BAND Approach to Optical Potentials

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CSWEG 2025

BAND Bayesian Analysis of Nuclear Dynamics

MICHIGAN STATE UNIVERSITY

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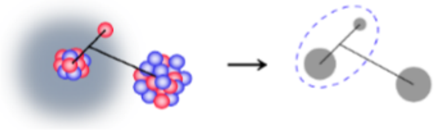
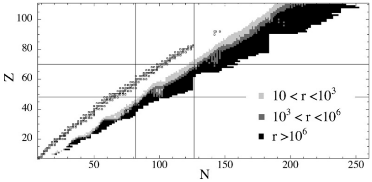
Few Body Reactions Group

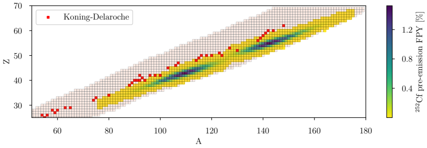
Nuclear reactions away from stability involves extrapolating the optical potential



- optical potential reduce many-body DOF in reactions to few
- phenomenological optical potentials are extrapolated away from β-stability
- along with NLDs, γSF, etc., they are necessary for prediction and evaluation in data-sparse regime



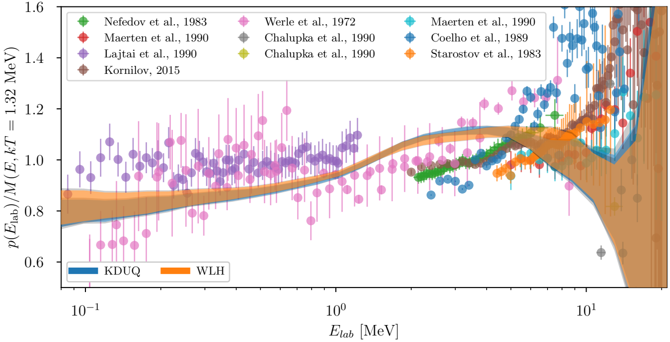
(n, γ) rates for r-process [1]



fission fragments [2]

[1] Goriely and Delaroche 2007, *Physics Letters B* 653(2-4), pp. 178–183
[2] Beyer et al. 2025, *Phys. Rev. C* 112, p. 024604

Past work: optical model uncertainty in CGMF fission observables



Optical model uncertainty in CGMF Monte Carlo Hauser-Feshbach calculations of ^{252}Cf PFNS [3]

[3] Beyer et al. 2025, *Phys. Rev. C* 112, p. 024604

Calibration of an uncertainty-quantified global optical potential

- Canonical KOH statistical approach to model calibration [4]

$$\underbrace{y_i + \epsilon_i}_{\text{observation with uncertainty}} = \underbrace{\zeta(x_i)}_{\text{latent truth}} = \underbrace{\eta(x_i;\alpha) + \delta(x_i)}_{\text{parametric model with discrepancy}} + \epsilon_i \tag{1}$$

- given priors

$$\epsilon_i \sim \mathcal{N}(0, \mathbf{\Sigma}^{\text{exp}})$$
$$\delta(x_i) \sim \mathcal{N}(0, \mathbf{\Sigma}^{\text{md}})$$

- and data set(s) $\mathcal{D} = \{x_i, y_i\}_{i=0}^{N}$
- the likelihood is

$$p(\alpha, \beta|\mathcal{D}) = \Big((2\pi)^N |\mathbf{V}(\beta)|\Big)^{-1/2} \exp\Big\{-\frac{1}{2}\mathbf{\Delta}^\top \mathbf{V}^{-1}(\beta)\mathbf{\Delta}\Big\},$$

  where $\Delta \equiv \mathbf{y} - \boldsymbol{\eta}(\boldsymbol{x}, \alpha)$ and $\boldsymbol{V}(\beta) \equiv \mathbf{\Sigma}^{\text{exp}} + \mathbf{\Sigma}^{\text{md}}(\beta)$
- Baye's rule provides posterior given priors $p(\alpha)$, $p(\beta)$
- for global nucleon-nucleus optical potentials, $x = \{A, Z, E, \theta, \dots\}$ and $y = d\sigma/d\Omega, A_y, \dots$

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

Statistical approach to optical potentials

- **1950s on**: Frequentist, least-squares fitting, a few parameters at a time. Parameter ambiguities observed. [a]
- **2003**: Koning-Delaroche [b] 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. [c])
- **2023:** First global Bayesian calibration: CHUQ and KDUQ (Pruitt et al.[d])

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[a] Satchler et al. 1964, *Physical Review* 136(3B), B637
[b] Koning and Delaroche 2003, *Nuclear Physics A* 713(3-4), pp. 231–310
[c] Lovell et al. 2017, *Physical Review C* 95(2), p. 024611
[d] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602

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

- systematic errors ignored!
- model discrepancy ignored (or treated with diagonal covariance)!
- non-identifiability not treated rigorously!

Can we trust the extrapolation into data-sparse regime?

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

- Resonable ansatz for isovector dependence of optical potential [5]:

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

Goal: uncertainty-quantified extrapolation in $(N-Z)/A$ using $(p,n)_{\text{IAS}}$ as a constraint and rigorous Bayesian approach

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

(p, n) to the isobaric analog state

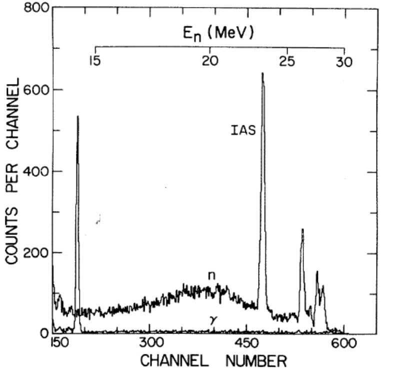
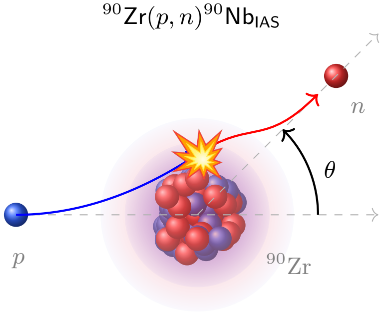


FIG. 1. Neutron (n) and γ-ray (γ) time-of-flight spectra at 0° for 35-MeV protons on ^{90}Zr. Each channel represents 0.1 nsec.

