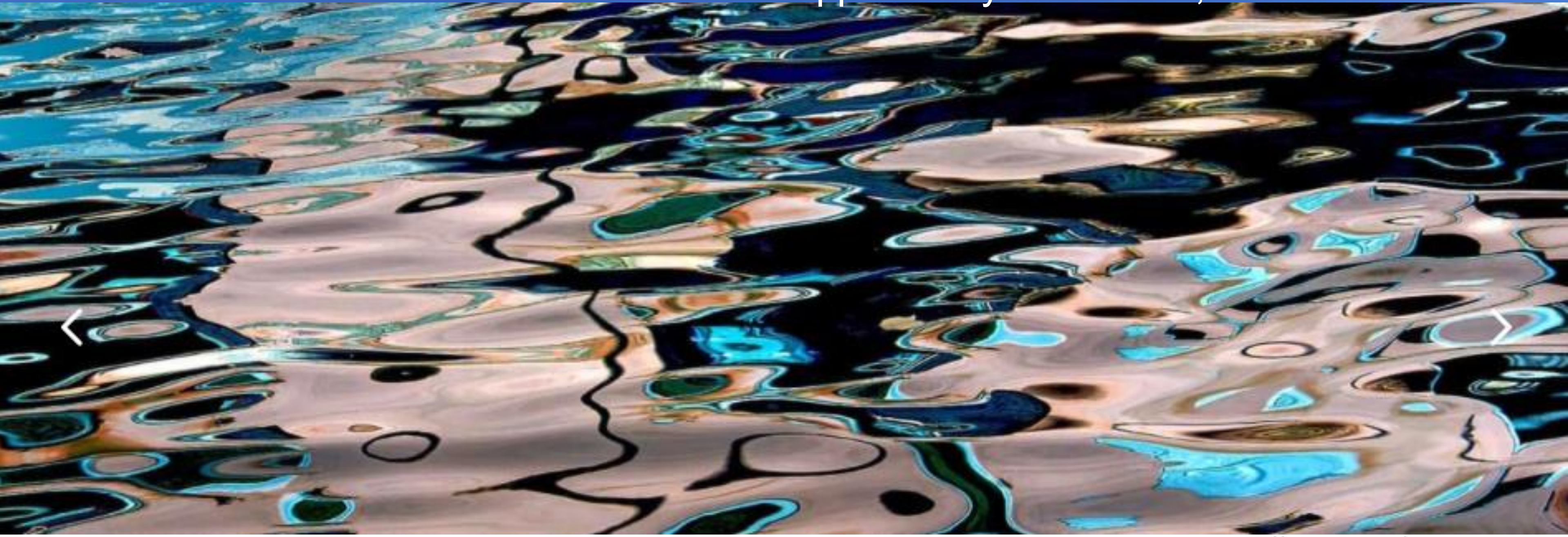
Work supported by NSF-CSSI, DOE-NP and MSU



https://imagesofvenice.com

Uncertainty quantification in nuclear reactions

Filomena Nunes
Michigan State University

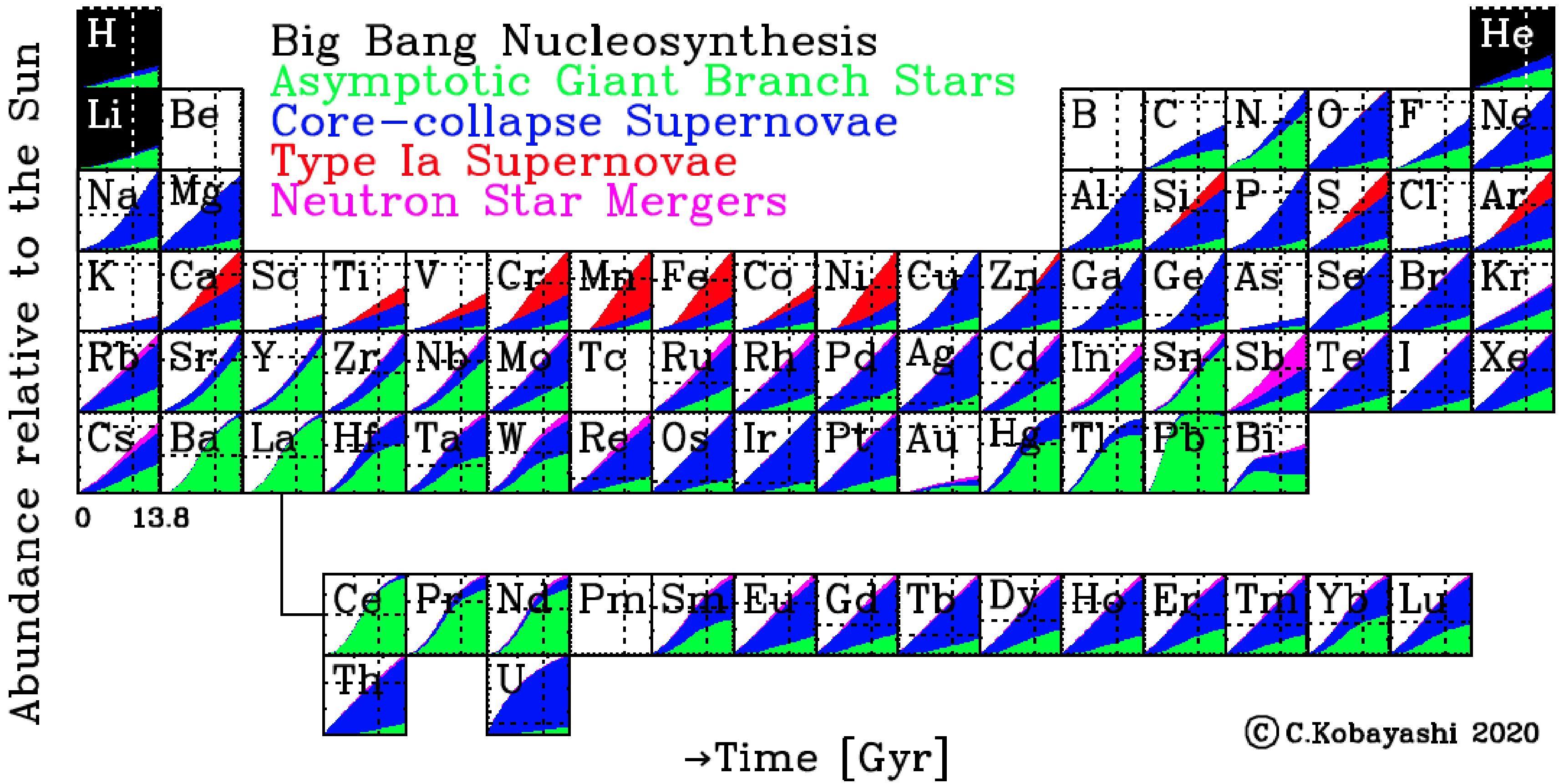
Michigan State University occupies the ancestral, traditional, and contemporary Lands of the Anishinaabeg–Three Fires Confederacy of Ojibwe, Odawa, and Potawatomi peoples. The University resides on Land ceded in the 1819 Treaty of Saginaw.

Outline

- The physical model
  - optical potentials in reactions
- Prior knowledge
- The evidence
- The likelihood
- Calibration: examples
- Conclusions

Color code:
Nuclear physics background
Statistical model

Where did nuclei come from?
How were they produced?

