Bayesian calibration, uncertainty quantification, and extrapolation of nuclear reaction models

Kyle Beyer
Collaborators: Filomena M Nunes

Seminar, Orsay 2025

Bayesian Analysis of Nuclear Dynamics

MICHIGAN STATE UNIVERSITY

FRIB

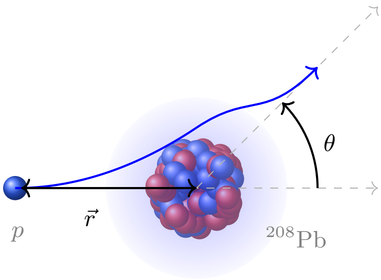
Few Body Reactions Group

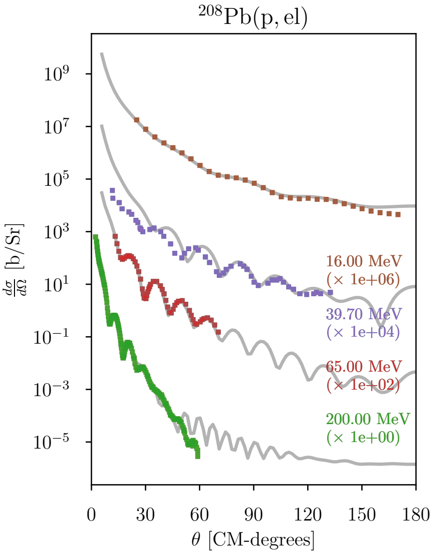
Overview

Introduction

Nuclear reactions and the optical potential

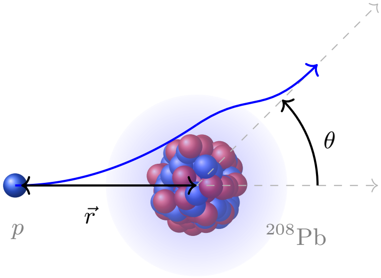
Can you reduce the many-body degrees of freedom of a nuclear reaction problem to few?

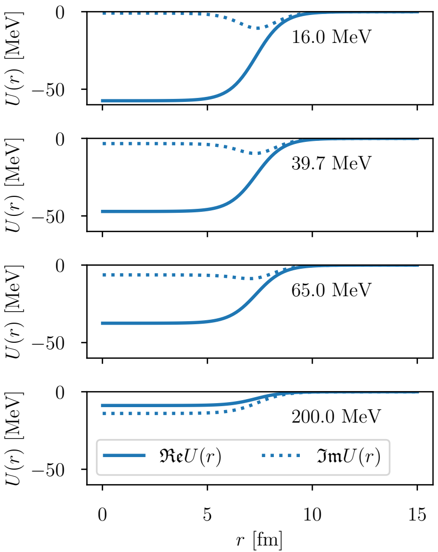




Nuclear reactions and the optical potential

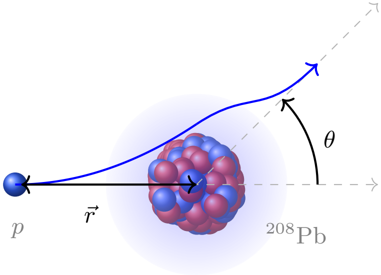
Can you reduce the many-body degrees of freedom of a nuclear reaction problem to few?
Yes, with the optical potential!

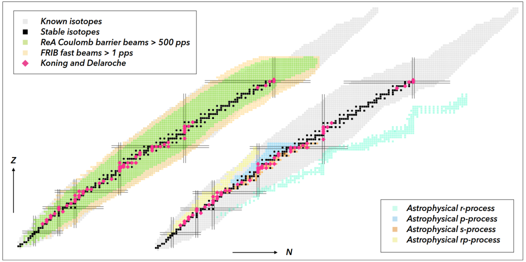




Nuclear reactions and the optical potential

Can you reduce the many-body degrees of freedom of a nuclear reaction problem to few?
Yes, with the optical potential!
...but it requires fitting and extrapolation

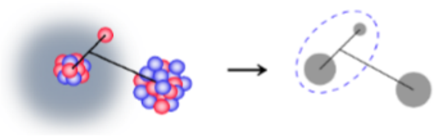




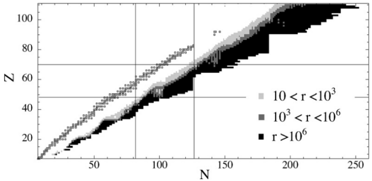
Optical potentials can be fit *locally* or *globally*, but only to stable isotopes[a]

[a] Hebborn et al. 2023, *Journal of Physics G: Nuclear and Particle Physics* 50(6), p. 060501

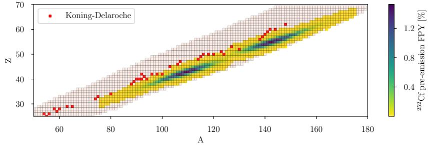
Nuclear reactions on rare isotopes involves extrapolating the optical potential



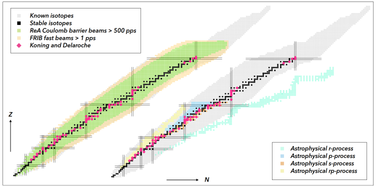
- Extrapolation of global optical potentials are ubiquitous in reaction analyses



(n, γ) rates for r-process [2]



de-excitation of fission fragments [1]



astrophysical processes, rare isotope beam experiments (and more!) [3]

[1] Beyer et al. 2025, *Phys. Rev. C* 112, p. 024604
[2] Goriely and Delaroche 2007, *Physics Letters B* 653(2-4), pp. 178–183
[3] Hebborn et al. 2023, *Journal of Physics G: Nuclear and Particle Physics* 50(6), p. 060501

Extrapolation off the line of stability is constrained by the charge-symmetry of the nuclear force

- Resonable ansatz for isovector dependence of optical potential [4]:

$$U(r) = U_0(r) + 4\frac{\boldsymbol{\tau}\cdot\mathbf{T}}{A}U_1(r)$$
$$= U_0(r) + \underbrace{4\frac{\tau_3 T_3}{A}U_1(r)}_{(N-Z)/A \text{ dependence in elastic scattering}} + \underbrace{4\frac{\tau_+ T_- + \tau_- T_+}{2A}U_1(r)}_{(p,n) \text{ to isobaric analog}}$$

- $\sim$10s of keV mass corrections for higher-order isospin terms suggests they are unimportant for scattering

Goal: improve extrapolation in $(N-Z)/A$ by using $(p,n)_{\text{IAS}}$ as a constraint in a global, uncertainty-quantified optical potential

[4] Lane 1962, *Nuclear Physics* 35, pp. 676–685

(p, n) to the isobaric analog state

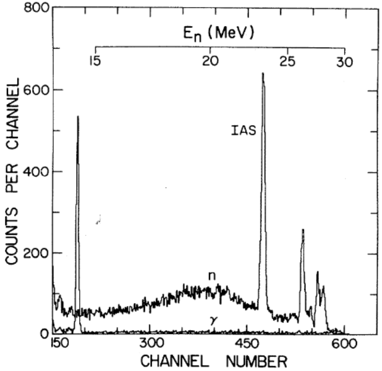
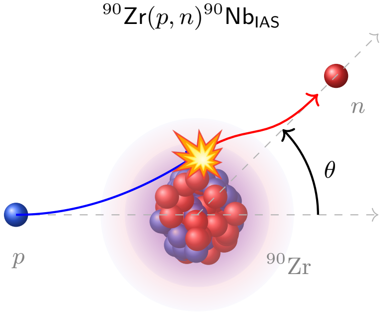


FIG. 1. Neutron (n) and γ-ray (γ) time-of-flight spectra at 0° for 35-MeV protons on ^{90}Zr. Each channel represents 0.1 nsec.