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

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

- New global, uncertainty quantified optical potential
- Lane consistent
- 24 parameters (compared to 48 for Koning-Delaroche)
- Coulomb correction to all orders
- open-source data curation (`exfor-tools`), solver (jit$\mathcal{R}$), and statistical modeling software (`rxmc`) as part BAND framework [6]

BAND
Bayesian Analysis of Nuclear Dynamics

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

github.com/beykyle/elm

[6] Beyer et al. 2025, (Version 0.5.0)

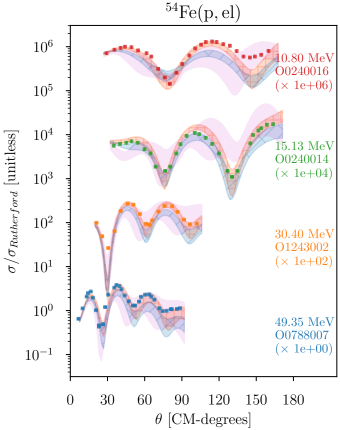
jit$\mathcal{R}$ allows for global calibration without needing emulators

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]

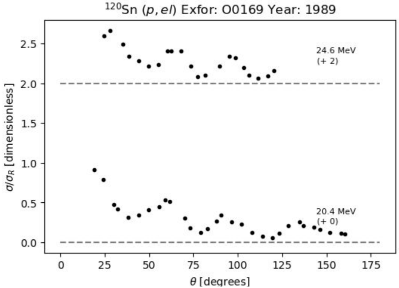
[a] Beyer et al. 2025, (Version 0.5.0)

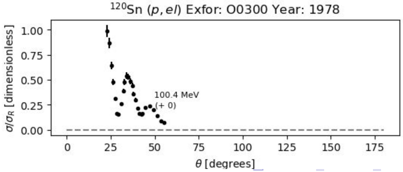
Curation of a body of experimental data

- $\sim$ 100 EXFOR entries, $\sim 10\text{K}$ data points
- sparse coverage of input space
- $40 \leq A \leq 208$
- $10\ \text{MeV} < \text{E}_{\text{lab}} < 200\ \text{MeV}$
- $d\sigma/d\Omega$ 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, built on top of David Brown's x4i package.

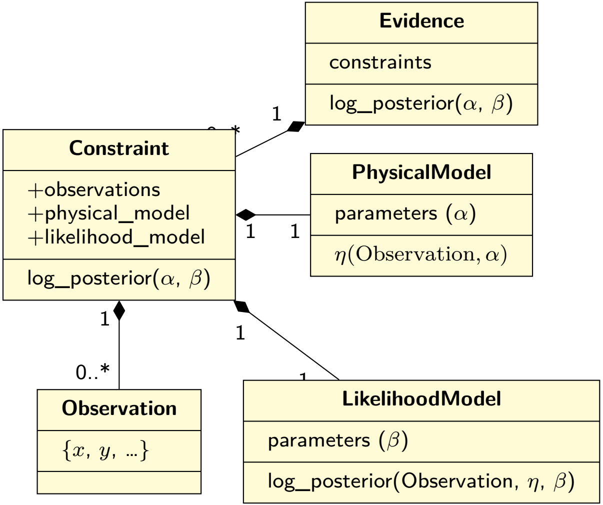
```
all_entries_pp = exfor_tools.get_exfor_differential_data(
    target=target,
    projectile=proton,
    quantity="dXS/dA",
    product="EL",
    energy_range=[10, 200],  # MeV
)
```





`rxmc`: flexible, hierarchal Bayesian calibration to heterogeneous data

- 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 sampler, or interface with external MCMC package
- handles parametric likelihood models with batched Metropolis-in-Gibbs sampling
- in alpha stage: https://github.com/beykyle/rxmc/



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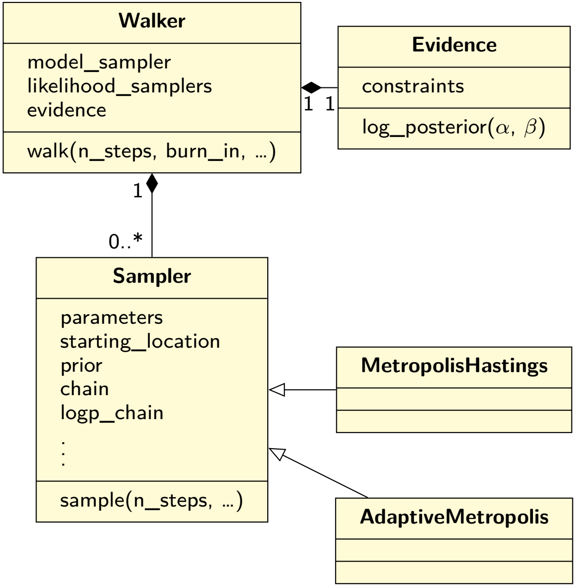

Statistical model for ELM

Likelihood model

$$\ln p(\mathcal{D}|\alpha, \mathcal{M}) = -\frac{1}{2}\left(\boldsymbol{\Delta}^\top \cdot \boldsymbol{V}^{-1} \cdot \boldsymbol{\Delta} + \ln\left((2\pi)^k |\boldsymbol{V}|\right)\right)$$
$$\Delta_i(\alpha) \equiv \eta(x_i, \alpha) - y_i$$
$$\boldsymbol{V}(\beta) = \boldsymbol{\Sigma}_{ij}^{\text{exp}} + \boldsymbol{\Sigma}_{ij}^{\text{MD}}(\beta)$$