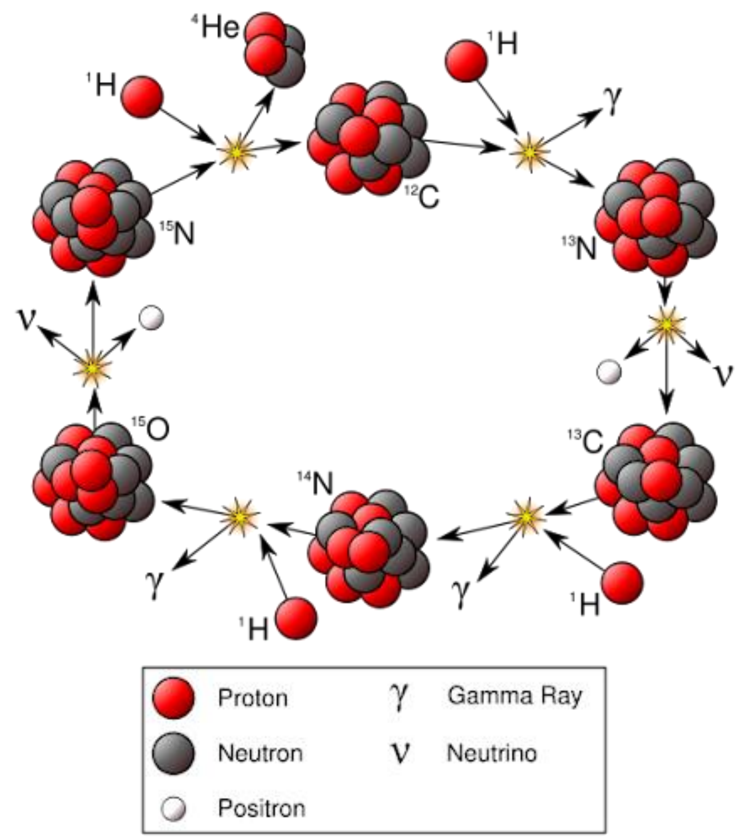


Kobayashi, Karakas, Lugaro, ApJ 2020

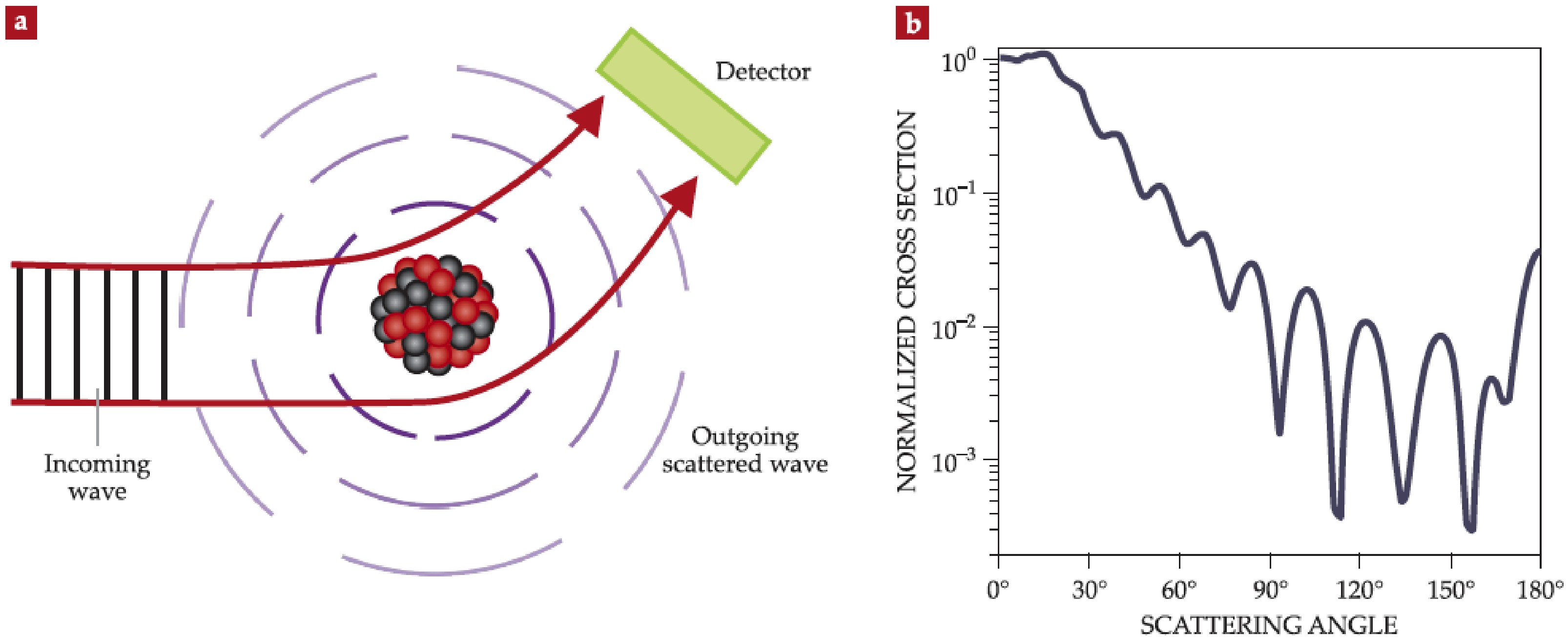
Reactions are key to answering these big science questions

It is through a bunch of reactions that we produce the elements we see on Earth

Example: CNO cycle which takes place in our favorite star

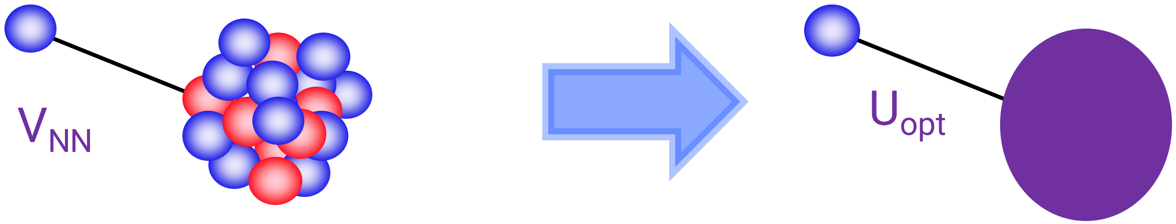


Nuclear reactions offer unique probes to explore our big science questions



We make beams of exotic rare isotopes and smash them onto a target!

The Optical Potential is an essential ingredient in reaction theory



It's the projection of the many-body scattering problem on the ground state: $$P\Psi(\vec{r},\vec{r}_1,\ldots,\vec{r}_A) = \phi_0(\vec{r})\Phi_0(\vec{r}_1,\ldots,\vec{r}_A)$$

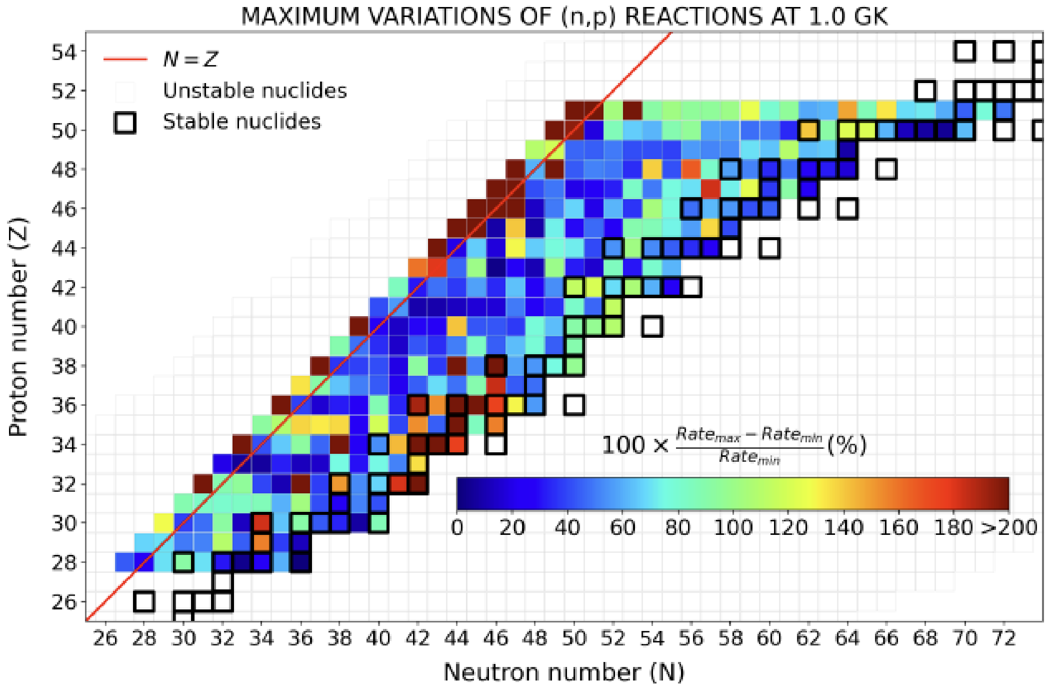
End up with a single-channel scattering equation with potential:

$$V_{\rm opt} = \mathcal{V}_{00} + \sum_{j,k\neq 0} \mathcal{V}_{0j}\frac{1}{E - H_{jk} + i\eta}\mathcal{V}_{k0}$$

Hebborn, Nunes, et al., JPG 50, 060501 (2023)

Optical potentials are pervasive in reaction models

Inputs necessary for (n,g); (p,g); (p,n); (n,p); (d,p); (d,n); …
Inputs also for breakup, knockout and transfer on heavier probes



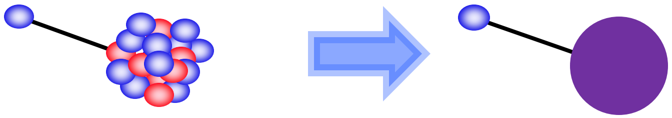
Reaction observables are very sensitive to details of the optical potential.

OP is a main source of uncertainty

Need uncertainty quantification!

Hebborn, Nunes, et al., JPG 50, 060501 (2023)

Physical model: optical model

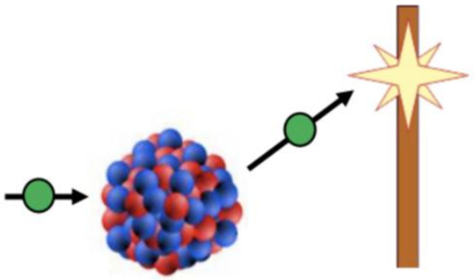


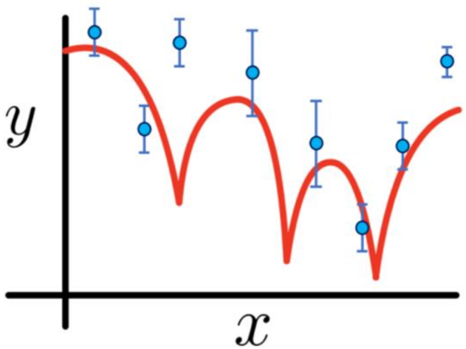
$$\boxed{[T+U_{opt}(R)-E]\psi=0}$$

The model has a set of parameters

$$U_{opt}(\ R\ )= V\ f(R,\ r,\ a) + W\ f(R,\ r_w,\ a_w) + W_s\ f(R,\ r_s,\ a_s) + V_{so} + V_C$$

