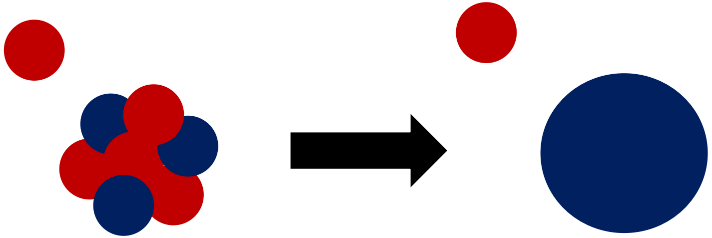
Effective potential



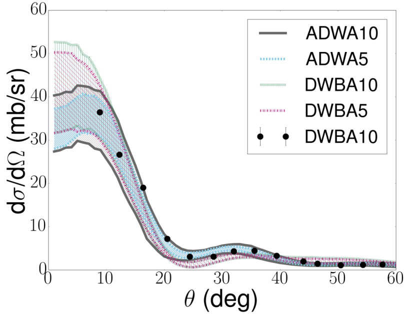
$$f(r; V_o, R_o, a_o) = -\frac{V_o}{1 + e^{(r - R_o)/a_o}}$$

Model uncertainties

Missing degrees of freedom



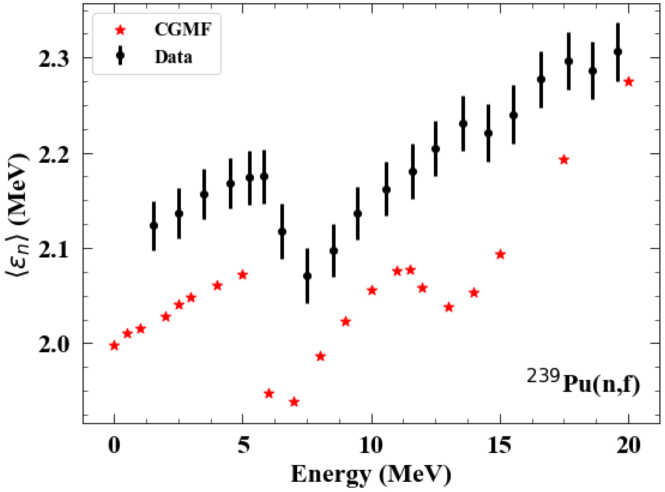
Approximations made



*Plus, numerical uncertainties coming from solving equations, sampling methods, etc.

Most theory/model UQ focus has been on parametric uncertainties but there are clearly other sources

Example: neutron energies from CGMF are systematically too low (comparison to Chi-Nu data)



WHY?

- Wrong fission fragment initial conditions?
- No scission neutrons?
- Simplified neutron emission?
- Missing nuclear levels?
- Incorrect level densities?
- Other missing physics?

A variety of optimization/UQ methods are in use

χ^2 optimization

- χ^2 metric is minimized

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

- Uncertainties are calculated by numerically constructing a parameter covariance matrix and sampling from that distribution

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

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

Bayesian optimization*

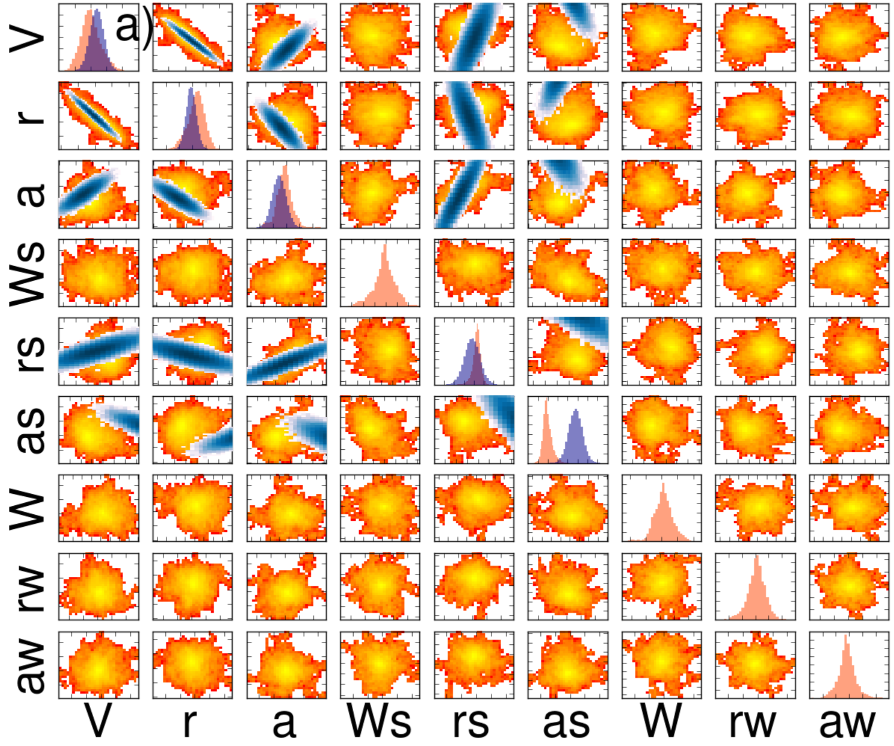
- Posterior distribution numerically sampled through a Markov Chain Monte Carlo
- Prior incorporates information about what is already known
- Likelihood compares data and model (typically through χ^2)