From measurements at MSU Cyclotron Lab [a]



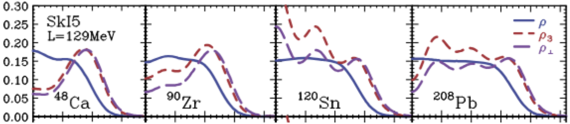
- good single-particle description: replacement of valence neutron orbital with incident proton
- probe of N, Z symmetry energy and neutron skins

[a] Doering et al. 1975, *Physical Review C* 12(2), p. 378

The East Lansing Model

$$U(r;E,A,Z) = U_0(r;E,A) + \left(\frac{N-Z}{N+Z}\right) U_1(r;E,A)$$

- 24 parameters (compared to 22 for CHUQ, 48 for KDUQ)
- Lane-consistent, spherical, global, energy dependent
- Coulomb correction to all orders
- relationship between (p,n), isovector/neutron skins, and symmetry energy by Danielewicz et al.[5]



visitlearn.msu.edu/resources/facility-for-rare-isotope-beams
photos.msu.edu

github.com/beykyle/elm

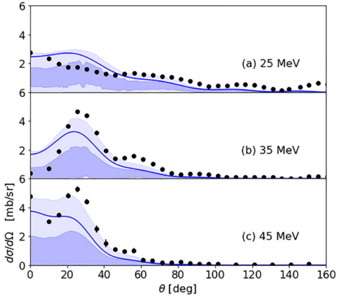
[5] Danielewicz et al. 2017, *Nuclear Physics A* 958, pp. 147–186

Calibration (and the software tools enabling it)

Progress on uncertainty quantification and extrapolation of the optical potential

Statistical approach to optical potentials

- **1950s on**: Frequentist, least-squares fitting, a few parameters at a time. Parameter ambiguities observed. [6]
- **2003**: Koning-Delaroche [7] is state-of-the-art: 50 parameter fit with computational steering, local, global hierarchy
- **2017**: Bayesian calibration and UQ with local potentials (Lovell et al. [8])
- **2023:** First global Bayesian calibration (Pruitt et al.[9])



^{48}Ca (p,n)^{48}Sc$_{IAS}$

- systematic errors, model discrepancy, errors in angle, identifiability, etc., have all been ignored
- Stable-target reactions poorly constrain U_1; large uncertainties for $(p, n)^{10}$ and for reactions on highly asymmetric isotopes [11]

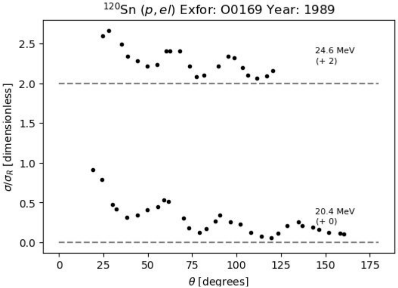
[6] Satchler et al. 1964, *Physical Review* 136(3B), B637
[7] Koning and Delaroche 2003, *Nuclear Physics A* 713(3-4), pp. 231–310
[8] Catacora-Rios et al. 2021, *Phys. Rev. C* 104, p. 9; Lovell et al. 2017, *Physical Review C* 95(2), p. 024611
[9] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602
[10] Smith et al. 2024, *Physical Review C* 110(3), p. 034602
[11] Goriely and Delaroche 2007, *Physics Letters B* 653(2-4), pp. 178–183

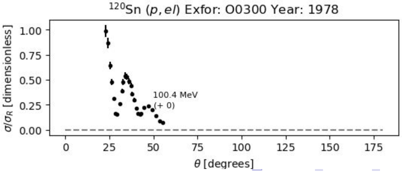
Curation of a body of experimental data

- $\sim$ 100 EXFOR entries, $\sim 10\text{K}$ data points
- $40 \leq A \leq 208$
- $10\text{ MeV} < \text{E}_{\text{lab}} < 200\text{ MeV}$
- $d\sigma/d\Omega$ and A_y from elastic (p,p), (n,n)
- $d\sigma/d\Omega$ with clean $\Delta J^\pi = 0^+$ from $(p,n)_{\text{IAS}}$
- manual ID & cleaning of outliers
- types of error reported inconsistent

github.com/beykyle/exfor_tools

```
all_entries_pp = exfor_tools.get_exfor_differential_data(
    target=target,
    projectile=proton,
    quantity="dXS/dA",
    product="EL",
    energy_range=[10, 200],  # MeV
)
```





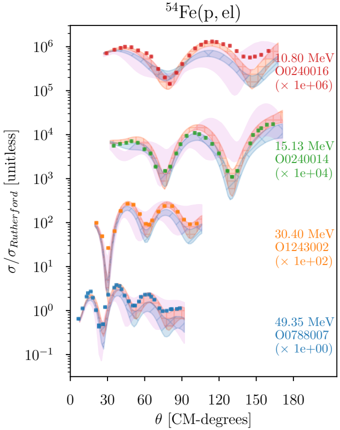
jit$\mathcal{R}$ allows for global calibration without needing emulators

philosophy:

Modular library for building workspaces which take in interaction models and spit out reaction observables

- calculable $\mathcal{R}$-matrix on Lagrange mesh [a]
- modular python library
- precompute everything you can
- `numba` just-in-time compilation, heavy `numpy` vectorization
- **2 orders of magnitude faster than comparable fortran codes**, just as fast as emulators [b] in UQ setting

[a] Baye 2015, *Physics reports* 565, pp. 1–107
[b] Odell et al. 2024, *Physical Review C* 109(4), p. 044612

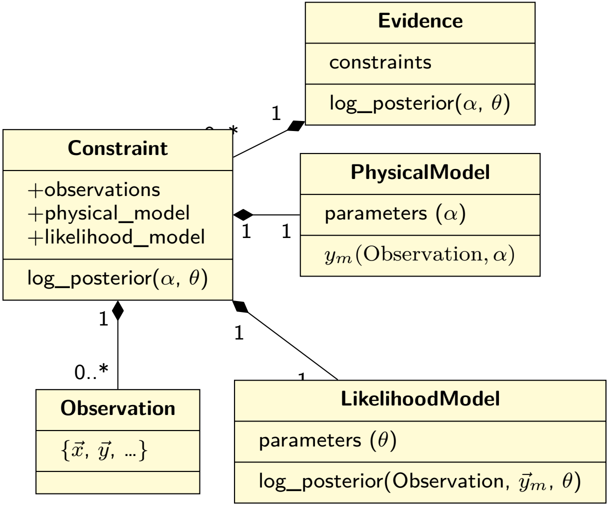


Open source, part of BAND framework [a]

[a] Beyer et al. 2023, (Version 0.3.0)

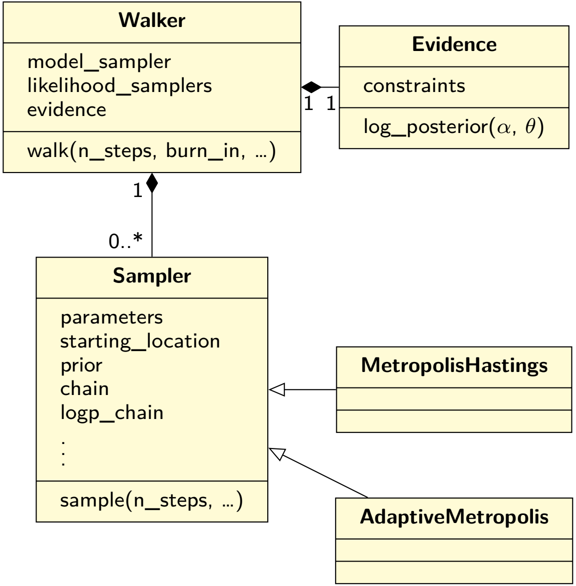
`rxmc`: spotlight on the body of evidence and the likelihood

- curating a body of evidence from multiple constraints
- Bayesian calibration with flexible likelihood models
- designed with `jit`$\mathcal{R}$ and `exfor-tools` in mind
- built-in MCMC, or interface with external MCMC package
- handles parametric likelihood models with batched Metropolis-in-Gibbs sampling
- alpha stage: https://github.com/beykyle/rxmc/