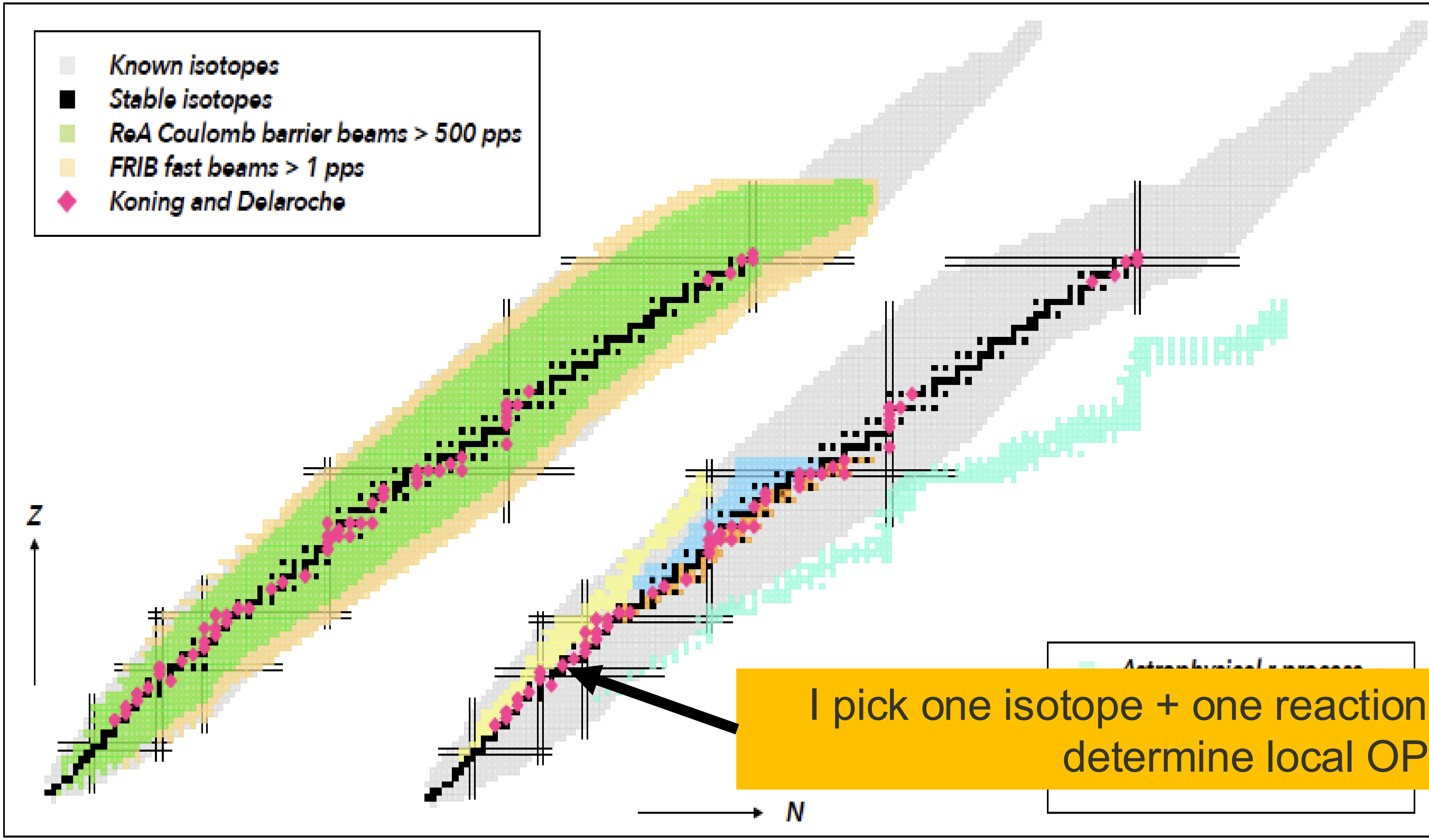
- calibrated with **reaction data** (**phenomenological** optical potentials)





A DEEPER UNDERSTANDING OF THE INPUTS FOR REACTION THEORY THROUGH UNCERTAINTY QUANTIFICATION
Amy Lovell (PhD thesis 2018)

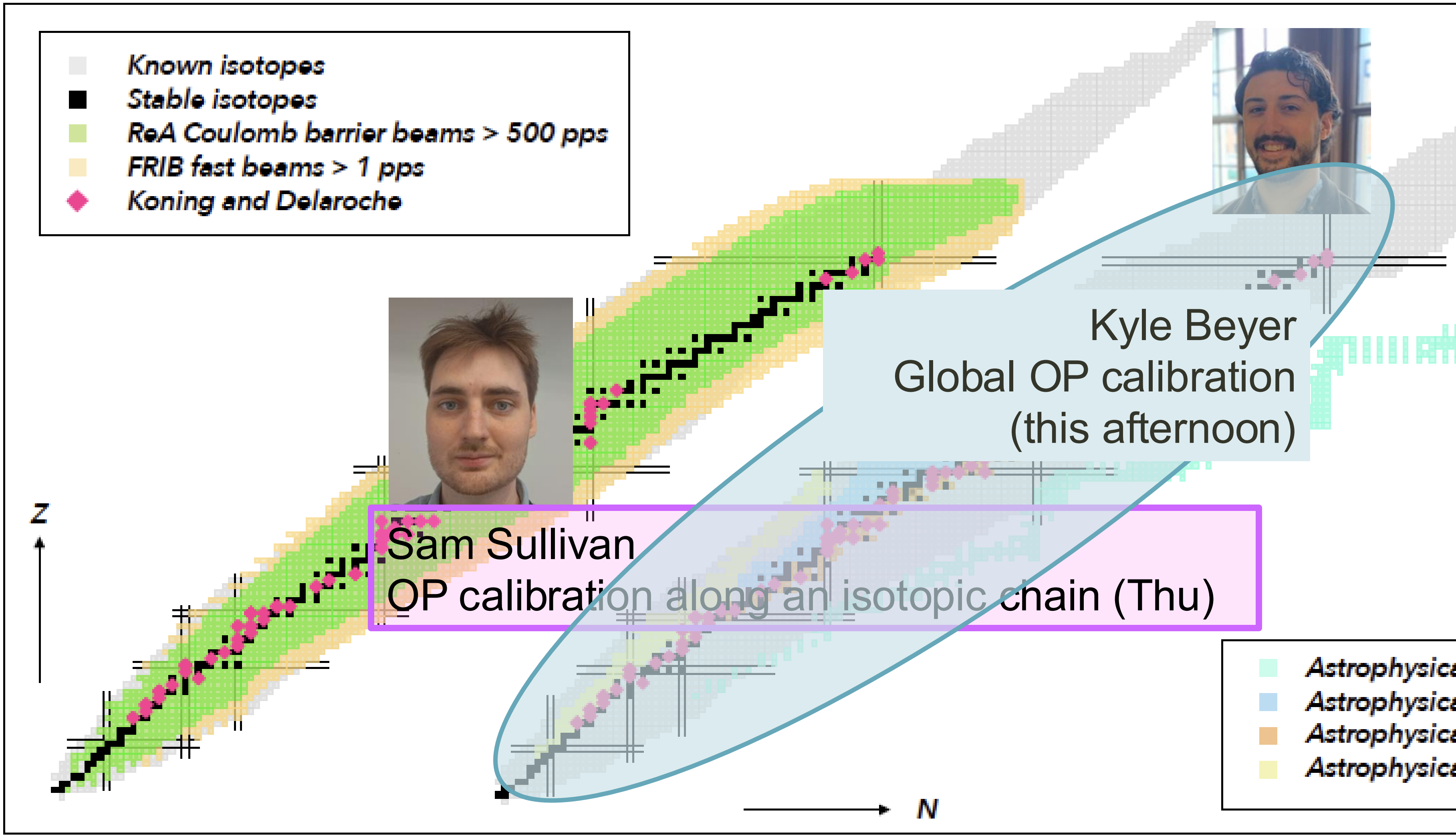
Phenomenological potentials fitted to stable nuclei



I pick one isotope + one reaction
determine local OP

Hebborn, Nunes, et al., JPG 50, 060501 (2023)

Phenomenological potentials fitted to stable nuclei



Hebborn, Nunes, et al., JPG 50, 060501 (2023)

Outline

- The physical model
  - optical potentials in reactions
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- The likelihood
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- Conclusions

Color code:
Nuclear physics background
Statistical model

Bayesian analysis: prior knowledge

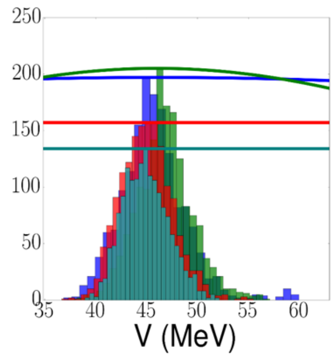
$$p(H|D,M) = \frac{p(D|H,M)p(H|M)}{p(D|M)}$$

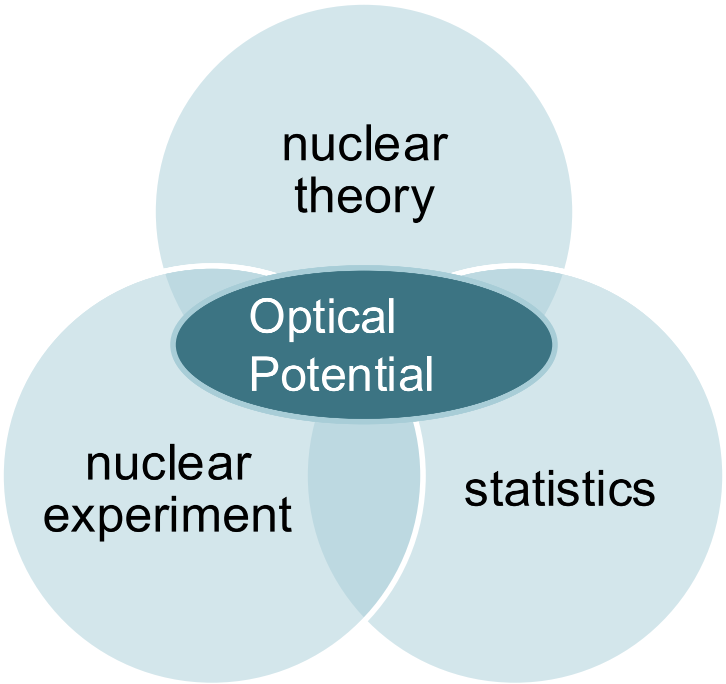
prior distribution of parameters H given model M

Gaussian distribution:

<u>Mean value</u>: global optical potential from global chi2 fits performed decades ago (BG, CH, KD)

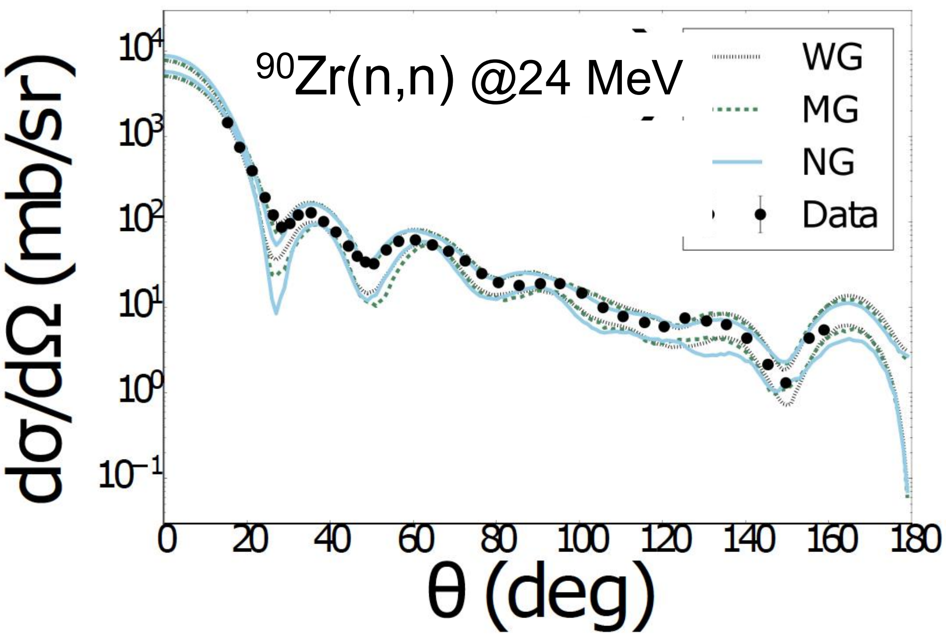
<u>Width</u>: 20% or 50% depending on the problem





What prior to use?