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

*linear approximation to Bayesian update in the Kalman filter

Los Alamos NATIONAL LABORATORY

Optimization methods matter, especially when parameter space is not well constrained



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

χ^2 minimization

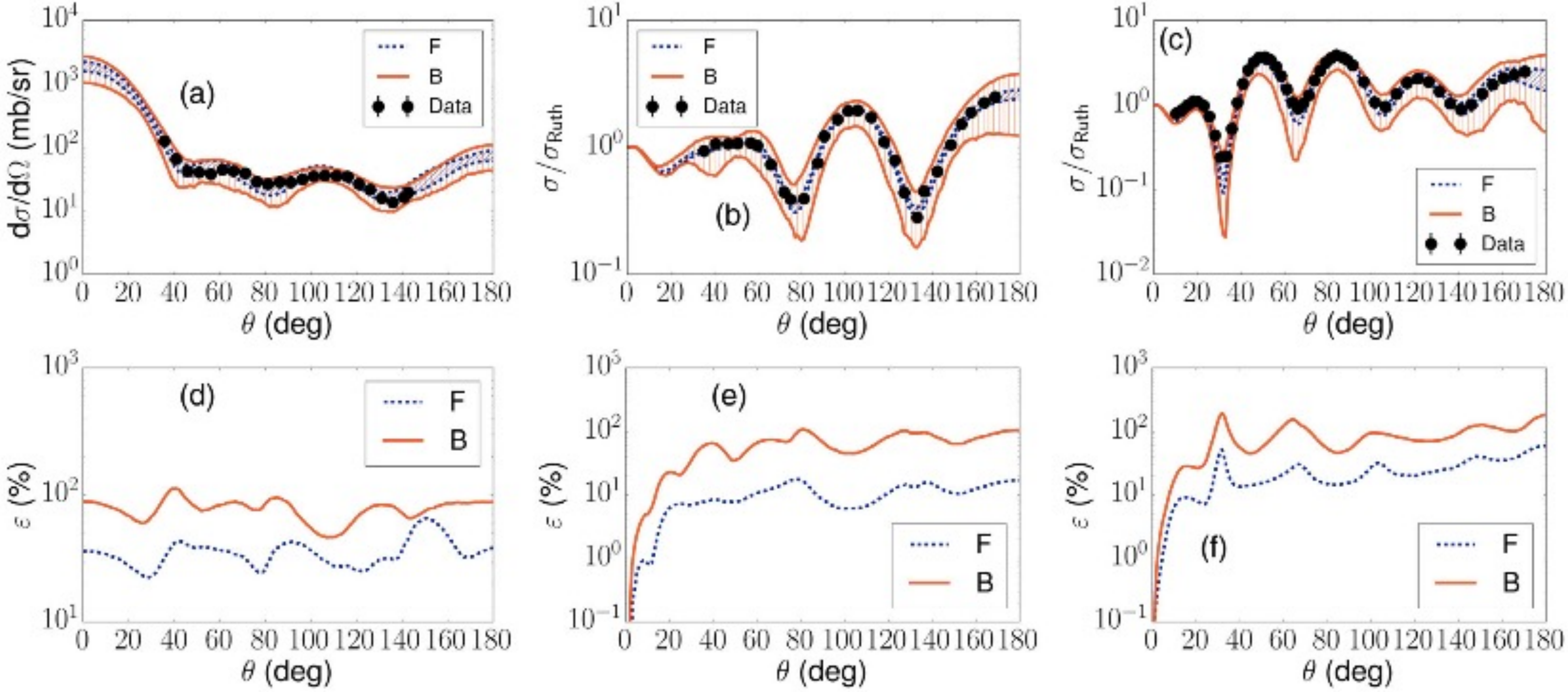
Bayesian

Gaussian approximations, reduced parameter space due to unconstrained parameters, etc., change parameter distributions and resulting observable uncertainties