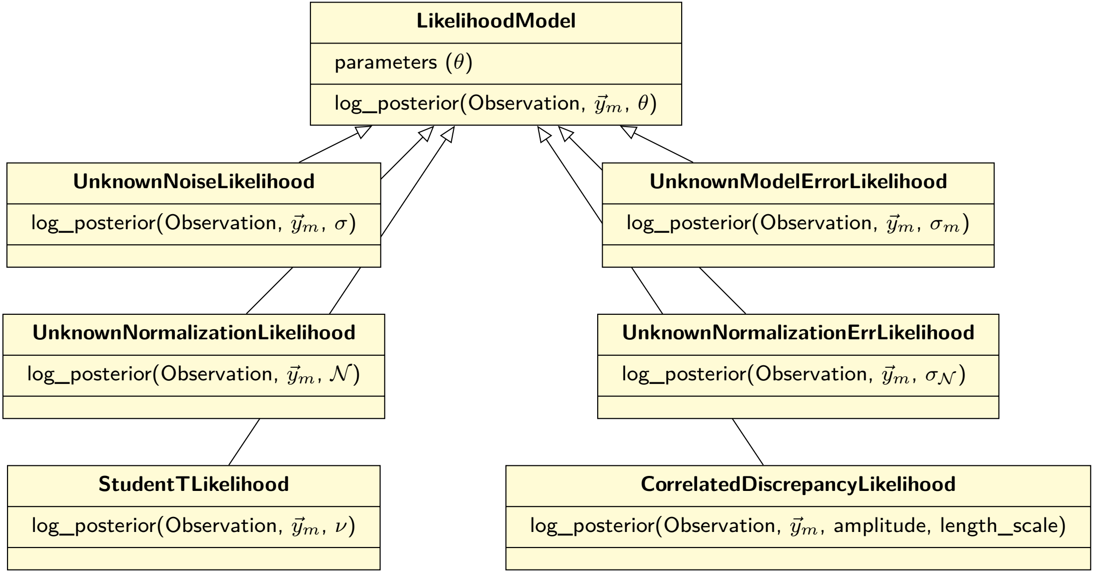


`rxmc`: spotlight on the body of evidence and the likelihood

- curating a body of evidence from multiple constraints
- Bayesian calibration with flexible likelihood models
- designed with `jit`$\mathcal{R}$ and `exfor-tools` in mind
- built-in MCMC, or interface with external MCMC package
- handles parametric likelihood models with batched Metropolis-in-Gibbs sampling
- alpha stage: https://github.com/beykyle/rxmc/



`rxmc`: spotlight on the body of evidence and the likelihood



Aside: systematic error in the likelihood

Common approach is to introduce a normalization parameter $\mathcal{N}$:

$$\chi^2(\alpha) = \sum_i \frac{(y_i - \mathcal{N} y_m(x_i;\alpha))^2}{\sigma_i^2} + \frac{(\mathcal{N}-1)^2}{\sigma_{\mathcal{N}}^2} \tag{1}$$

This is incorrect! The correct approach is actually[12]:

$$\chi^2(\alpha) = \sum_i \frac{(\mathcal{N} y_i - y_m(x_i;\alpha))^2}{(\mathcal{N}\sigma_i)^2} + \frac{(\mathcal{N}-1)^2}{\sigma_{\mathcal{N}}^2} \tag{2}$$

One can implicitly marginalize over $\mathcal{N}$, which requires use of a non-diagonal covariance[13]. This relates to Peelle's Pertinent Puzzle in nuclear data evaluation[14].

[12] Giulio D'Agostini (1994). "On the use of the covariance matrix to fit correlated data". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346.1-2, pp. 306–311; Ian J Thompson and Filomena M Nunes (2009). *Nuclear reactions for astrophysics: principles, calculation and applications of low-energy reactions*. Cambridge University Press.

[13] Roger Barlow (2021). "Combining experiments with systematic errors". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864.

[14] R Frühwirth et al. (2012). "Peelle's pertinent puzzle and its solution". In: *EPJ Web of Conferences*. Vol. 27. EDP Sciences, p. 00008; Denise Neudecker et al. (2012). "Peelle's pertinent puzzle: A fake due to improper analysis". In: *Nuclear science and engineering* 170.1, pp. 54–60.

Handling multiple constraints with systematic errors

- statistical only:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2$$

- statistical error is fit parameter:

$$\Sigma_{ij} = \delta_{ij}(\eta\, y_m(x_i;\alpha))^2$$

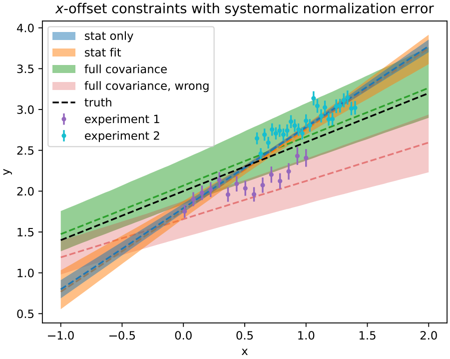
- full covariance:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_m(x_i;\alpha) y_m(x_j;\alpha)$$

- full covariance, wrong:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_i y_j$$

We have a high-schooler working on calibrating optical potentials accounting properly for systematic error!



https://github.com/beykyle/rxmc/blob/main/examples/systematic_err_demo.ipynb

Statistical model for ELM

$$\underbrace{p(\boldsymbol{\alpha}|\mathcal{D},\mathcal{M})}_{\text{posterior}} \propto \underbrace{p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\alpha})}_{\text{prior}}$$

Likelihood model [15]

$$y_{i,\exp} + \delta_{i,\exp} = y_{\mathcal{M}}(x_i;\boldsymbol{\alpha}) + \delta_{MD}(x;\boldsymbol{\alpha})$$

$$\ln p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M}) = -\frac{1}{2}\left(\boldsymbol{\Delta}^{\top}\cdot\boldsymbol{\Sigma}\cdot\boldsymbol{\Delta} + \ln\left((2\pi)^{k}\,|\boldsymbol{\Sigma}|\right)\right)$$

$$\Delta_i(\alpha) = y_{\mathcal{M}}(x_i,\boldsymbol{\alpha}) - y_i$$

$$\boldsymbol{\Sigma} \equiv \boldsymbol{\Sigma}_{\exp} + \boldsymbol{\Sigma}_{\mathrm{MD}}$$

Prior model

- estimated from posterior of prior calibrations w/out (p,n) [16]

Calibration

- Adaptive Metropolis-Hastings in Gibbs with `rxmc`
- Goodman-Weare from `emcee`[17]
- massively parallel computation

[15] Kennedy and O'Hagan 2001, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 63(3), pp. 425–464

[16] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602

[17] Foreman-Mackey et al. 2013, *PASP* 125(925), p. 306; Goodman and Weare 2010, *Communications in applied mathematics and computational science* 5(1), pp. 65–80

Likelihood model

$$\ln p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M}) = -\frac{1}{2}\left(\boldsymbol{\Delta}^\top \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{\Delta} + \ln\left((2\pi)^k |\boldsymbol{\Sigma}|\right)\right) \qquad \Delta_i(\alpha) \equiv y_{\mathcal{M}}(x_i,\boldsymbol{\alpha}) - y_i$$

- learn model (uncorrelated) discrepancy from data

$$\Sigma_{\mathrm{exp,ij}}(\alpha) \equiv \delta_{ij}\sigma^2_{\mathrm{exp,i}}$$
$$\Sigma_{\mathrm{MD,ij}}(\eta) \equiv \delta_{ij}\left[\epsilon\left(y_{\mathcal{M}}(x_i;\boldsymbol{\alpha}) + y_{i,\mathrm{exp}}\right)/2\right]^2$$

- ϵ is a free parameter

To re-scale or not to re-scale the log-likelihood?