- diagonal model discrepancy, learned from data (following [7]).

$$\boldsymbol{\Sigma}_{ij}^{\text{exp}} \equiv \delta_{ij}\sigma^2_{\text{exp,i}}$$
$$\boldsymbol{\Sigma}_{ij}^{\text{MD}}(\beta) \equiv \delta_{ij}\left(\beta\tilde{y}_i\right)^2, \quad \tilde{y}_i \equiv \left(\eta(x_i;\alpha) + y_{i,\text{exp}}\right)/2$$

- β are free parameters (one per data sector)

Prior

- estimated from CHUQ

Sampling

- Adaptive Metropolis-in-Gibbs with `rxmc`
- Goodman-Weare from `emcee`[8]
- massively parallel

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

[8] 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

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

- Pruitt et al. re-scaled the log likelihood by k/N (# of free parameters / # of experimental data points $\sim 20/10000$):

$$\ln p(\mathcal{D}|\alpha,\mathcal{M}) \rightarrow$$

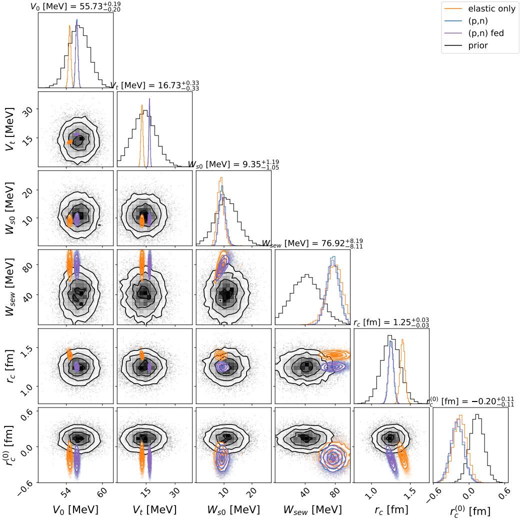
$$\frac{k}{N}\ln p(\mathcal{D}|\alpha,\mathcal{M})$$

- re-scaling is equivalent to “cold” posterior with $\lambda = k/N < 1$ (post-Bayesian approach) [8]

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

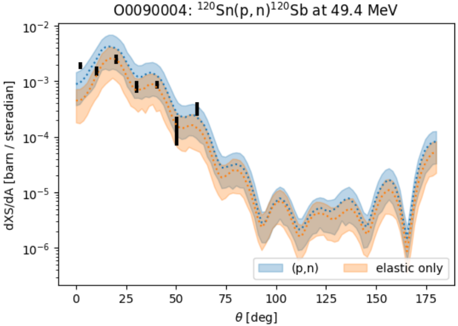
[7] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602
[8] Grünwald 2011, vol. 19, pp. 397–420

Effect of (p, n)

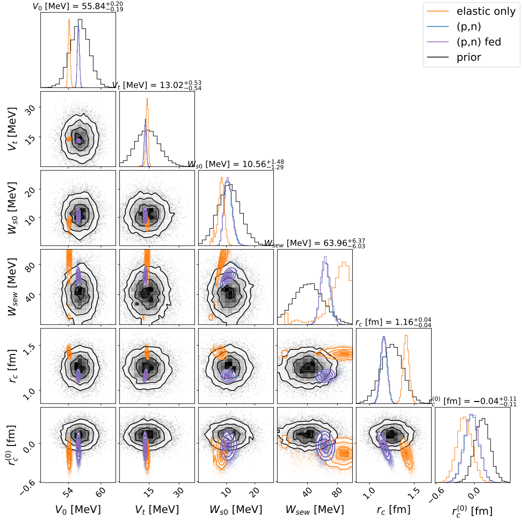


Corner plot for subset of posterior with and without (p, n)

- Introduction of (p, n) constraint doesn't make a huge difference . . .



Effect of independent isovector geometry



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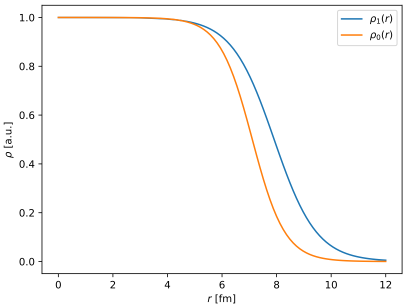

- Independent isoscalar and isovector geometries suggestd by Danieliwicz et. al. [a]
- Convergence only reached when (p, n) constraint is included

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

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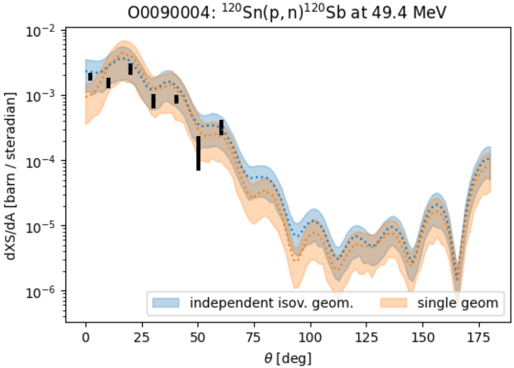