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

Optimization methods matter, especially when parameter space is not well constrained

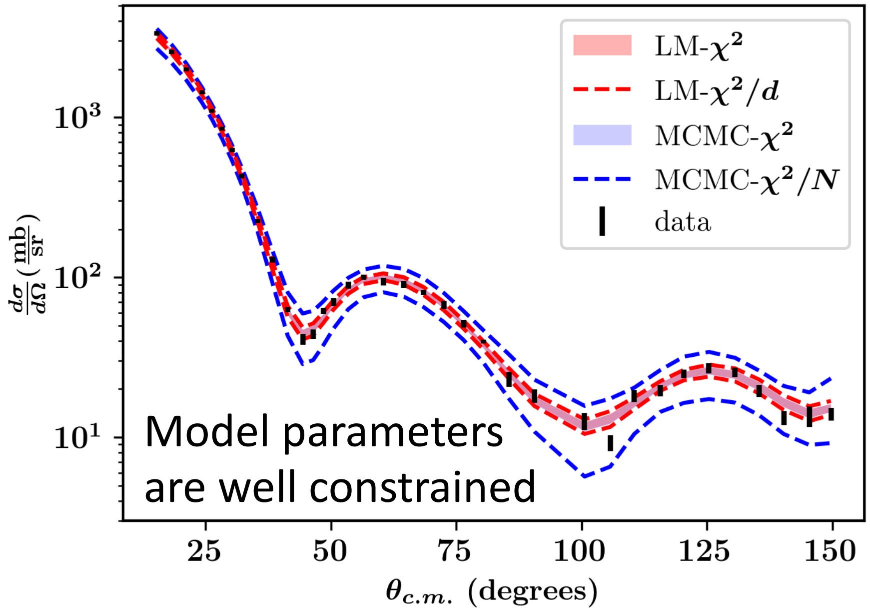
^{48}Ca(n,n) @ 12 MeV ^{48}Ca(p,p) @ 14.03 MeV ^{48}Ca(p,p) @ 25 MeV

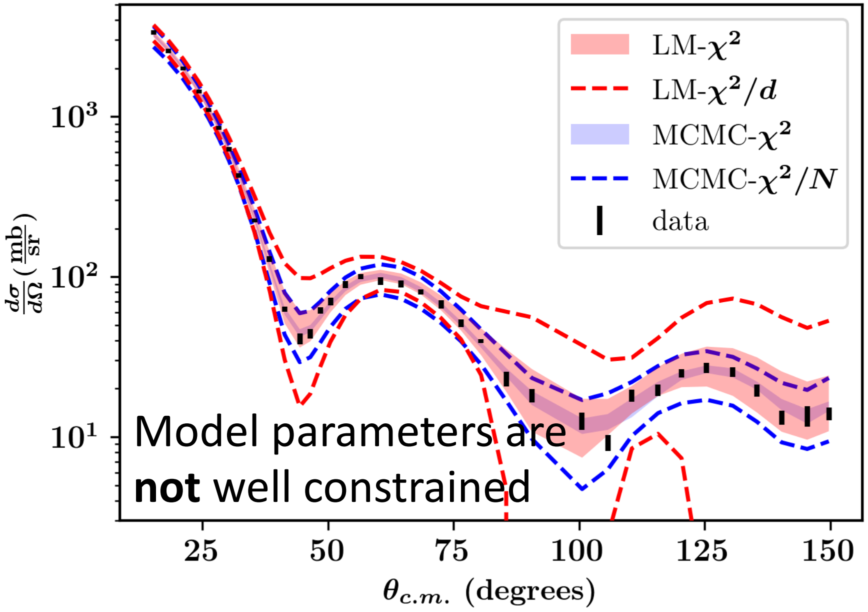


G.B. King, A.E. Lovell, L. Neufcourt, F.M. Nunes, *PRL* **122**, 232502 (2019)