- Pruitt et al[a] re-scaled the log likelihood by k/N (# of free parameters / # of experimental data points):

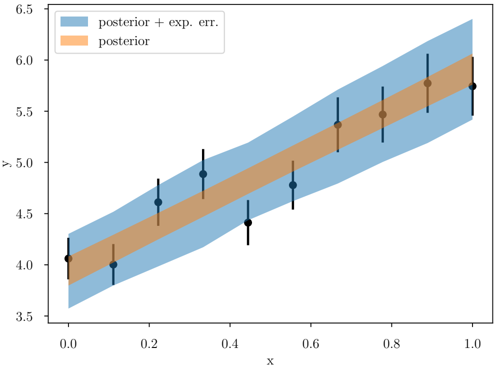
$$\ln p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M}) \to -\left(\frac{k}{N}\right)\frac{1}{2}\left(\boldsymbol{\Delta}^\top \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{\Delta} + \ln\left((2\pi)^k |\boldsymbol{\Sigma}|\right)\right)$$

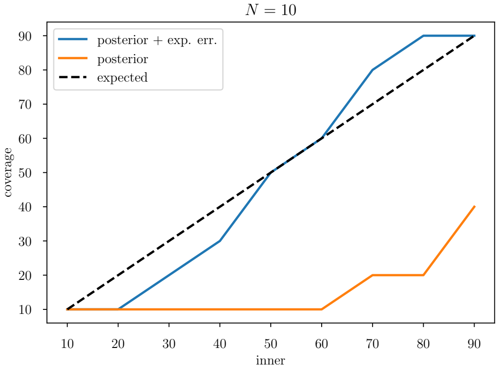
- Are we overconfident if posterior credible intervals are narrow?
- re-scaling is equivalent to "cold" posterior with $\lambda = k/N < 1$ (post-Bayesian approach) [b]

$$p_\lambda(\boldsymbol{\alpha}|\mathcal{D},\mathcal{M}) \propto p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M})^\lambda p(\boldsymbol{\alpha})$$

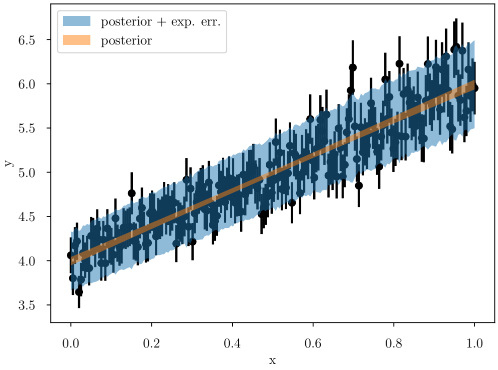
[a] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602
[b] Grünwald 2011, vol. 19, pp. 397–420

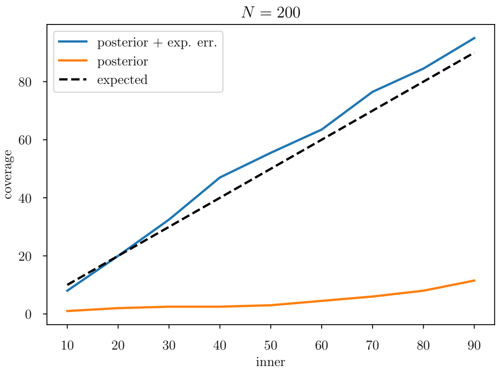
Empirical coverage



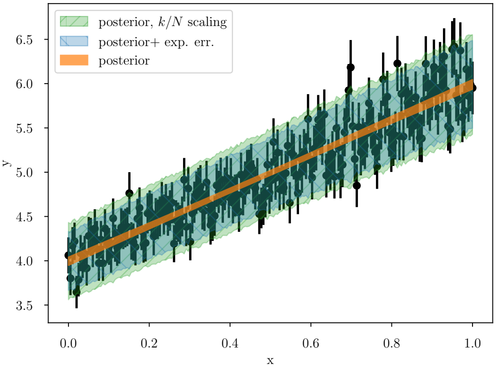


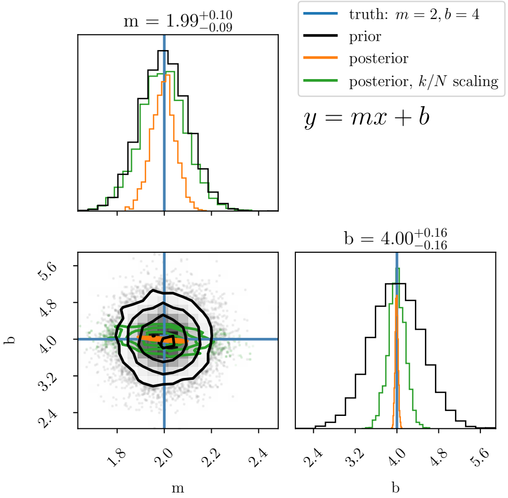
Empirical coverage



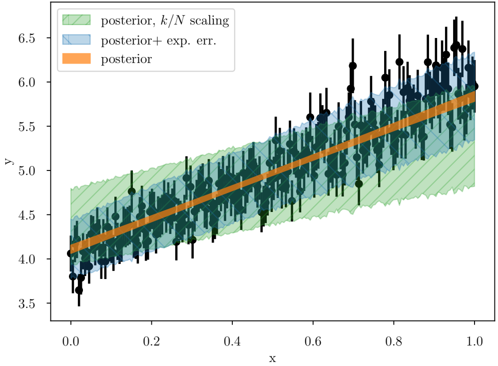


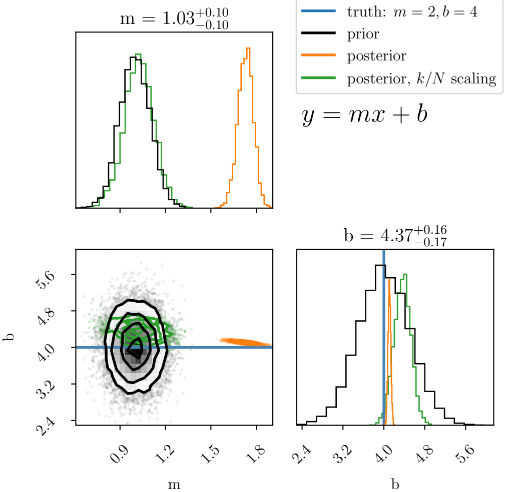
"Cold" posterior





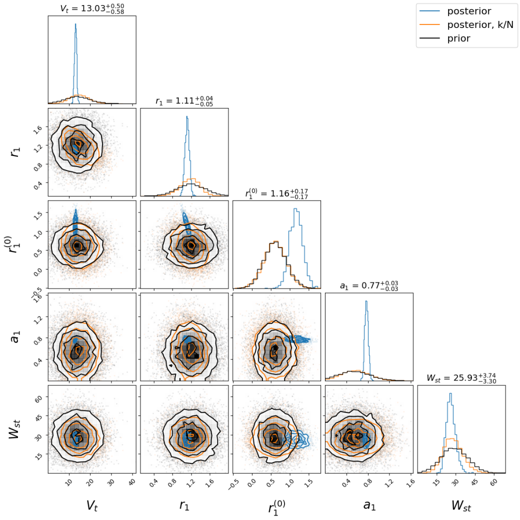
"Cold" posterior: over-emphasis on the prior