How confident are you in your prior knowledge?



Lovell and Nunes PRC (2018)

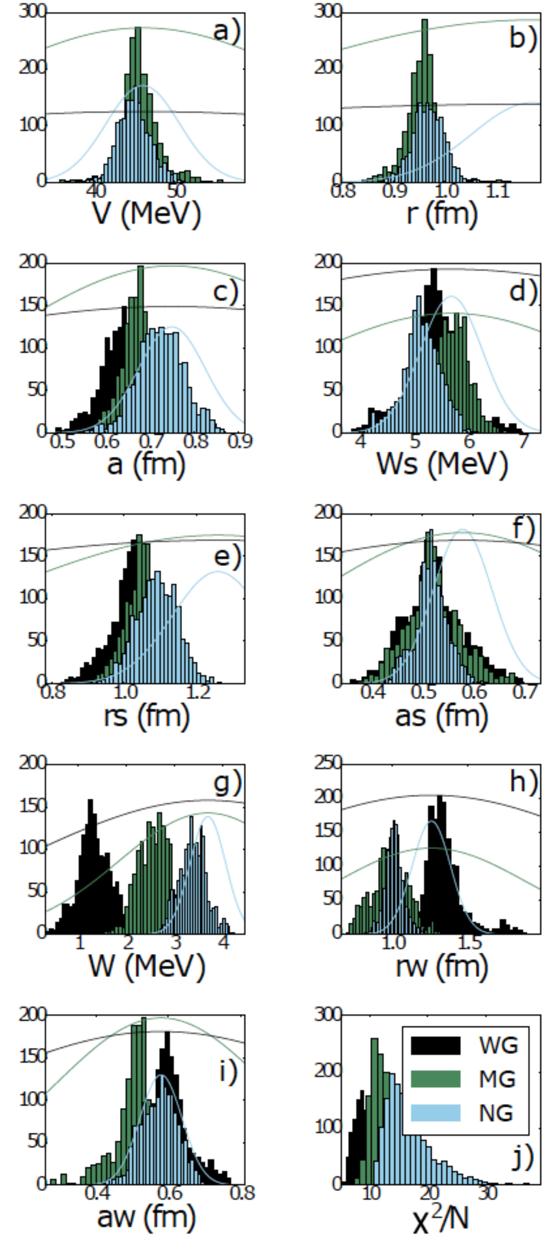


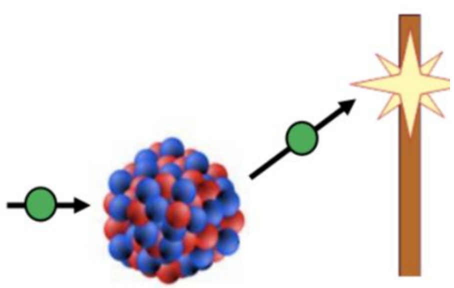
FIG. 2: (Color online) Comparison of the posterior distributions (histograms) resulting from various prior distributions (corresponding solid lines) for a wide Gaussian (WG), medium Gaussian (MG), and narrow Gaussian (NG) as defined in Table II for ^{90}Zr(n,n)^{90}Zr at 24.0 MeV.

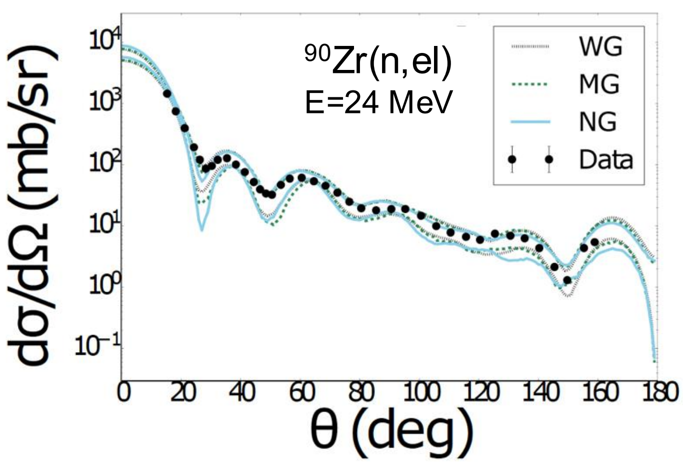
Bayesian analysis: the data

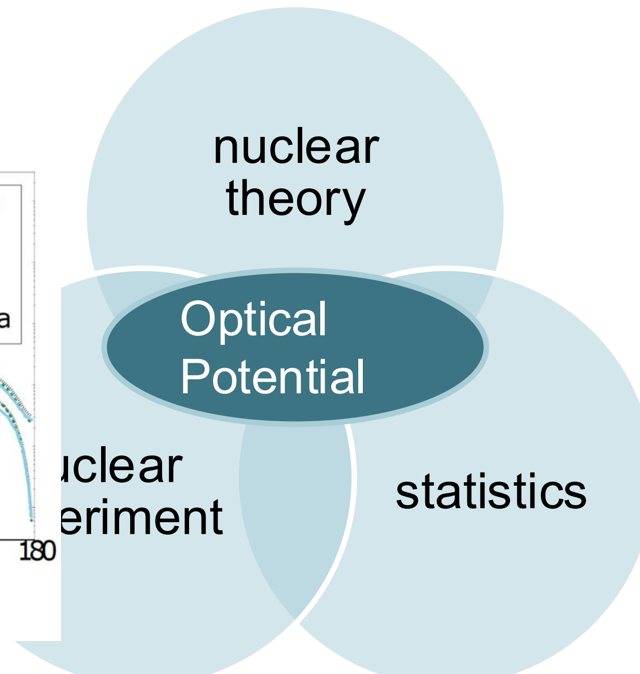
$$p(H|D,M) = \frac{p(D|H,M)\,p(H|M)}{p(D|M)}$$

Data constraints

elastic scattering: angular distributions
total cross sections, polarization data, etc
- real exp data with evaluated errors
- mock data using KD with 10% errors







Bayesian analysis: the likelihood

- no correlations and errors normally distributed

$$\boxed{p(D|H,M) = \exp[-\chi^2/2]}$$

$$\chi^2 = \sum_{i=1}^{N} \frac{[\sigma_{\exp}(\theta_i) - \sigma_{\mathrm{th}}(\theta_i, x)]^2}{[\Delta\sigma_{\exp}(\theta_i)]^2}$$

- rescale chi2 by the degrees of freedom χ^2/d
  ($d = N_{data} - N_{parameters}$)

- If $N_{data} >> N_{parameters}$ $\boxed{p(D|H,M) = \exp[-\chi^2/(2N)]}$

Bayesian analysis: the likelihood with correlations (the real thing)

Including data correlations in likelihood:

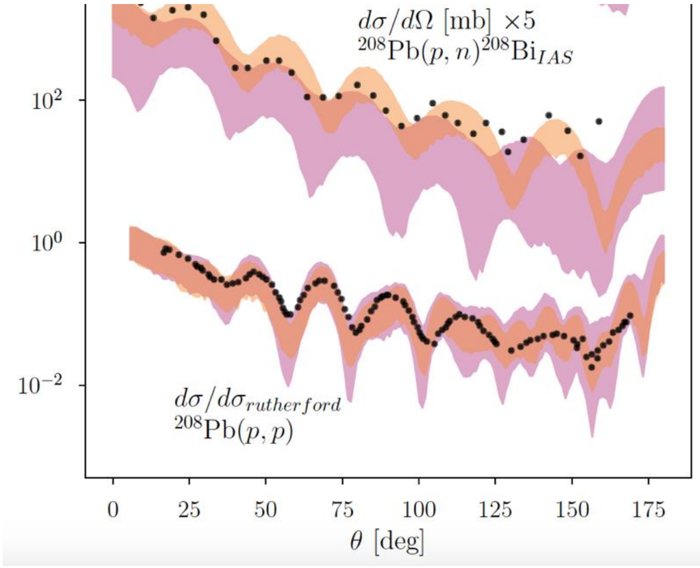
$$\chi^2 = [\sigma_{\text{exp}}(\theta_i) - \sigma_{\text{th}}(\theta_i, x)]\mathbb{C}^{-1}[\sigma_{\text{exp}}(\theta_i) - \sigma_{\text{th}}(\theta_i, x)]^T$$

$$\boxed{p(D|H, M) = \exp[-\chi^2/2]}$$

typically not used because covariance is usually not known in reactions experiments

Recognition that doubling the angles in the measurement contains essentially the same information – introduction of 1/N scaling

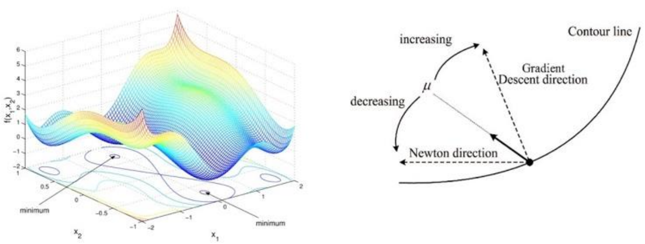
$$\boxed{p(D|H, M) = \exp[-\chi^2/(2N)]}$$



Frequentist versus Bayesian approach

Frequentist Chi2 minimization

$$\chi^2 = \sum_{i=1}^{N} \frac{[\sigma_{\mathrm{exp}}(\theta_i) - \sigma_{\mathrm{th}}(\theta_i, x)]^2}{[\Delta\sigma_{\mathrm{exp}}(\theta_i)]^2}$$



Levenberg–Marquardt algorithm explained

Interpolates between Newton and gradient-descent: better numerical stability and converges faster than standard gradient descent.