How the optimization is performed is important (method and inputs)

χ^2 (LM) vs Bayesian (MCMC), using a 1/N scaling factor in the likelihood or not





Los Alamos NATIONAL LABORATORY

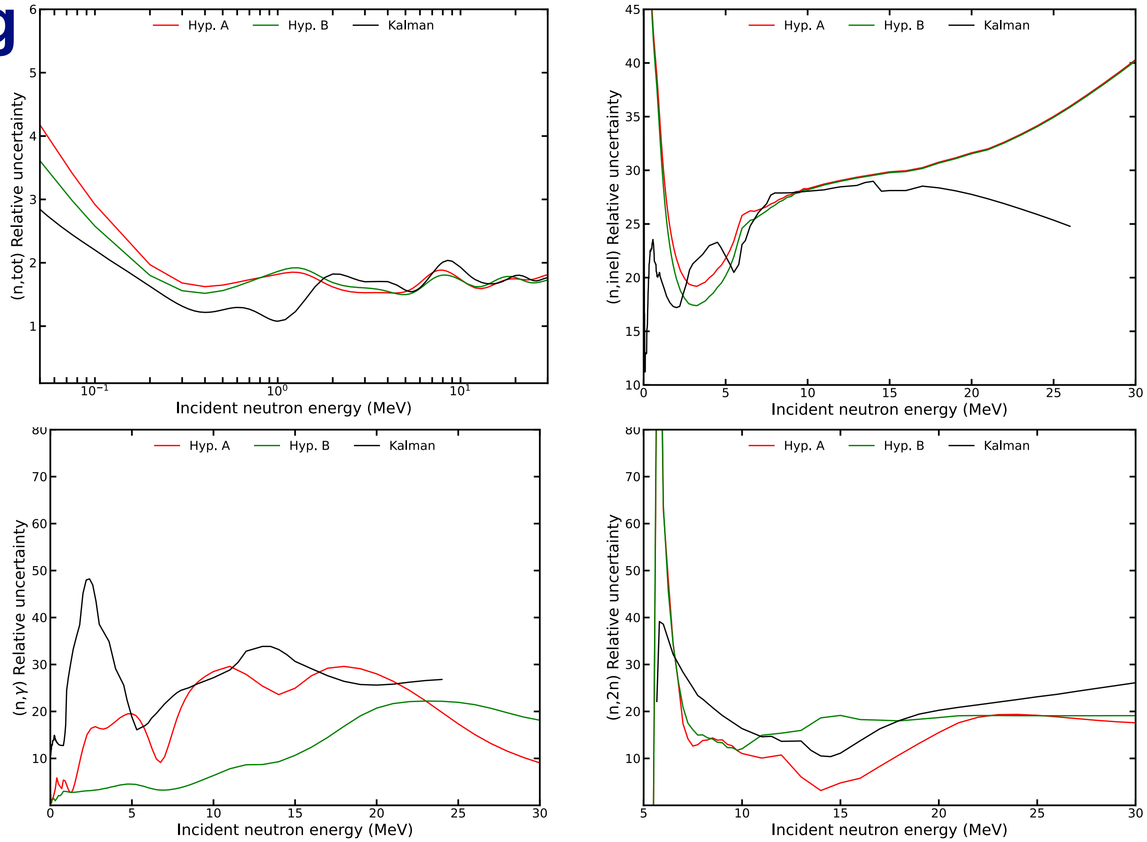
C.D. Pruitt, *et al.*, arXiv:2403.00753, LLNL-JRNL-86063, LA-UR-24-21479

Experimental inputs to optimization/UQ are important, especially weighting

Relative uncertainty on ^{239}Pu cross sections, from a Bayesian method vs Kalman filter

Hyp. A treats all data sets equally

Hyp. B assigns a normalization factor that is marginalized over



Work by M.R. Mumpower

Experimental inputs to the optimization and covariance procedure matter

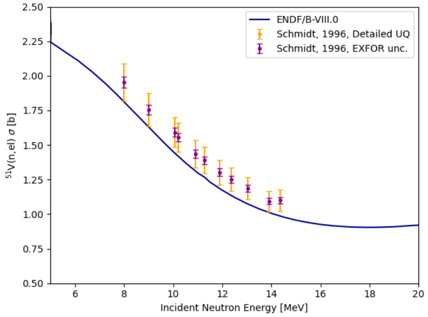
Templates of Expected Measurement Uncertainties: a CSEWG Effort,
Cyrille De Saint Jean and Denise Neudecker (Guest editors)