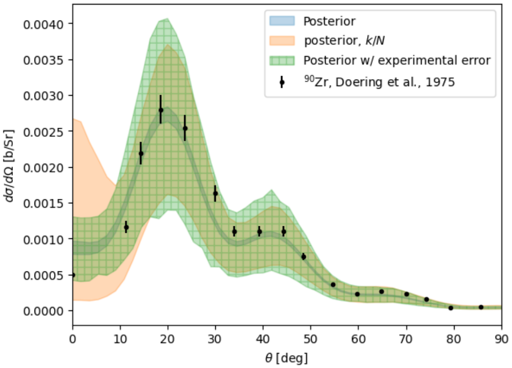




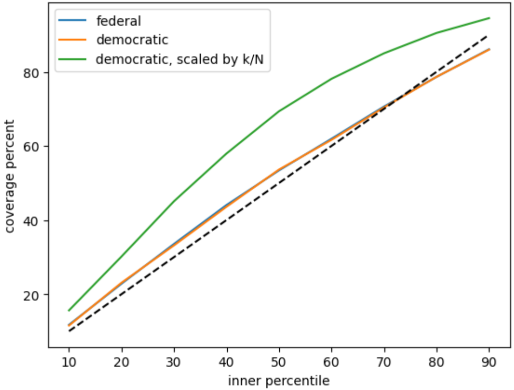
Results

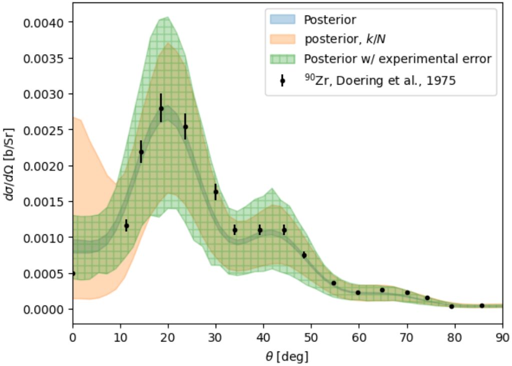
"Cold" posterior: over-emphasis on the prior



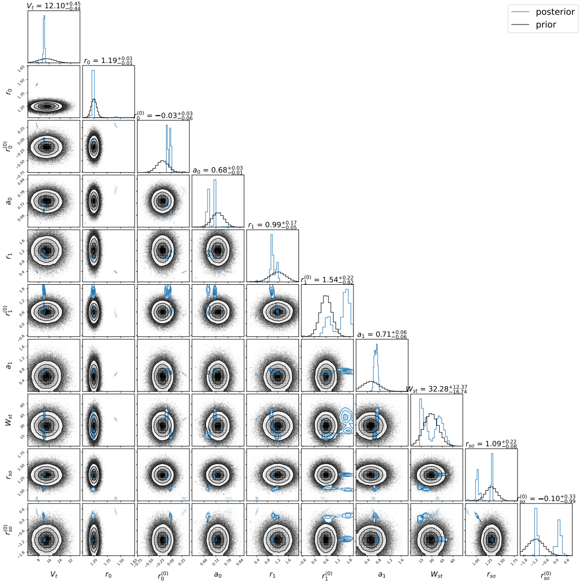


Predictive posteriors and empirical coverage

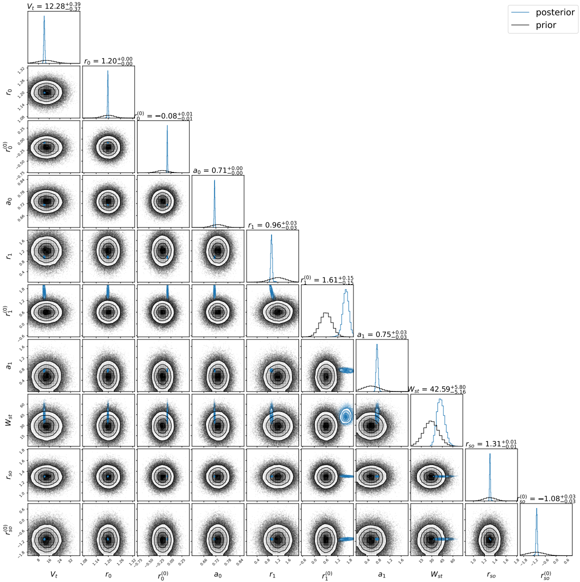




Multimodality, parameter ambiguity in radii

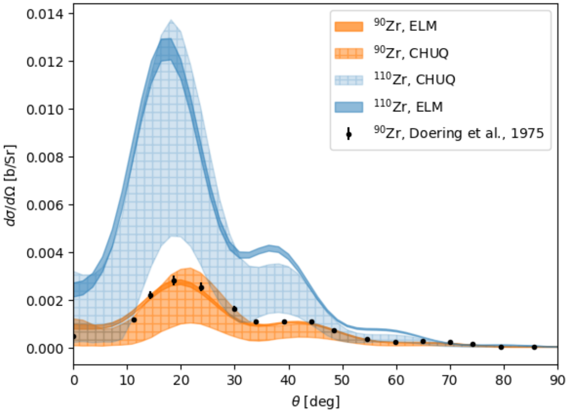


Multimodality, parameter ambiguity in radii



Extrapolation and uncertainty quantification

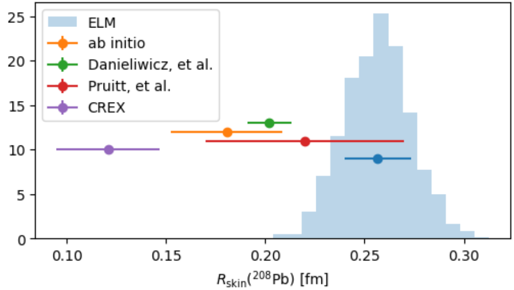
Extrapolation in $(N-Z)/A$

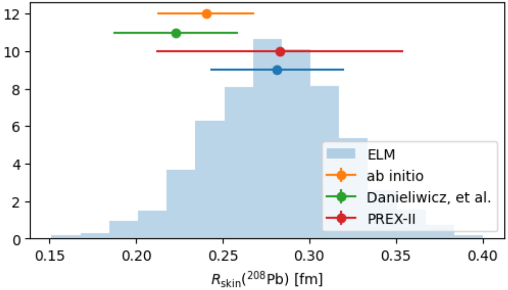


Problem: Model is function of $(N-Z)/A$, but model discrepancy model has no dependence on input space at all!

Bayesian inference of neutron skins

Preliminary ...





Summary and outlook

ELM coming soon!

- reasonable posteriors without re-scaling, prediction of $R_{\text{skin}}(^{A}Z)$
- an open-source software ecosystem for reaction phenomenology has been developed

Outlook and stuff I'd like to do (or am doing)

- correlated experimental error, model discrepancy, errors in angle
- multi-modality in full model calibration? What orthogonal constraints can we fold in?
- model mixing
- microscopic (Skyrme-based) and ab-initio (NCSM) optical potentials for (p, n)
- ELM dispersive

Thank you for your time!

In collaboration with Filomena Nunes and the Few Body Reactions Group

BAND Bayesian Analysis of Nuclear Dynamics

MICHIGAN STATE UNIVERSITY

FRIB

Few Body Reactions Group

References I

- Barlow, Roger (2021). "Combining experiments with systematic errors". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864.
- Baye, Daniel (2015). "The Lagrange-mesh method". In: *Physics reports* 565, pp. 1–107.
- Bentley, Michael A (2022). "Excited States in Isobaric Multiplets—Experimental Advances and the Shell-Model Approach". In: *Physics* 4.3, pp. 995–1011. ISSN: 2624-8174. DOI: 10.3390/physics4030066. URL: https://www.mdpi.com/2624-8174/4/3/66.
- Beyer, Kyle et al. (2023). *BANDFramework: An Open-Source Framework for Bayesian Analysis of Nuclear Dynamics*. Tech. rep. Version 0.3.0. URL: https://github.com/bandframework/bandframework.
- Beyer, Kyle A. et al. (2025). "Uncertainty quantification of optical models in fission fragment deexcitation". In: *Phys. Rev. C* 112 (2), p. 024604. DOI: 10.1103/4kny-mj7g. URL: https://link.aps.org/doi/10.1103/4kny-mj7g.
- Catacora-Rios, M. et al. (2021). "Statistical tools for a better optical model". In: *Phys. Rev. C* 104, p. 9. URL: https://doi.org/10.1103/PhysRevC.104.064611.
- D'Agostini, Giulio (1994). "On the use of the covariance matrix to fit correlated data". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346.1-2, pp. 306–311.