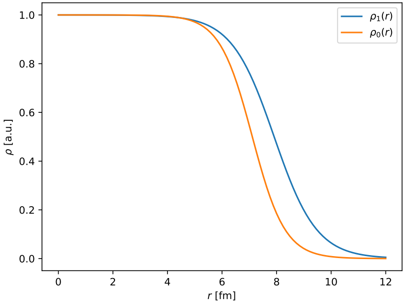

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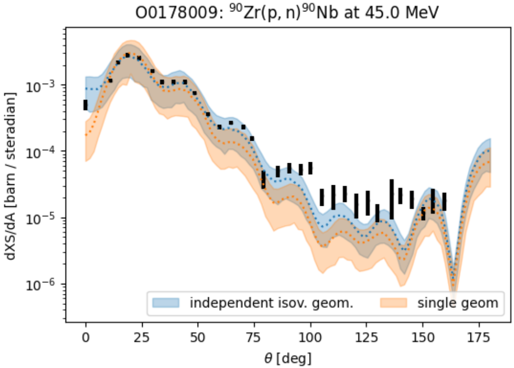

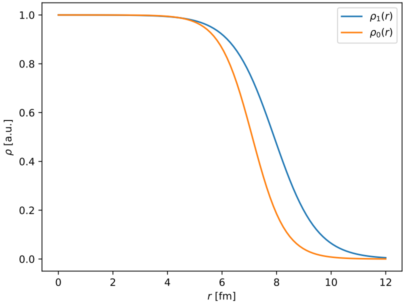

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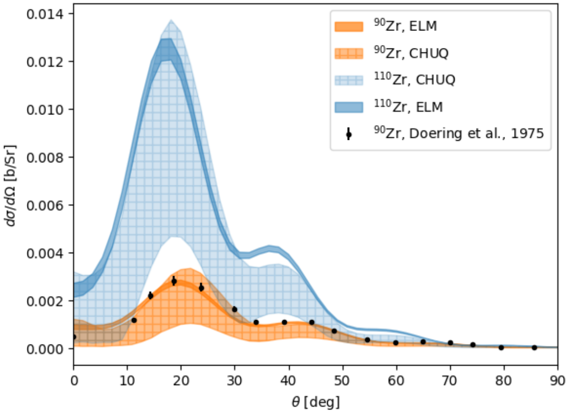
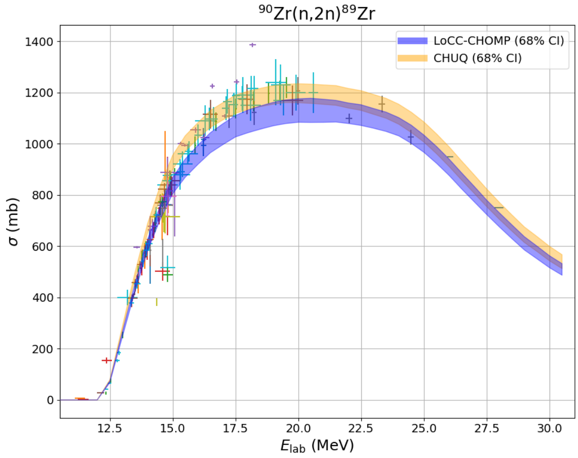
Extrapolation in $(N - Z)/A$ with reduced uncertainties compared to CHUQ



$(p, n)_{IAS}$ for Zr isotopes

We've begun propagating uncertainties to Hauser-Feshbach calculations



BAND Fellow, Samuel Sullivan
(PhD student at University of Surrey)

- Lane-consistent potential calibrated to $d\sigma_{el}/d\Omega$ and Ay for (n, n), (p, p) along isotopic chains from 10-50 MeV using `rxmc`
- propagation to compound channels using TALYS
- covariances can be obtained empirically from posterior predictive

Summary and outlook

ELM coming soon!

- need both (p, n) constraints and independent isoscalar and isovector geometries
- developed open-source software ecosystem for Bayesian inference in nuclear reactions

Future work:

- systematic experimental error, model discrepancy, errors in angle
- handle non-identifiability of spin-orbit potential, geometric parameters
- dispersion relation and structure constraints
- UQ of nuclear level density

Thank you for your time!

In collaboration with Filomena Nunes and the Few Body Reactions Group

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Bayesian Analysis of Nuclear Dynamics

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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. (2025a). *BANDFramework: An Open-Source Framework for Bayesian Analysis of Nuclear Dynamics*. Tech. rep. Version 0.5.0. URL: https://github.com/bandframework/bandframework.

Beyer, Kyle A. et al. (2025b). "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.

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.

Danielewicz, Paweł et al. (2017). "Symmetry energy III: Isovector skins". In: *Nuclear Physics A* 958, pp. 147–186.

References II

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].

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.

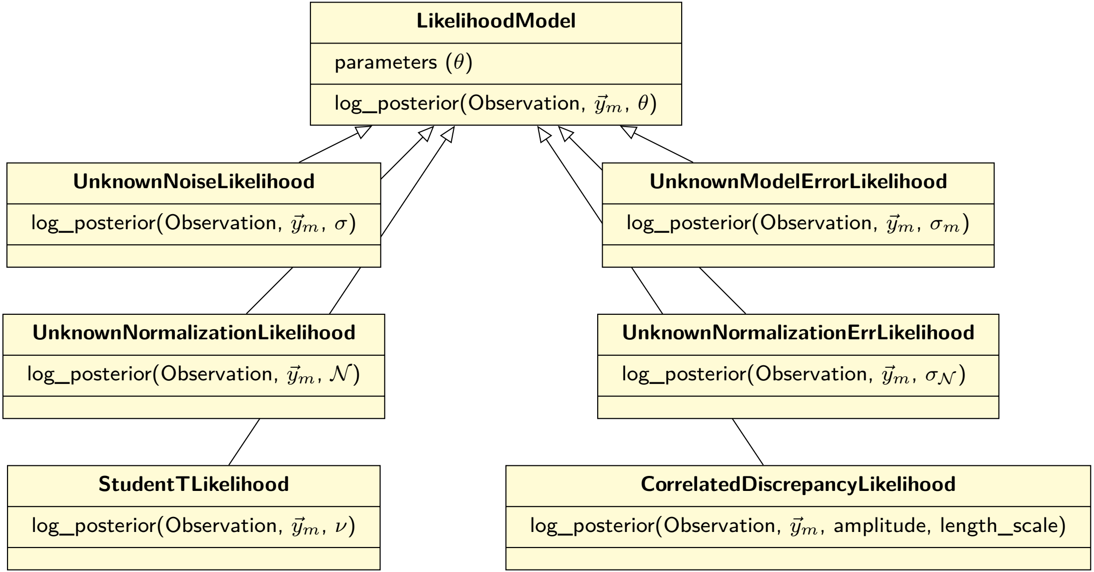
Kennedy, Marc C and Anthony O'Hagan (2001). "Bayesian calibration of computer models". In: *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 63.3, pp. 425–464. DOI: http://dx.doi.org/10.1111/1467-9868.00294.