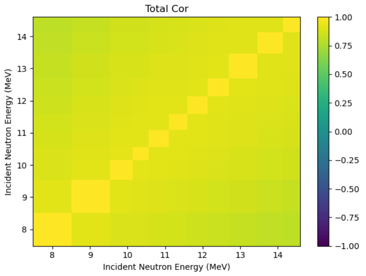
Available online at:
https://www.epj-n.org

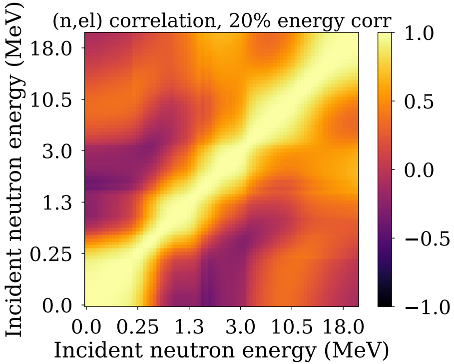
REGULAR ARTICLE OPEN ACCESS

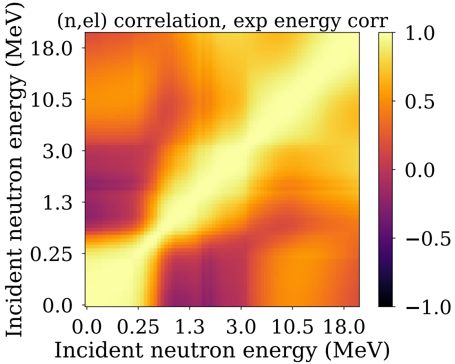
Templates of expected measurement uncertainties

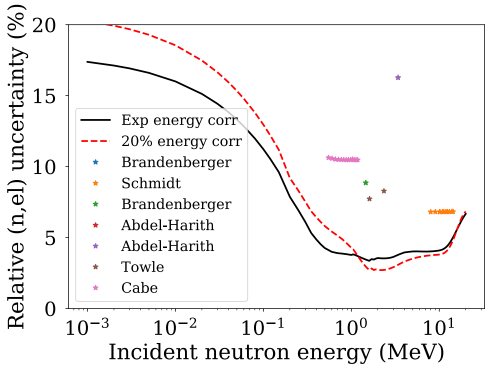
Denise Neudecker[1,*], Amanda M. Lewis[2], Eric F. Matthews[3], Jeffrey Vanhoy[4], Robert C. Haight[1], Donald L. Smith[5], Patrick Talou[1], Stephen Croft[6], Allan D. Carlson[7], Bruce Pierson[8], Anton Wallner[9], Ali Al-Adili[10], Lee Bernstein[3,11], Roberto Capote[12], Matthew Devlin[1], Manfred Drosg[13], Dana L. Duke[1], Sean Finch[14,15], Michal W. Herman[1], Keegan J. Kelly[1], Arjan Koning[12], Amy E. Lovell[1], Paola Marini[16,17], Kristina Montoya[1], Gustavo P.A. Nobre[18], Mark Paris[1], Boris Pritychenko[18], Henrik Sjöstrand[10], Lucas Snyder[19], Vladimir Sobes[20], Andreas Solders[10] and Julien Taieb[16,21]