References II

- Danielewicz, Paweł et al. (2017). "Symmetry energy III: Isovector skins". In: *Nuclear Physics A* 958, pp. 147–186.
- Doering, RR et al. (1975). "Microscopic description of isobaric-analog-state transitions induced by 25-, 35-, and 45-MeV protons". In: *Physical Review C* 12.2, p. 378.
- Foreman-Mackey, Daniel et al. (Mar. 2013). "emcee: The MCMC Hammer". In: *PASP* 125.925, p. 306. DOI: 10.1086/670067. arXiv: 1202.3665 [astro-ph.IM].
- Frühwirth, R et al. (2012). "Peelle's pertinent puzzle and its solution". In: *EPJ Web of Conferences*. Vol. 27. EDP Sciences, p. 00008.
- Goodman, Jonathan and Jonathan Weare (2010). "Ensemble samplers with affine invariance". In: *Communications in applied mathematics and computational science* 5.1, pp. 65–80.
- Goriely, Stéphane and J-P Delaroche (2007). "The isovector imaginary neutron potential: A key ingredient for the r-process nucleosynthesis". In: *Physics Letters B* 653.2-4, pp. 178–183.
- Grünwald, Peter (2011). "Safe Learning: bridging the gap between Bayes, MDL and statistical learning theory via empirical convexity". In: *Proceedings of the 24th Annual Conference on Learning Theory*. Ed. by Sham M. Kakade and Ulrike von Luxburg. Vol. 19. Proceedings of Machine Learning Research. Budapest, Hungary: PMLR, pp. 397–420. URL: https://proceedings.mlr.press/v19/grunwald11a.html.

References III

- Hebborn, C et al. (2023). "Optical potentials for the rare-isotope beam era". In: *Journal of Physics G: Nuclear and Particle Physics* 50.6, p. 060501. DOI: 10.1088/1361-6471/acc348. URL: https://dx.doi.org/10.1088/1361-6471/acc348.
- Kennedy, Marc C and Anthony O'Hagan (2001). "Bayesian calibration of computer models". In: *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 63.3, pp. 425–464. DOI: http://dx.doi.org/10.1111/1467-9868.00294.
- Koning, AJ and JP Delaroche (2003). "Local and global nucleon optical models from 1 keV to 200 MeV". In: *Nuclear Physics A* 713.3-4, pp. 231–310.
- Lane, AM (1962). "Isobaric spin dependence of the optical potential and quasi-elastic (p, n) reactions". In: *Nuclear Physics* 35, pp. 676–685.
- Lovell, Amy E et al. (2017). "Uncertainty quantification for optical model parameters". In: *Physical Review C* 95.2, p. 024611.
- Neudecker, Denise et al. (2012). "Peelle's pertinent puzzle: A fake due to improper analysis". In: *Nuclear science and engineering* 170.1, pp. 54–60.
- Odell, Daniel et al. (2024). "ROSE: A reduced-order scattering emulator for optical models". In: *Physical Review C* 109.4, p. 044612.
- Pruitt, CD et al. (2023). "Uncertainty-quantified phenomenological optical potentials for single-nucleon scattering". In: *Physical Review C* 107.1, p. 014602.

References IV

Satchler, GR et al. (1964). "Optical-Model Analysis of" Quasielastic"(p, n) Reactions". In: *Physical Review* 136.3B, B637.

Schery, SD et al. (1974). "The (p, n) reaction to the isobaric analogue state of high-Z elements at 25.8 MeV". In: *Nuclear Physics A* 234.1, pp. 109–129.

Smith, AJ et al. (2024). "Uncertainty quantification in (p, n) reactions". In: *Physical Review C* 110.3, p. 034602.

Thompson, Ian J and Filomena M Nunes (2009). *Nuclear reactions for astrophysics: principles, calculation and applications of low-energy reactions*. Cambridge University Press.

Extra slides: ELM physical model

$$U(r,E,A,Z) = U_0(r,E,A) \pm \frac{N-Z}{N+Z} U_1(r,E,A) + V_C$$

$$\begin{aligned}
U_0(r,E,A) &= V_0(E) f((r - R_0(A))/a_0) + iW_0(E) f((r - R_w(A))/a_w) \\
&\quad - 4ia_w W_{s,0}(E) \frac{d}{dr} f((r - R_w(A))/a_w) + 2\,(\boldsymbol{\sigma} \cdot \boldsymbol{\ell})\; V_{so} \frac{1}{r} \frac{d}{dr} f((r - R_{so}(A))/a_{so}) \\
U_1(r,E,A) &= V_1(E) f((r - R_1(A))/a_1) - 4ia_w W_{s,1}(E) \frac{d}{dr} f((r - R_w(A))/a_w)
\end{aligned}$$

$$f(x) = \frac{1}{1+\exp(x)} \qquad R_i(A) = r_{i,0} + r_{i,A} A^{1/3} \qquad E_C = 6Z\alpha\hbar c/5R_C$$

$$\begin{aligned}
V_{0(1)}(E) &= V_{0(1)} - \alpha(E - E_C) \\
W(E) &= W \Big/ \left(1 + \exp\left(\frac{\eta_W - (E - E_C)}{\lambda_W}\right)\right) \\
W_{s,0(1)}(E) &= W_{s,0(1)} \Big/ \left(1 + \exp\left(\frac{(E - E_C) - \eta_s}{\lambda_s}\right)\right)
\end{aligned}$$

Extra slides: ELM statistical model and calibration

- Goodman-Weare [18] affine-invariante stretch move sampler from `emcee`[19], using default step-size ($a = 2$)
- 256 chains, 200,000 samples each
- massively parallel calibration requires ~ 3 days to run
- priors taken from CHUQ posterior
- priors for r_1^0, r_1^A and a_1 taken from Danielewicz[20]
- each data sector re-scaled to be equally important
- fractional uncertainties reasonably consistent with CHUQ: $\frac{d\sigma^{(n,n)}}{d\Omega}$: 35%, $\frac{d\sigma^{(p,p)}}{d\Omega}$: 44%, $A_y^{(n,n)}$: 140%, $A_y^{(p,p)}$: 155%, $\frac{d\sigma^{(p,n)}}{d\Omega}$: 55%

[18] Goodman and Weare 2010, *Communications in applied mathematics and computational science* 5(1), pp. 65–80
[19] Foreman-Mackey et al. 2013, *PASP* 125(925), p. 306
[20] Danielewicz et al. 2017, *Nuclear Physics A* 958, pp. 147–186

To re-scale or not to re-scale (the likelihood)

Pruitt et al[21] re-scaled the log likelihood by k/N (# of free parameters / # of experimental data points):

$$\ln p(\mathcal{D}|\boldsymbol{\alpha}, \mathcal{M}) = -\frac{k}{N}\frac{1}{2}\left(\boldsymbol{\Delta}^\top \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{\Delta} + \ln\left((2\pi)^k |\boldsymbol{\Sigma}|\right)\right)$$

We do not re-scale for ELM

[21] CD Pruitt et al. (2023). "Uncertainty-quantified phenomenological optical potentials for single-nucleon scattering". In: *Physical Review C* 107.1, p. 014602.

Charge exchange to isobaric analog states

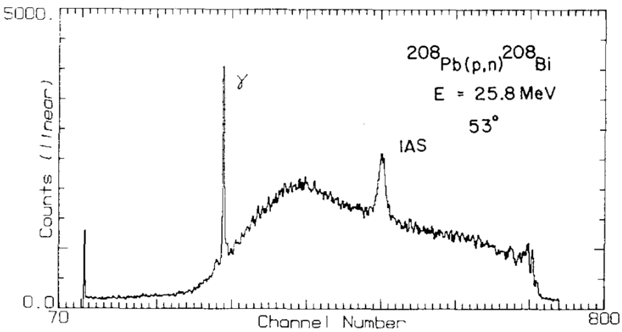
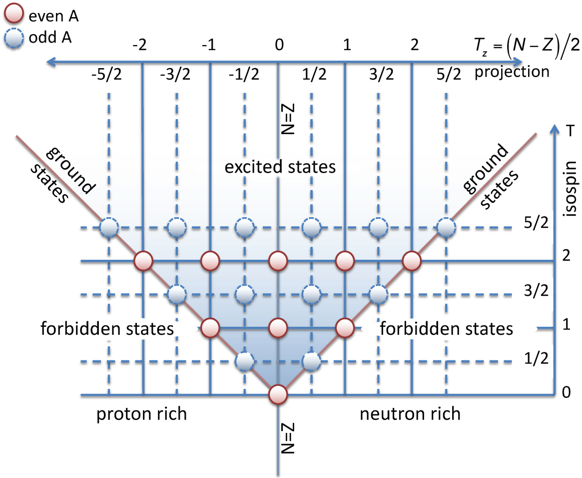


Fig. 1. Time-of-flight neutron spectrum for the reaction ^{208}Pb(p, n)^{208}Bi at 25.8 MeV showing the broad peak of the isobaric analogue state (IAS) and a narrow peak caused by incomplete rejection of γ-rays. The abscissa gives the time with units of 0.50 nsec per channel; higher energy neutrons are to the right in the spectrum. The flight path was approximately 9 m.