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.

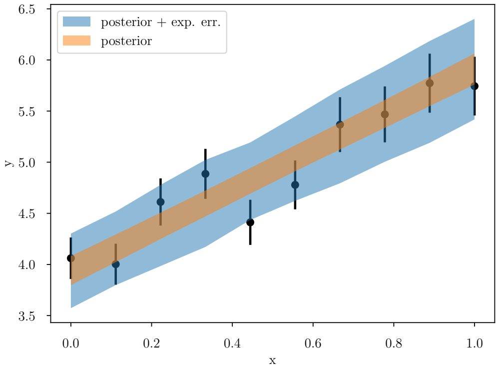
References III

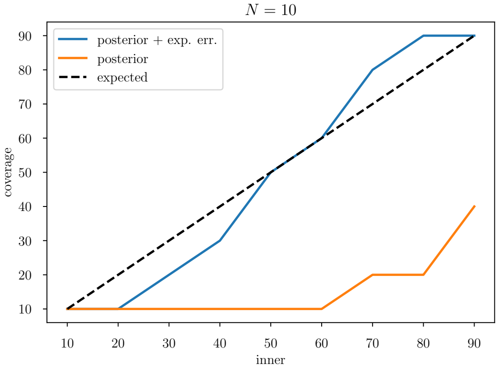
- Lane, AM (1962). “Isobaric spin dependence of the optical potential and quasi-elastic (p, n) reactions”. In: *Nuclear Physics* 35, pp. 676–685.
- Lovell, Amy E et al. (2017). “Uncertainty quantification for optical model parameters”. In: *Physical Review C* 95.2, p. 024611.
- Neudecker, Denise et al. (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.
- 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.

rxmc: building and composing likelihood models



Empirical coverage





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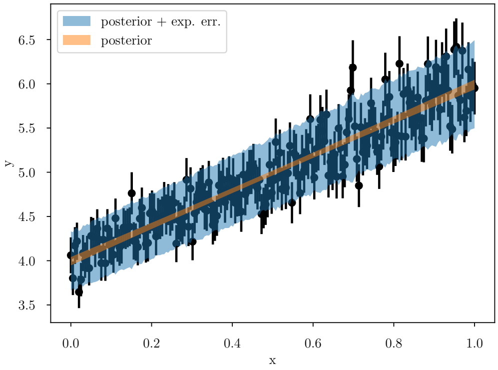
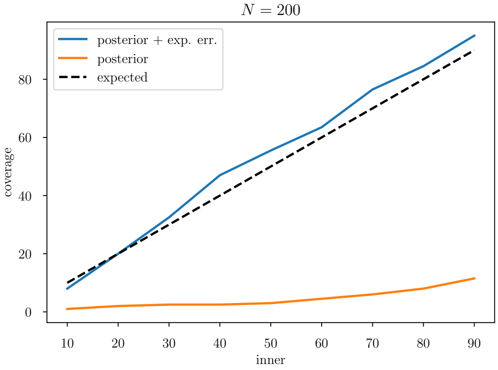
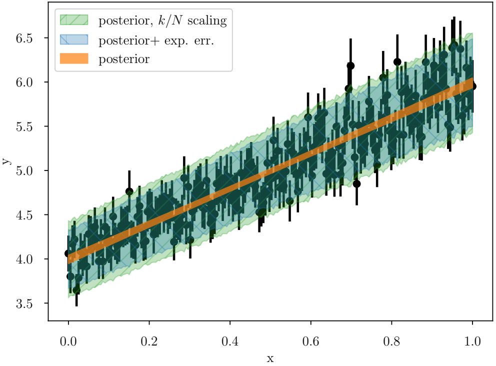
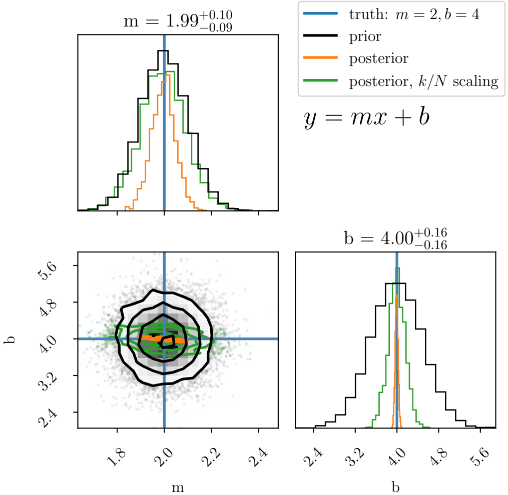