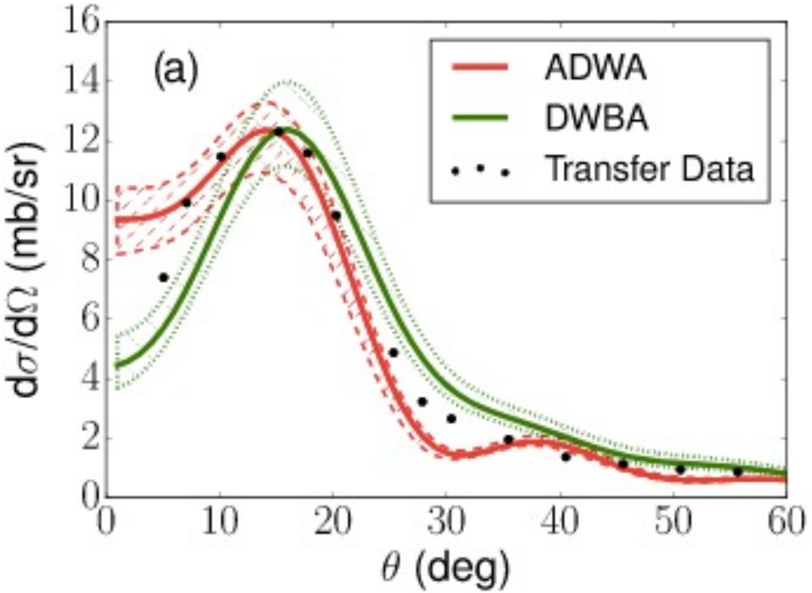


Example of ^{51}V total and elastic cross sections

Work with D. Neudecker and A. Khatiwada (LANL)

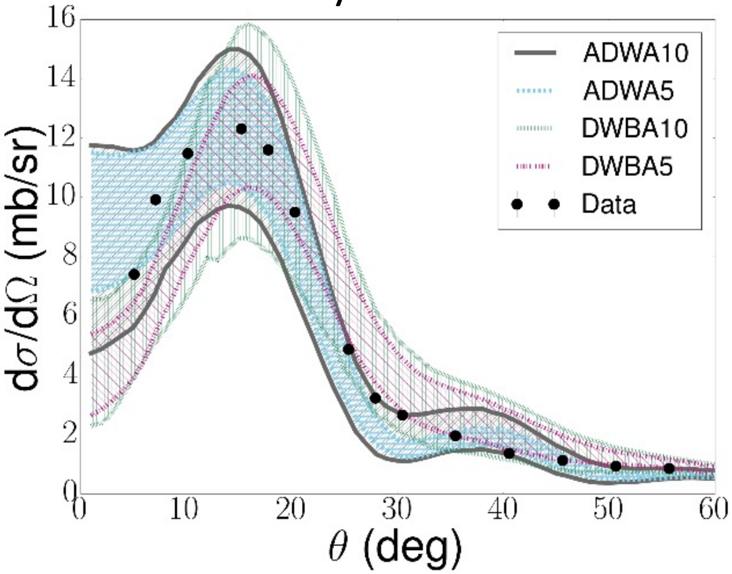
Larger sources of uncertainty likely come from model simplifications/missing degrees of freedom

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



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

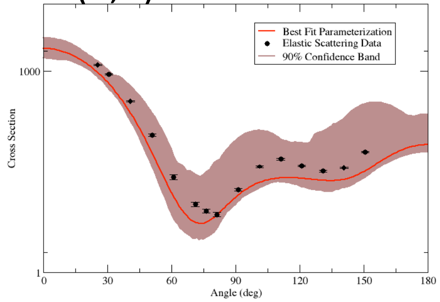
$^{90}Zr(d,p)^{91}Zr$(g.s) @ 22.0 MeV
Bayesian



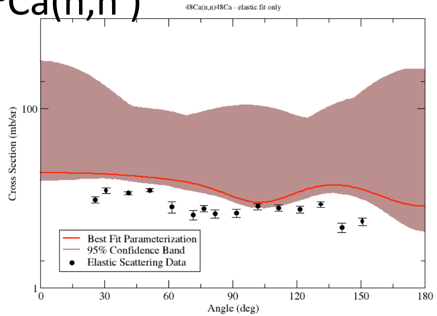
A.E. Lovell, MSU/NSCL Thesis (2018)

Larger sources of uncertainty likely come from model simplifications/missing degrees of freedom

^{48}Ca(n,n)

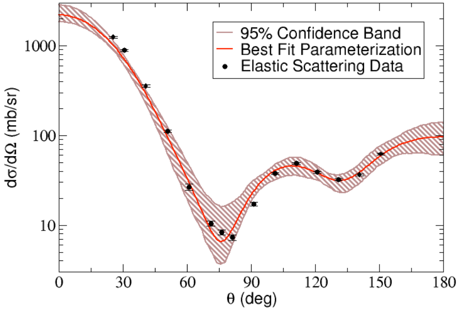


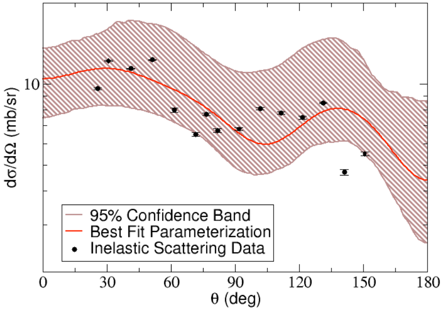
^{48}Ca(n,n')