Reprinted from[22]

[22] SD Schery et al. (1974). "The (p, n) reaction to the isobaric analogue state of high-Z elements at 25.8 MeV". In: *Nuclear Physics A* 234.1, pp. 109–129.

Charge exchange to isobaric analog states



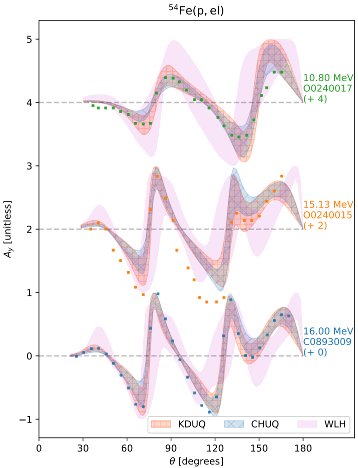
Reprinted from[23]

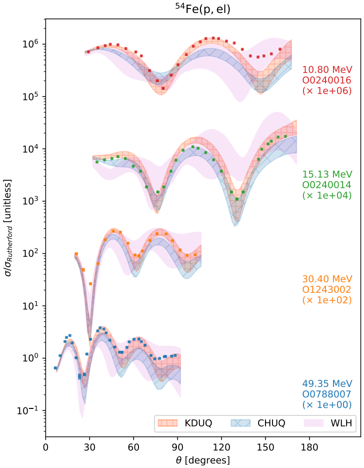
[23] Michael A Bentley (2022). "Excited States in Isobaric Multiplets—Experimental Advances and the Shell-Model Approach". In: *Physics* 4.3, pp. 995–1011. ISSN: 2624-8174. DOI: 10.3390/physics4030066. URL: https://www.mdpi.com/2624-8174/4/3/66.

jit$\mathcal{R}$ demos and tutorials: built-in optical potentials

```
[2]: from jitr.optical_potentials import chuq, kduq, wlh
```

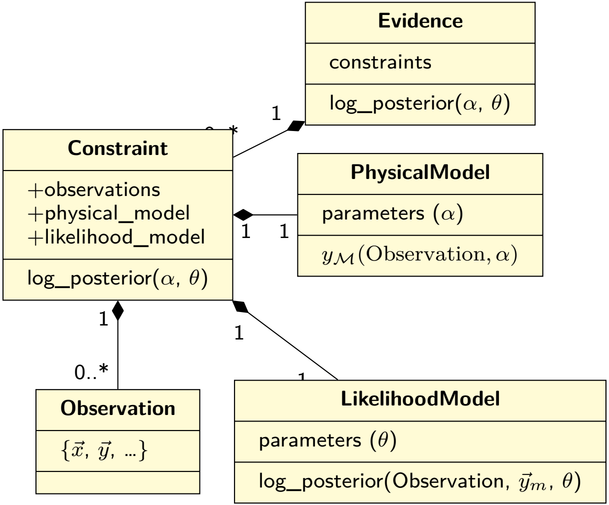
https://github.com/beykyle/jitr/blob/main/examples/notebooks/builtin_omps_uq.ipynb





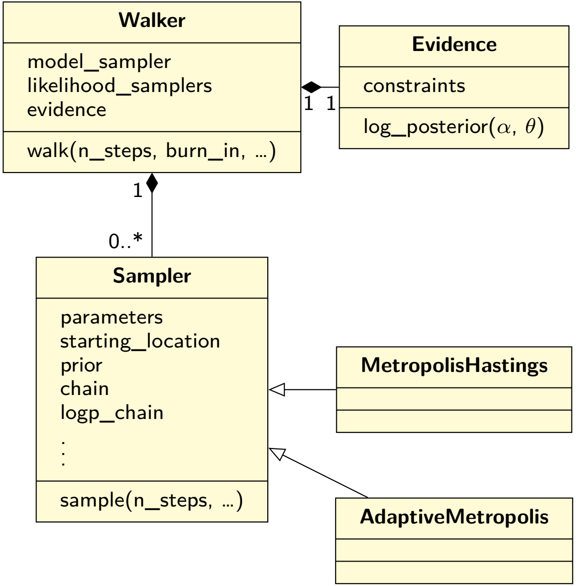
`rxmc`: spotlight on the body of evidence and the likelihood

- curating a body of evidence from multiple constraints
- Bayesian calibration with flexible likelihood models
- designed with `jit`$\mathcal{R}$ and `exfor-tools` in mind
- built-in MCMC, or just calculate the log posterior as input to another MCMC package (e.g. `surmise`)
- handles parametric likelihood models with Gibbs sampling
- alpha stage: https://github.com/beykyle/rxmc/

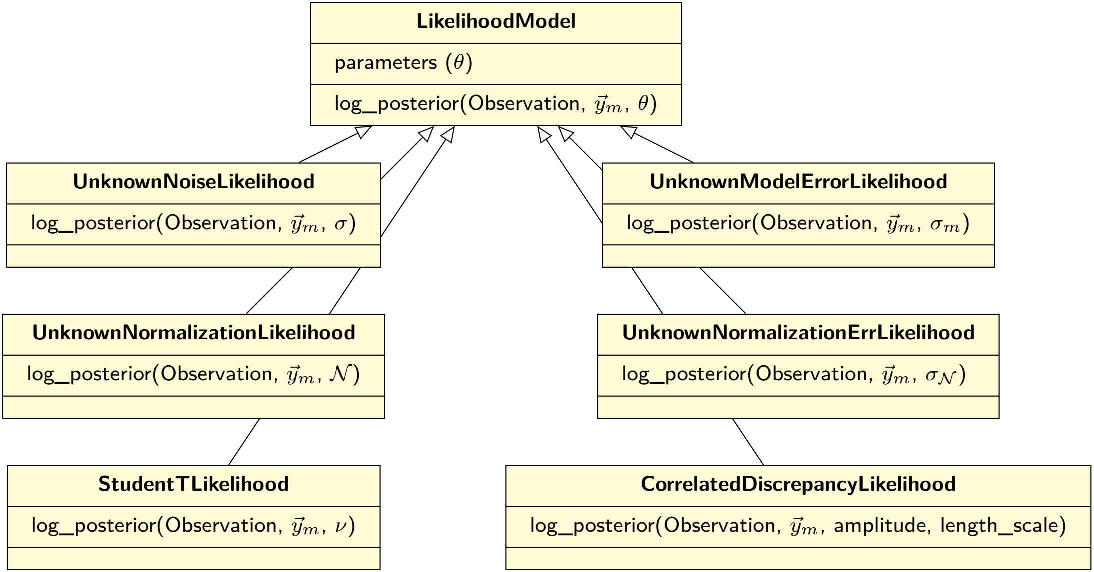


rxmc: spotlight on the body of evidence and the likelihood

- curating a body of evidence from multiple constraints
- Bayesian calibration with flexible likelihood models
- designed with jit$\mathcal{R}$ and `exfor-tools` in mind
- built-in MCMC, or just calculate the log posterior as input to another MCMC package (e.g. `surmise`)
- handles parametric likelihood models with Gibbs sampling
- alpha stage: https://github.com/beykyle/rxmc/



`rxmc`: spotlight on the body of evidence and the likelihood



Aside: systematic error in the likelihood

Common approach is to introduce a normalization parameter $\mathcal{N}$:

$$\chi^2(\alpha) = \sum_i \frac{(y_i - \mathcal{N} y_{\mathcal{M}}(x_i;\alpha))^2}{\sigma_i^2} + \frac{(\mathcal{N}-1)^2}{\sigma_{\mathcal{N}}^2} \tag{3}$$

This is incorrect! The correct approach is actually[24]:

$$\chi^2(\alpha) = \sum_i \frac{(\mathcal{N} y_i - y_{\mathcal{M}}(x_i;\alpha))^2}{(\mathcal{N}\sigma_i)^2} + \frac{(\mathcal{N}-1)^2}{\sigma_{\mathcal{N}}^2} \tag{4}$$

One can implicitly marginalize over $\mathcal{N}$, which requires use of a non-diagonal covariance[25]. This relates to Peelle's Pertinent Puzzle in nuclear data evaluation [26].