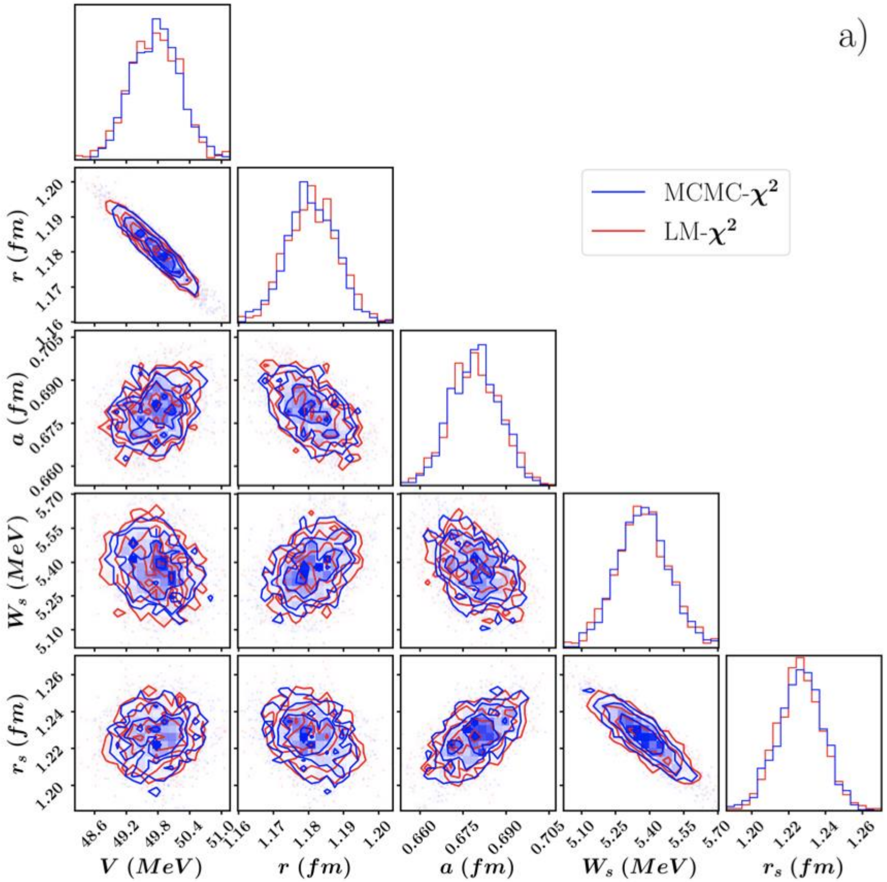
Bayesian MCMC:

emcee - Goodman-Weare stretch-move proposal distribution

- affine-invariant (not affected by the scaling or shape of the target distribution)
- uses an ensemble of walkers to propose moves
- more efficient, especially for highly skewed or badly scaled problems, due to a lower autocorrelation time

Study lead by Cole Pruitt
in collaboration with
Amy Lovell,
Chloe Hebborn,
Filomena Nunes
PRC (2024)

Application: OP with 5 parameters



^{90}Zr(n,n) @10 MeV

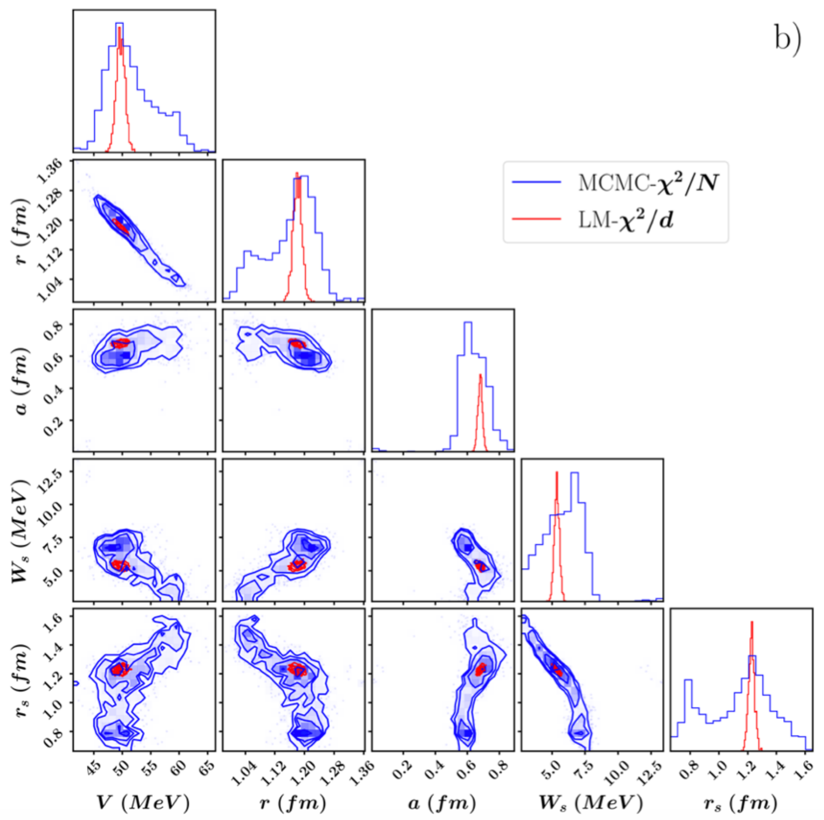
N_{data}=36

Frequentist (red)
Bayesian (blue)

same likelihoods+priors produce same posteriors

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Application: OP with 5 parameters scaled



^{90}Zr(n,n) @10 MeV

Frequentist (red)
Bayesian (blue)

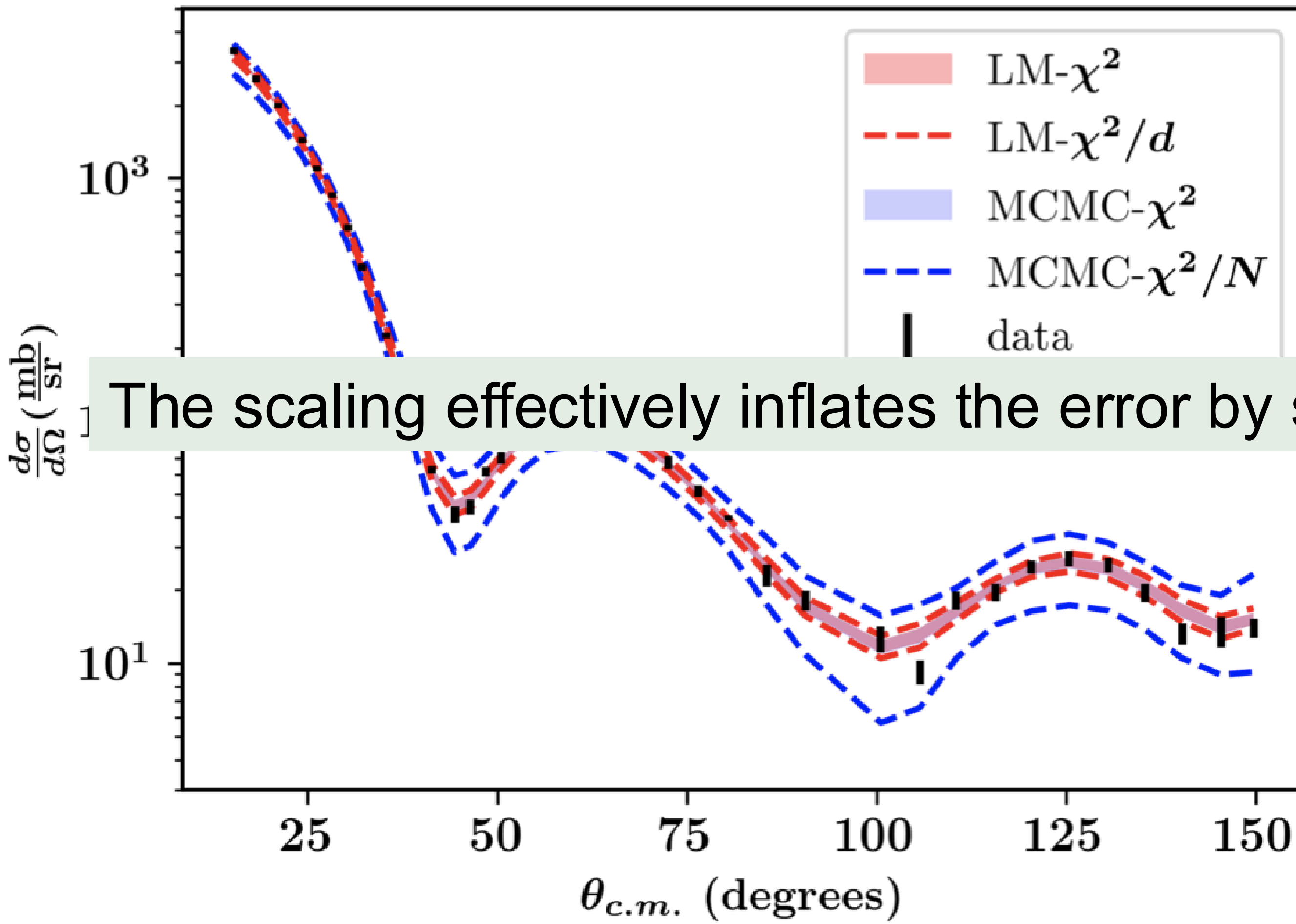
Different likelihood scaling allows MCMC to sample a wider region of parameters space

And results in different posteriors

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Application: OP with 5 parameters