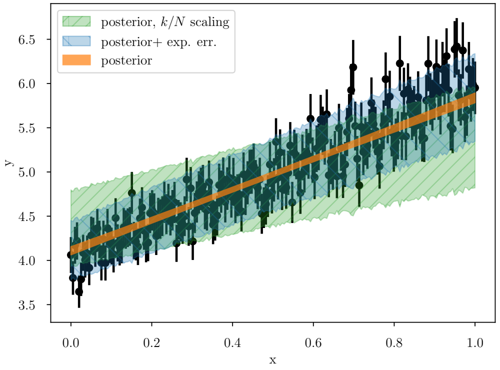


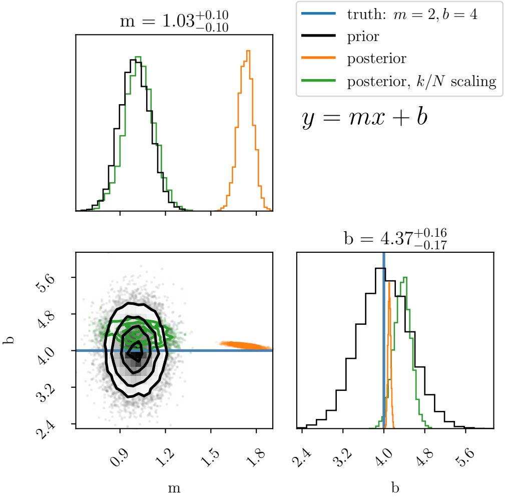
“Cold” posterior





“Cold” posterior: over-emphasis on the prior





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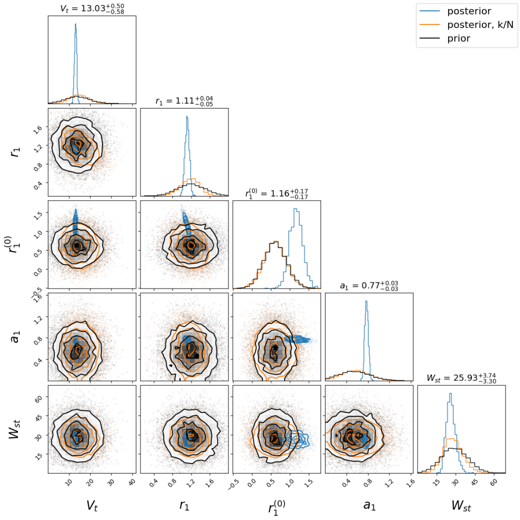
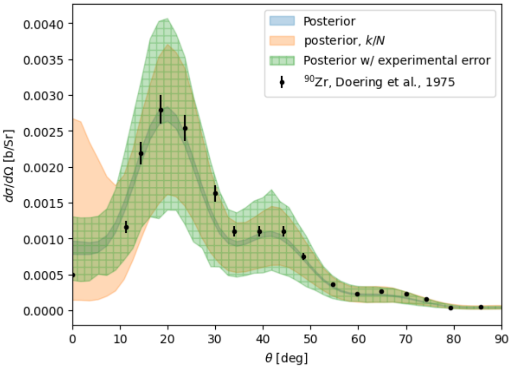
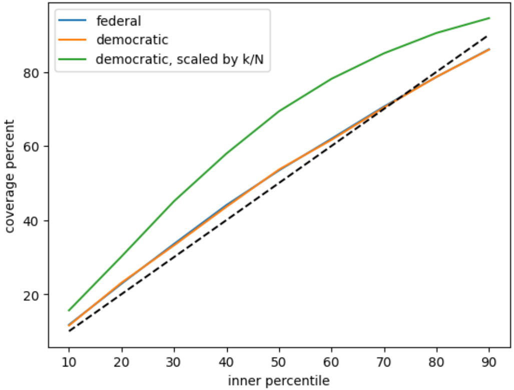
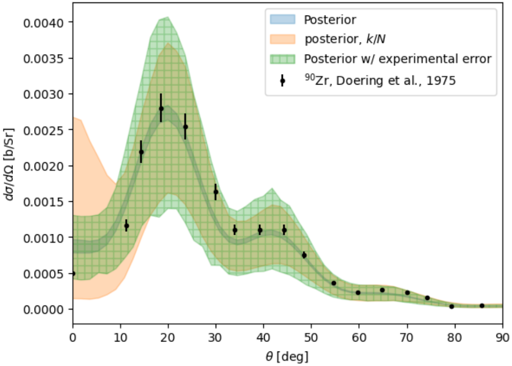