χ^2 minimization

Only elastic scattering fitted





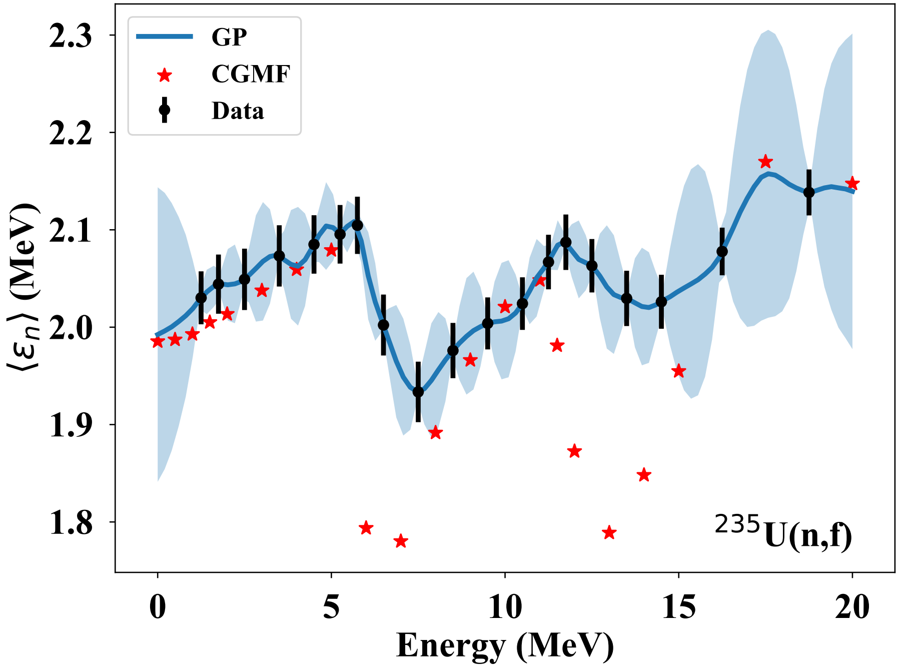
Elastic and inelastic fitted with coupled channel calculation

Los Alamos NATIONAL LABORATORY

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

How can we quantify what is missing from our models if we don’t have the ground truth from theory?

Gaussian processes (and other methods) can be used to systematically "correct" between theory and experiment



Preliminary GP studies: 2020 XCP Computational Workshop (S. Blade and S. Ozier) emulated the discrepancy between CGMF and experimental data for the average neutron energy (with I. Stetcu and M. Grosskopf)

But can we get enough trends to make predictions? Does this type of correction give us any insight into better modeling or how to include more physics?

Bayesian evidence can give a measure of the impact of different data or models

$$p(\mathcal{D}|\mathcal{M}) = \int_{\Omega_{\mathcal{M}}} p(\mathcal{D}|\alpha, \mathcal{M}) p(\alpha|\mathcal{M}) d\alpha_{\mathcal{M}}$$

TABLE I. Bayesian evidence (multiplied by 10^{-3}) for the surface model (second row) and the volume model (third row) for both beam energies considered (first row). The ratio between the Bayesian evidence of the volume model over that with the surface model is in the fourth row (the Bayes' factor).

Energy	9 MeV	65 MeV
Evidence (surface)	1.06	0.02
Evidence (volume)	0.65	0.13
Bayes' factor	0.6	6.9

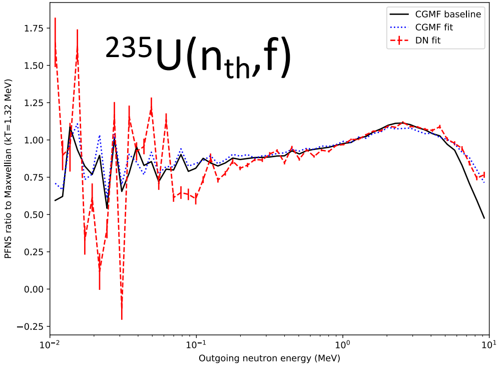
Here, we looked at the difference between the imaginary surface and volume terms in the optical potential for two scattering energies, where volume OR surface absorption should dominate