$^{90}Zr(n,n)$ @10 MeV



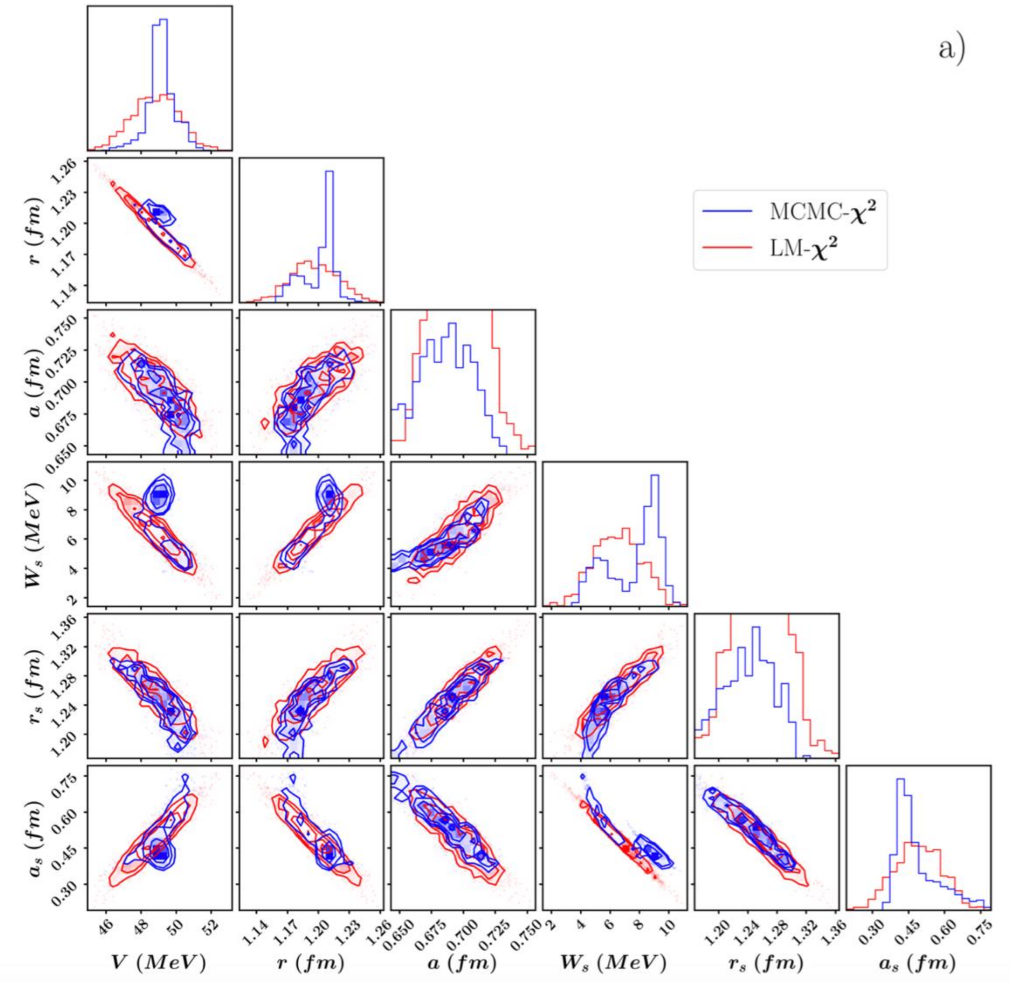
The scaling effectively inflates the error by sqrt(N)

MCMC with 1/N scaling produces credible intervals roughly sqrt(N) wider

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Application: OP with 6 parameters

$^{90}Zr(n,n)$ @10 MeV



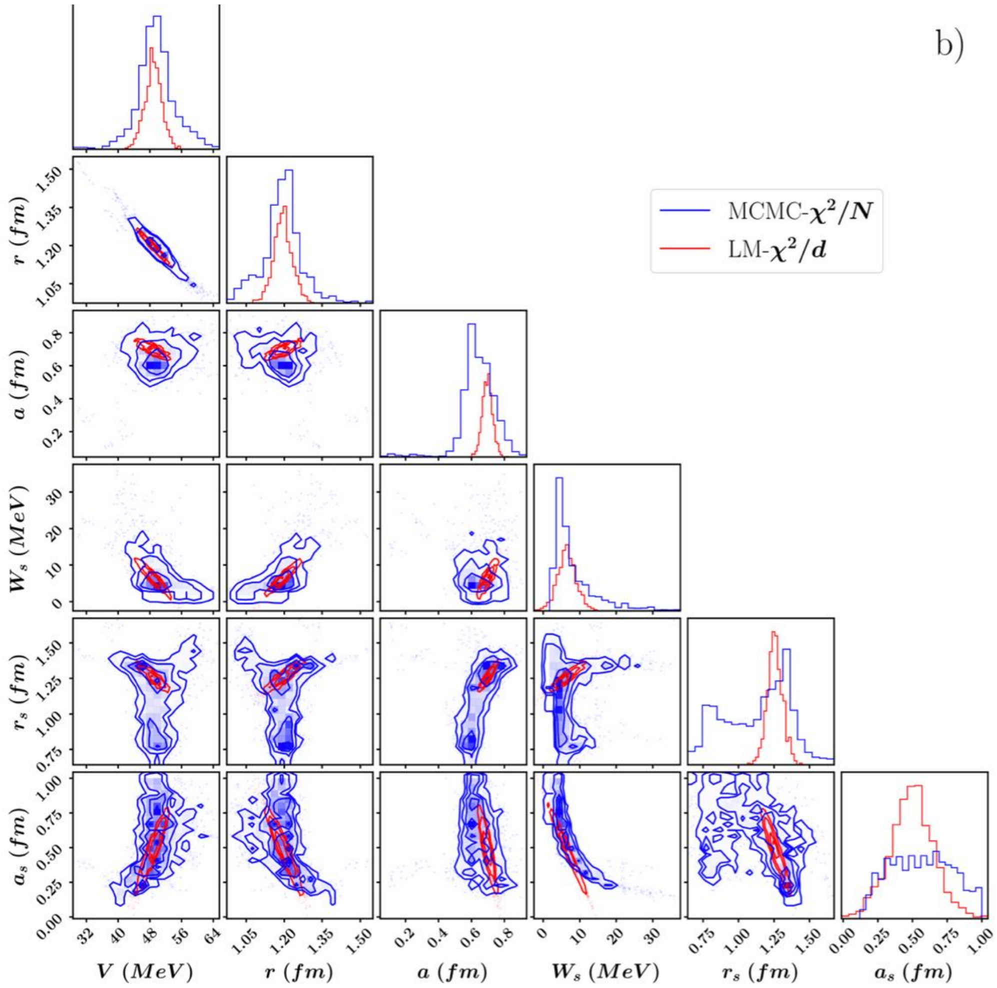
Frequentist (red)
Bayesian (blue)

same likelihoods+priors
different posteriors

frequentist approach is unable to capture the complex parameter dependencies in the model

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Application: OP with 6 parameters scaled



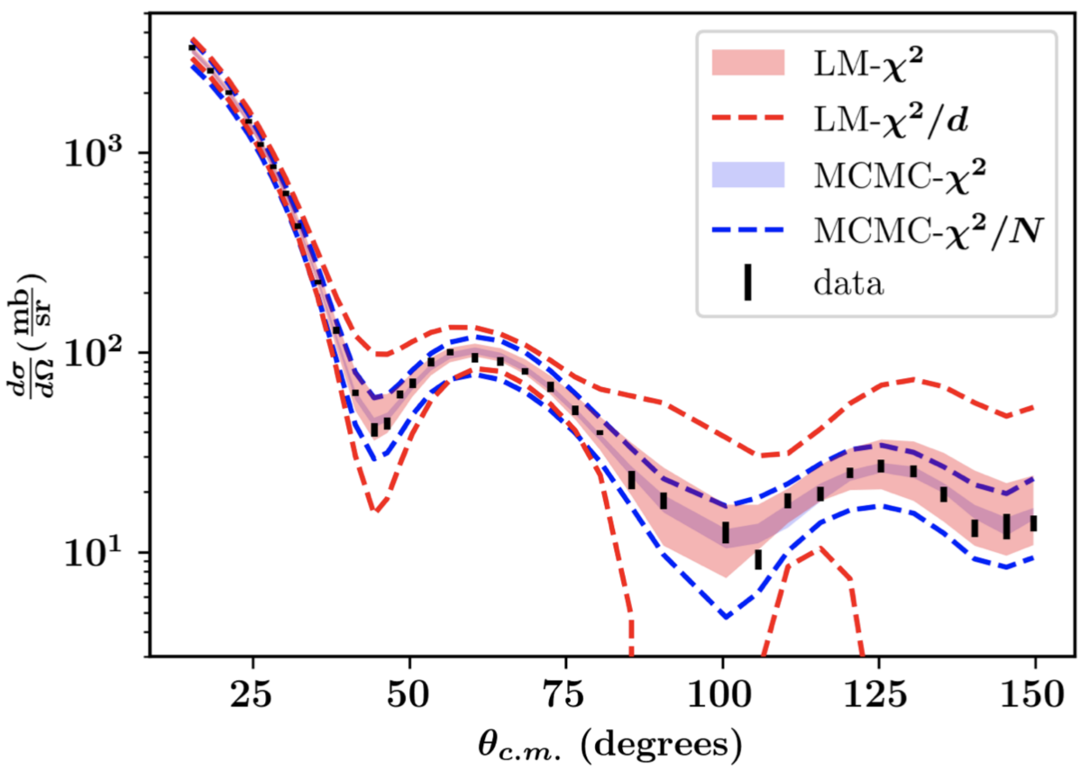
$^{90}Zr(n,n)$ @10 MeV

Frequentist (red)
Bayesian (blue)

The different scaling has a more dramatic effect on the posteriors

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Application: OP with 6 parameters



^{90}Zr(n,n) @10 MeV

For this example, frequentist credible intervals are larger than the Bayesian and not a reliable estimate

Many applications have much more than 6 parameters

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Likelihood: how to pick the right one?