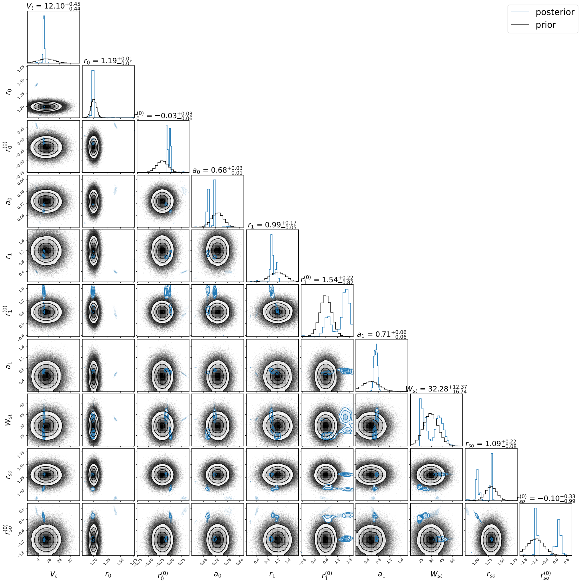


Predictive posteriors and empirical coverage

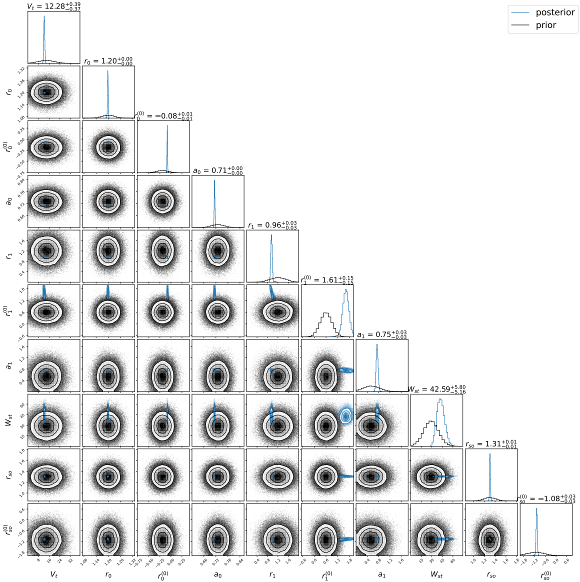




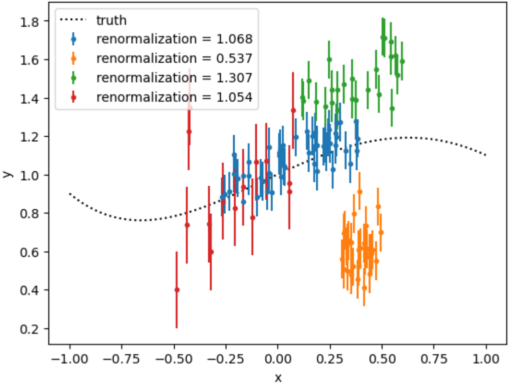
Multimodality, parameter ambiguity in radii



Multimodality, parameter ambiguity in radii



Handling multiple constraints with systematic errors



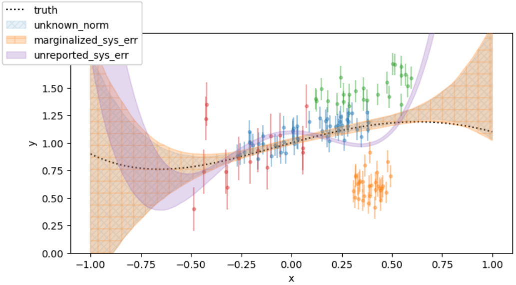
Each synthetic data set j has it's own systematic error σ_j

- treat data normalization as free parameter: $y_{i \in \mathcal{D}_j} = \zeta(x_i) + \epsilon_i = \rho_j \eta(x_i; \alpha) + \delta(x_i)$
- explicitly marginalize over $\rho_j \sim \mathcal{N}(1, \sigma_j)$, leads to *model-dependent* covariance matrix: $\Sigma_{lm} = \delta_{lm}\sigma^2_{stat,l} + \sigma_j^2 \eta(x_l; \alpha)\eta(x_m; \alpha)$. Note: doing this wrong leads to Peelle's Pertinent Puzzle [9]!

Adapted from open source demos in https://github.com/beykyle/rxmc

[9] Barlow 2021, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864; D'Agostini 1994, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346(1-2), pp. 306–311; Neudecker et al. 2012, *Nuclear science and engineering* 170(1), pp. 54–60

Handling multiple constraints with systematic errors



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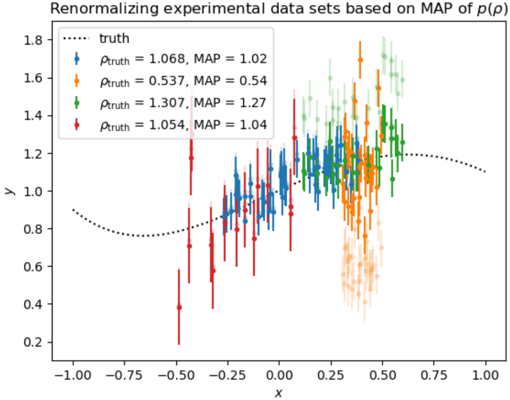
- compare to ignoring systemtic error

Adapted from open source demos in https://github.com/beykyle/rxmc

[9] Barlow 2021, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864; D'Agostini 1994, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346(1-2), pp. 306–311; Neudecker et al. 2012, *Nuclear science and engineering* 170(1), pp. 54–60



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- advantage of keeping ρ_j free is the ability to renormalize experimental data to be consistent with each other

Adapted from open source demos in https://github.com/beykyle/rxmc

[9] Barlow 2021, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864; D'Agostini 1994, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346(1-2), pp. 306–311; Neudecker et al. 2012, *Nuclear science and engineering* 170(1), pp. 54–60

- statistical only:

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

- fit (fractional) statistical error:

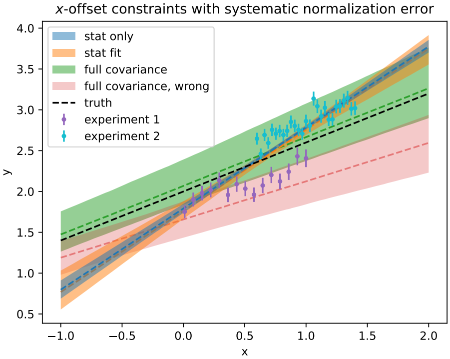
$$\Sigma_{ij} = \delta_{ij}(\eta\, y_{\mathcal{M}}(x_i;\alpha))^2$$

- full covariance:

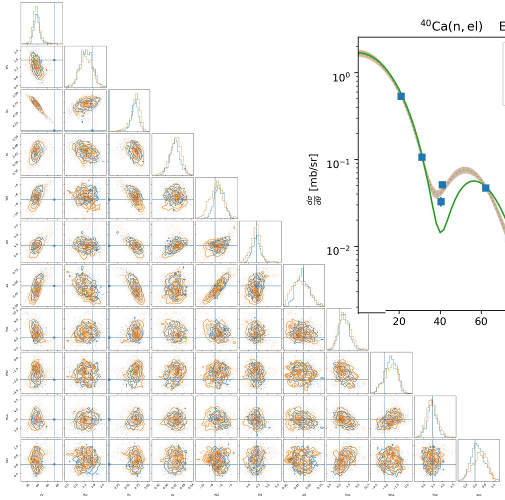
$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_{\mathcal{M}}(x_i;\alpha) y_{\mathcal{M}}(x_j;\alpha)$$