[24] D'Agostini 1994, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346(1-2), pp. 306–311; Thompson and Nunes 2009

[25] Barlow 2021, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864

[26] Frühwirth et al. 2012, vol. 27, p. 00008; Neudecker et al. 2012, *Nuclear science and engineering* 170(1), pp. 54–60

`rxmc` demos and tutorials: handling multiple constraints with systematic errors

- statistical only:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2$$

- fit (fractional) statistical error:

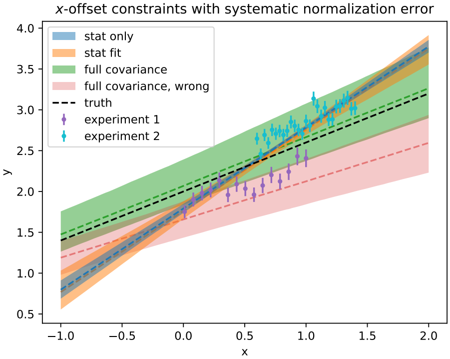
$$\Sigma_{ij} = \delta_{ij}(\eta\, y_{\mathcal{M}}(x_i;\alpha))^2$$

- full covariance:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_{\mathcal{M}}(x_i;\alpha) y_{\mathcal{M}}(x_j;\alpha)$$

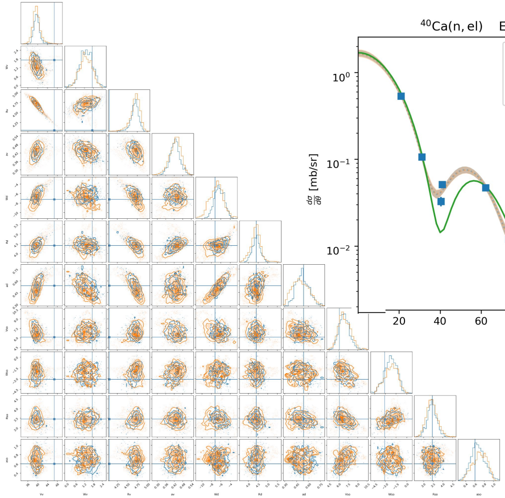
- full covariance, wrong:

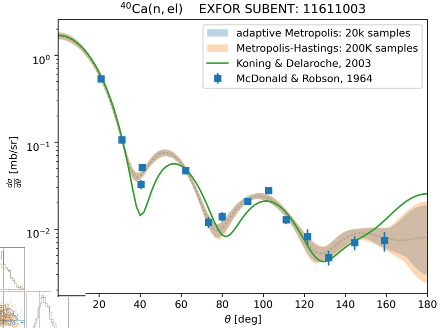
$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_i y_j$$

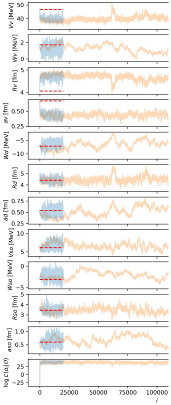


https://github.com/beykyle/rxmc/blob/main/examples/systematic_err_demo.ipynb

`rxmc` demos and tutorials: compare sampling algorithms for fitting an optical potential







https://github.com/beykyle/rxmc/blob/main/examples/fitting_an_optical_potential.ipynb

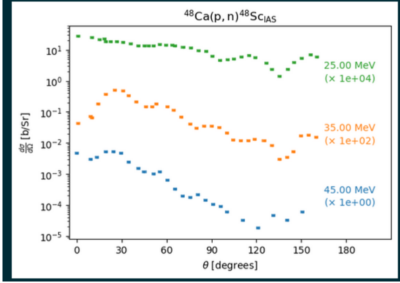
Curating a body of evidence

```
entry_pn = ExforEntry(
    entry="00178",
    reaction=ca48_pn,
    quantity="dXS/dA",
    vocal=True,
    parsing_kwargs={
        "statistical_err_labels": ["DATA-ERR"],
        "systematic_err_labels": ["ERR-1"],
    },
)
```

```
Found subentry 00178006 with the following columns:
['ERR-1', 'ERR-2', 'ERR-3', 'ERR-4', 'EN', 'Q-VAL', 'ANG-ERR', 'DATA-ERR', 'ANG-CM', 'DATA', 'ERR-T']
Found subentry 00178007 with the following columns:
['ERR-1', 'ERR-2', 'ERR-3', 'ERR-4', 'EN', 'Q-VAL', 'ANG-ERR', 'DATA-ERR', 'ANG-CM', 'DATA', 'ERR-T']
Found subentry 00178008 with the following columns:
['ERR-1', 'ERR-2', 'ERR-3', 'ERR-4', 'EN', 'Q-VAL', 'ANG-ERR', 'DATA-ERR', 'ANG-CM', 'DATA']
```

```
fig, ax = plt.subplots(1, 1, figsize=(6, 4))
entry_pn.plot(
    ax, offsets=100, label_kwargs={"label_xloc_deg": 165, "label_offset_factor": 0.0001}
)
ax.set_xlim([-5, 210])
ax.set_title(ax.title.get_text() + r"$_\text{IAS}$")
```

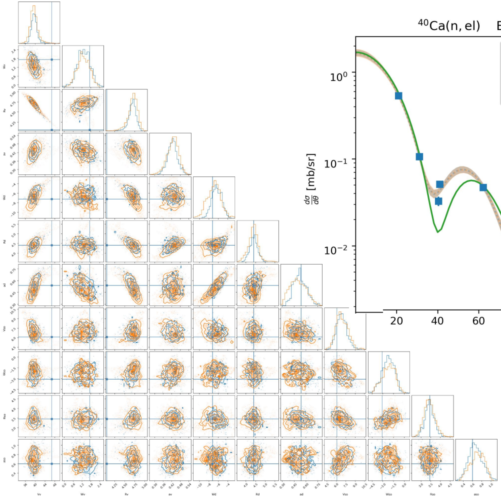
```
Text(0.5, 1.0, '$^{48} \\rm{Ca}(p,n)^{48} \\rm{Sc}$$_\\text{IAS}$')
```

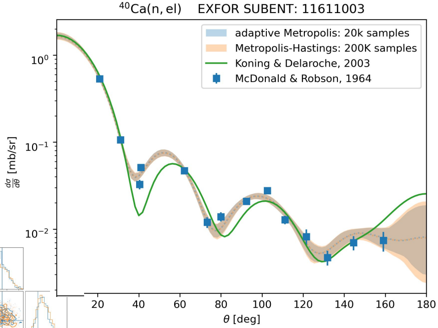


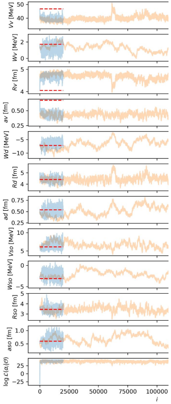
https://github.com/beykyle/exfor_tools

- reproducible curation
- systematically improvable with new evaluations

Comparison of sampling algorithms for fitting an optical potential







https://github.com/beykyle/rxmc/blob/main/examples/fitting_an_optical_potential.ipynb