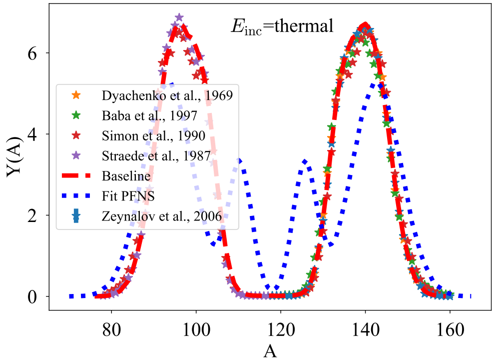
The differences in Bayesian evidence reflects those model differences

M. Catacora-Rios, G.B. King, A.E. Lovell, F.M. Nunes, *PRC* **104**, 064611 (2021)

WARNING: Parameters can try to compensate for model deficiencies

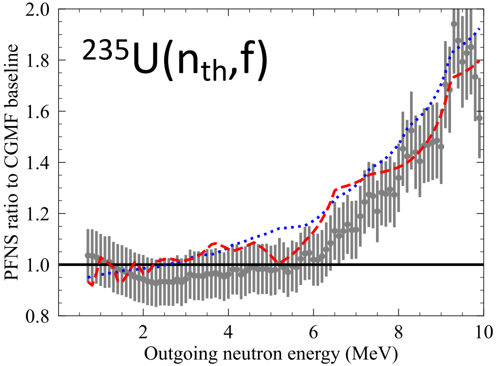
Mass distributions

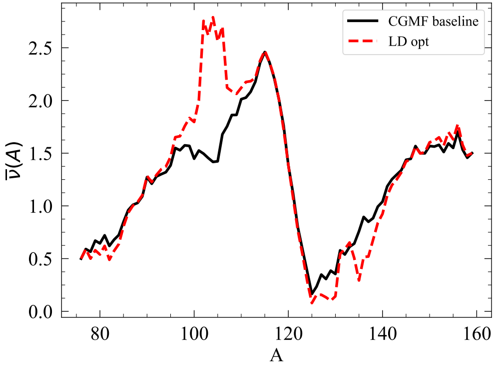




Lovell and Neudecker, LA-UR-21-30882

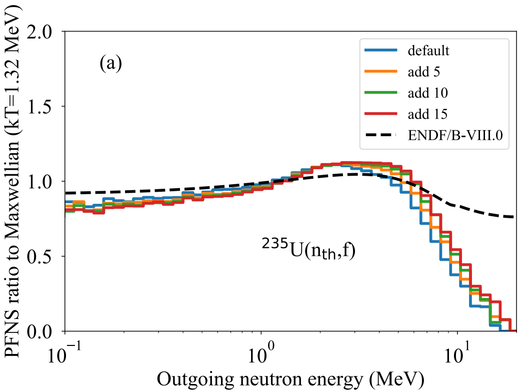
Level densities





Lovell, 20220532ECR

Discrete levels



Discrete nuclear levels have not been measured for all of the neutron-rich nuclei that are produced by fission; we can use some model to include more

Conclusions and outlook

- Uncertainty quantification is important for a variety of applications and basic science, basic theory has been catching up
- Most focus has been – from theory in particular – on parametric uncertainties but these are only part of the total model uncertainty, which should be taken into account
- Quantifying model uncertainties is hard, especially when missing physics might not be easily described or a simplified model is not a subset of a more accurate model
- Tools are being developed to begin to investigate some of these challenges
- Model uncertainty should not be ignored just because it's difficult

Acknowledgements

- F.M. Nunes, M. Catacora-Rios, C. Hebborn (MSU/FRIB)
- S.M. Wild, J. Sarich (formerly ANL)
- G.B. King (WUStL, formerly MSU)
- C.D. Pruitt (LLNL)
- I. Stetcu, P. Talou, T. Kawano, M.R. Mumpower, D. Neudecker, A. Khatiwada, K.J. Kelly, M. Grosskopf (LANL)
- S. Blade, S. Ozier (LANL XCP Computational Workshop 2020)

- Funding from ASC, NCSP, LDRD (20220532ECR), DOE NNSA SSGF (pre-LANL)

Thank you!

Questions?