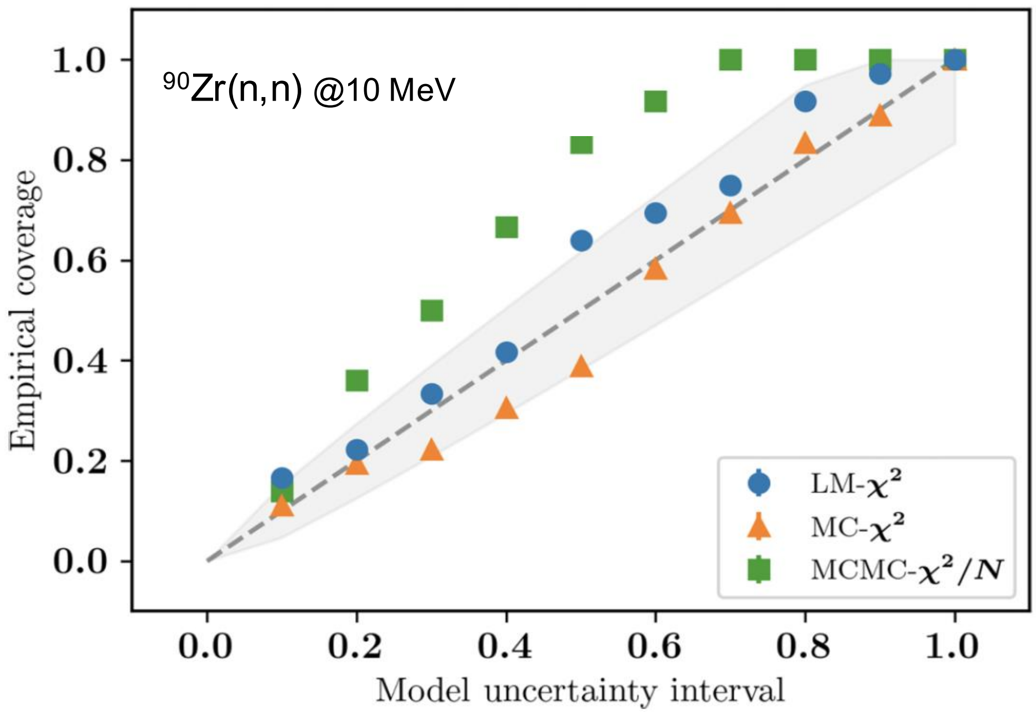
Complications:

- data correlations
- systematic errors on data underestimated
- model correlations
- model uncertainties

$$p(D|H,M) = \exp\left[-\chi^2/(2N)\right] \textbf{?} \qquad p(D|H,M) = \exp\left[-\chi^2/2\right] \textbf{?}$$

How to combine sets of angular distributions?
How to combine different types of reaction data?

Empirical coverage can discern likelihoods



^{90}Zr(n,n) @10 MeV (6 parameter)

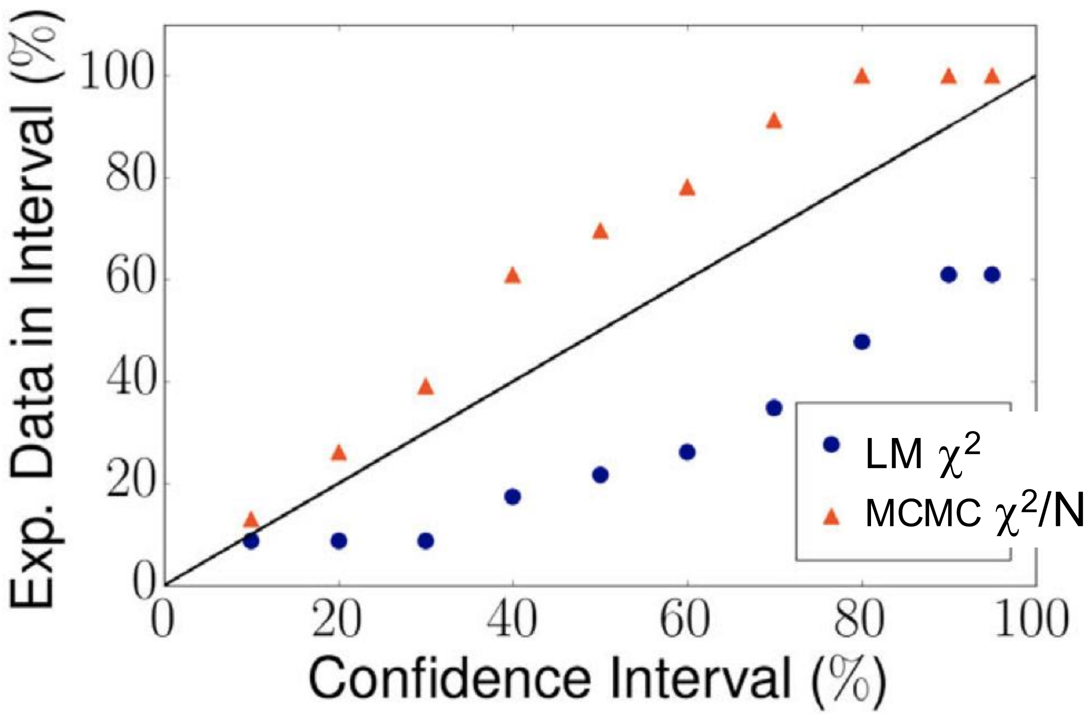
Empirical coverage evaluates the fraction of experimental data that fall within the estimated model uncertainty intervals

$\Delta\sigma_{\mathrm{exp}}(\theta_i)$ added to the model's parametric uncertainty in quadrature

For this reaction, the the unscaled chi2 has expected coverage

Pruitt, Lovell, Hebborn, Nunes, PRC **110**, 064606 (2024)

Empirical coverage can discern likelihoods



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

For this example, the unscaled chi2 underestimates uncertainty for 95% C.I. – an indication that uncertainties are larger than assumed

$$\Delta\sigma_{\exp}(\theta_i) \longrightarrow \Delta\sigma_{\exp}(\theta_i) + \Delta\sigma_{\mathrm{UFU}}$$

The unaccounted-for uncertainties will contain unreported experimental errors (systematic) and/or model errors

King et al., PRL 2019

What are the alternatives to these 'likelihoods'?

Should we be tempering the weight of the data?

Post-Bayesian Inference

Optimisation-centric posteriors /
Generalised Variational Inference ~~(A1)~~, ~~(A2)~~, ~~(A3)~~

$$q_n^*(\theta) = \arg\min_{q \in \mathcal{Q}} \Big\{ \underbrace{\mathcal{L}(q, x_{1:n})}_{\text{Data-fitting}} + \underbrace{\mathrm{D}(q, \pi)}_{\text{Prior regularisation}} \Big\};$$

$\mathcal{Q} \subseteq \mathcal{P}(\Theta)$

[See Knoblauch, Jewson, & Damoulas (2019/2022)]

Predictively oriented Inference VI

Gibbs/Generalised/
Pseudo Posterior ~~(A1)~~, (A2), (A3)

$$\pi_n^{\mathsf{L}}(\theta \mid x_{1:n}) = \frac{\exp\{-\mathsf{L}(x_{1:n}, p_\theta)\} \cdot \pi(\theta)}{\int \exp\{-\mathsf{L}(x_{1:n}, p_\theta)\} \cdot \pi(\theta) d\theta}$$

Power/Fractional/
Cold Posterior ~~(A1)~~, (A2), (A3)

$$\pi_n^{(\lambda)}(\theta \mid x_{1:n}) = \frac{p(x_{1:n} \mid \theta)^{\lambda} \cdot \pi(\theta)}{\int p(x_{1:n} \mid \theta)^{\lambda} \cdot \pi(\theta) d\theta}$$

Parameter Inference III

See Knoblauch's talk from Monday

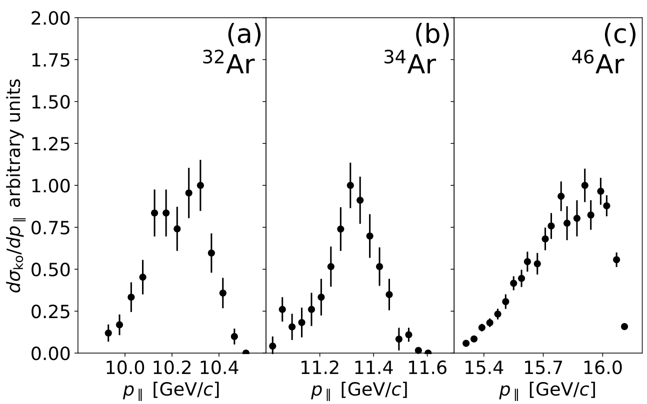
Conclusion

- Optical potential calibrations are essential for determining uncertainties in reaction observables
- Frequentist approach fails as complexity of parameter space increases
- How to account for the complexity in the statistical model with reduced information - choice of likelihood

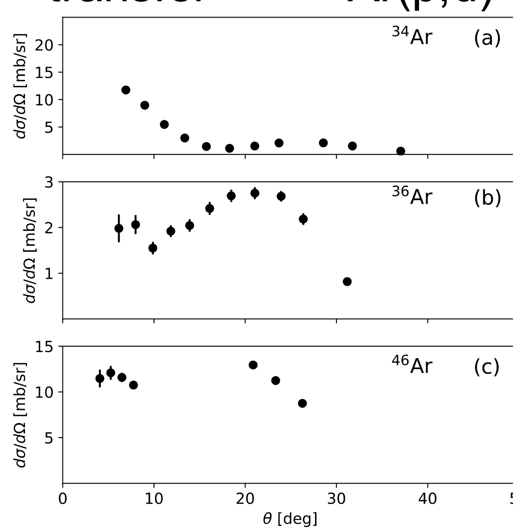
Empirical coverage is an important validation tool!

knockout

^{32,34,46}Ar on ^{9}Be @ ~70 MeV A

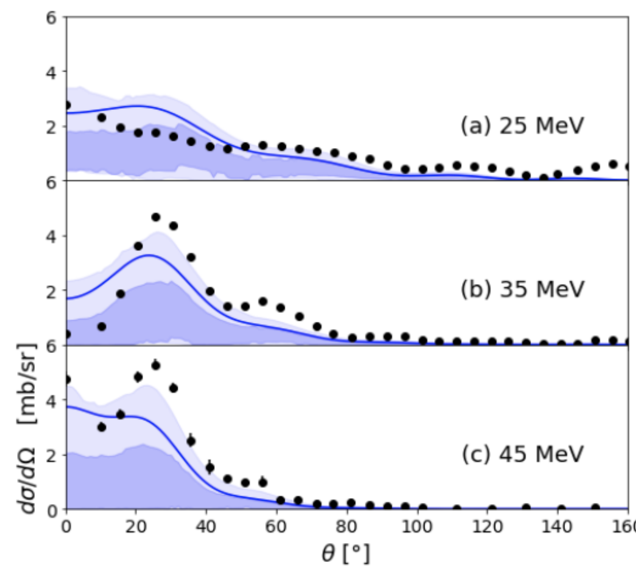


transfer ^{34,26,46}Ar(p,d)