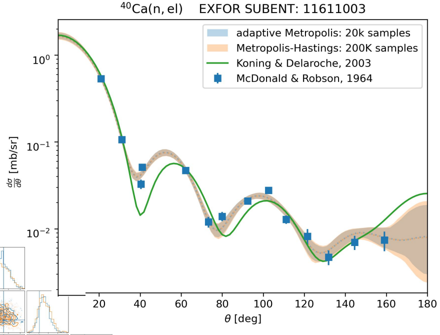
- full covariance, wrong:

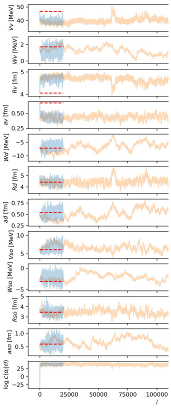
$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_i y_j$$



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







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

Extra slides: ELM physical model

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

$$\begin{aligned}
U_0(r, E, A) = {} & V_0(E) f((r - R_0(A))/a_0) + i W_0(E) f((r - R_w(A))/a_w) \\
& - 4 i a_w W_{s,0}(E) \frac{d}{dr} f((r - R_w(A))/a_w) + 2\,(\boldsymbol{\sigma} \cdot \boldsymbol{\ell})\; V_{so} \frac{1}{r} \frac{d}{dr} f((r - R_{so}(A))/a_{so}) \\
U_1(r, E, A) = {} & V_1(E) f((r - R_1(A))/a_1) - 4 i a_w W_{s,1}(E) \frac{d}{dr} f((r - R_w(A))/a_w)
\end{aligned}$$

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

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

- Goodman-Weare [10] affine-invariante stretch move sampler from `emcee`[11], 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[12]
- 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%

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

Charge exchange to isobaric analog states

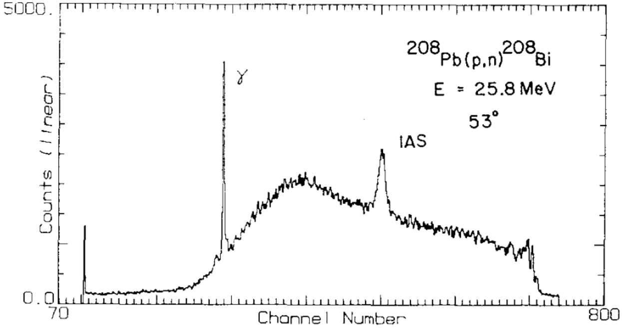
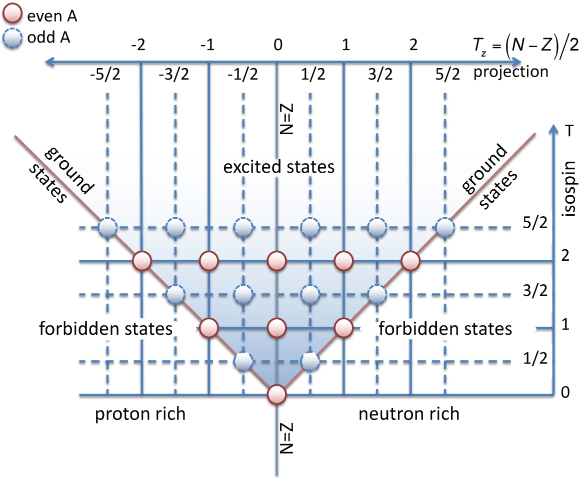


Fig. 1. Time-of-flight neutron spectrum for the reaction ^{208}Pb(p, n)^{208}Bi at 25.8 MeV showing the broad peak of the isobaric analogue state (IAS) and a narrow peak caused by incomplete rejection of γ-rays. The abscissa gives the time with units of 0.50 nsec per channel; higher energy neutrons are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

Reprinted from[13]

[13] 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



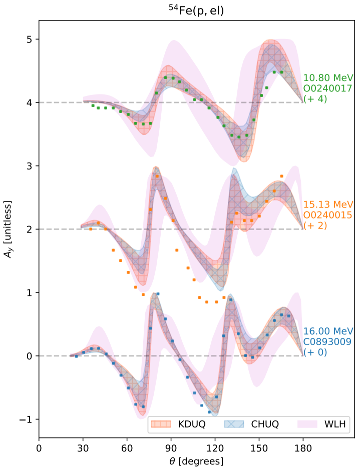
Reprinted from[14]

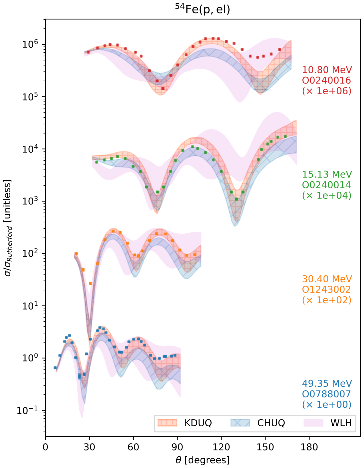
[14] Michael A Bentley (2022). "Excited States in Isobaric Multiplets—Experimental Advances and the Shell-Model Approach". In: *Physics* 4.3, pp. 995–1011. ISSN: 2624-8174. DOI: 10.3390/physics4030066. URL: https://www.mdpi.com/2624-8174/4/3/66.

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





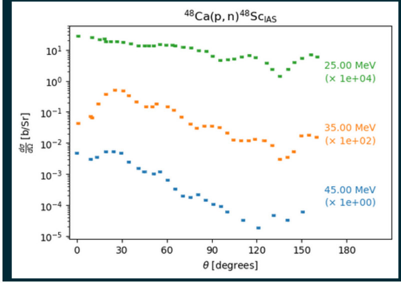
Curating a body of evidence

```
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