Charge exchange

^{48}Ca(p,n) ^{48}Sc



Work supported by NSF-CSSI, DOE-NP and MSU

The future is the young people working in the field


Filomena Nunes


Chloë Hebborn


Kyle Beyer


Patrick McGlynn

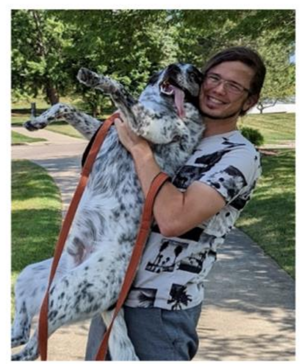

Ibrahim Abdurrahman


Cate Beckman


Manuel Catacora Rios


Andy Smith


Daniel Shiu


Pablo Giuliani


Grigor Sargsyan

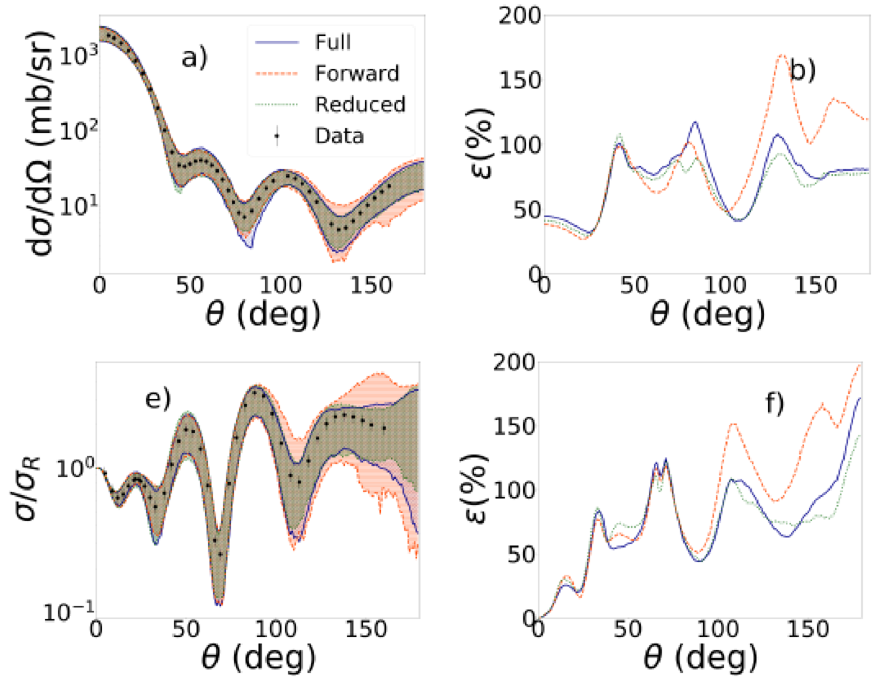

Zetian Ma

The few-body reactions group at FRIB

Chloe Hebborn@Orsay

BACKUP

What angular information needed?



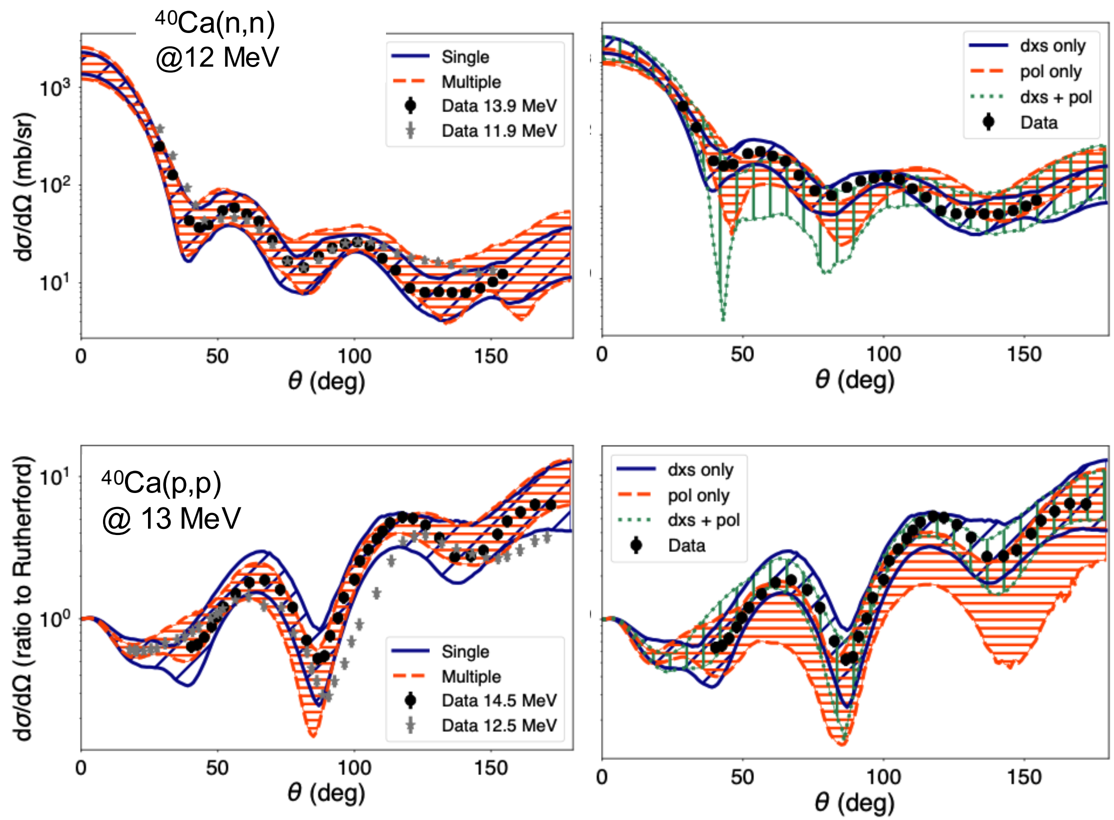
^{48}Ca(n,n)^{48}Ca at 12 MeV

^{48}Ca(p,p)^{48}Ca at 21 MeV

Catacora-Rios, King, Lovell and Nunes, PRC (2019)

Single energy versus multiple energy sets? Polarization versus differential cross sections?

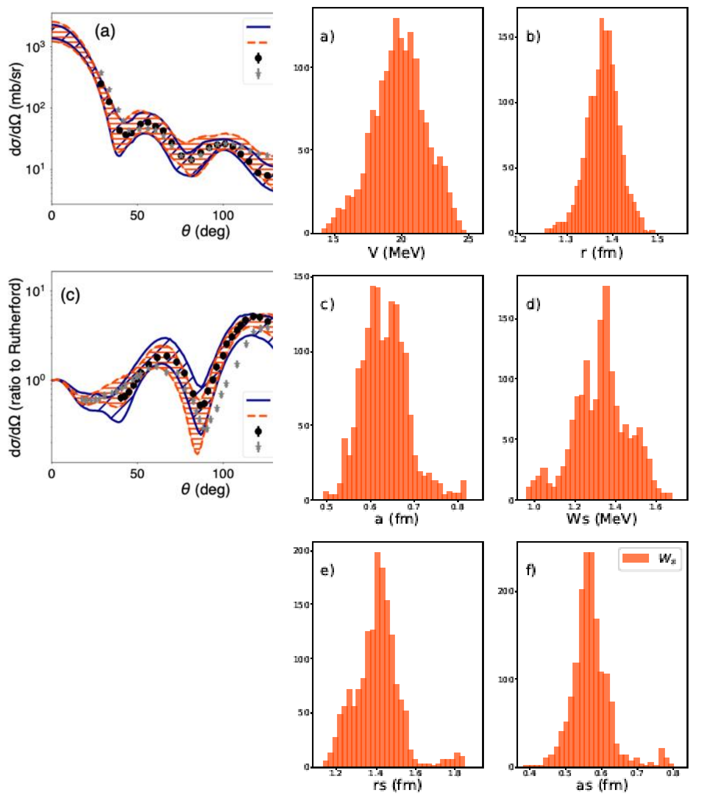
95% credible intervals



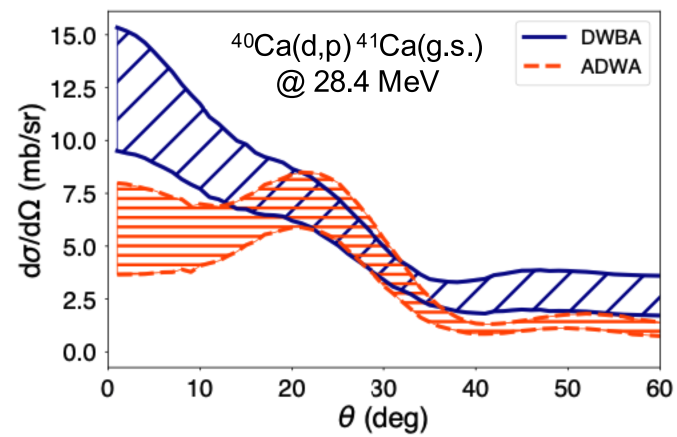
King, Lovell, Neufcourt, Nunes PRL (2019)
Catacora-Rios et al. PRC 100, 064615 (2019)
Lovell, Nunes, Catacora-Rios, King, JPG (2020)
Catacora-Rios et al. PRC 104, 064611 (2021)

Propagating uncertainties to transfer

OP constrained with elastic scattering to obtain posterior distributions for parameters



Propagate to other reaction observables

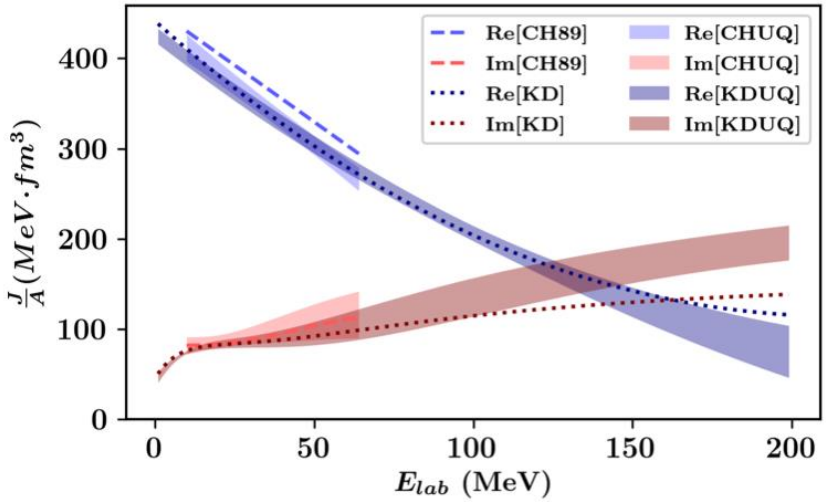


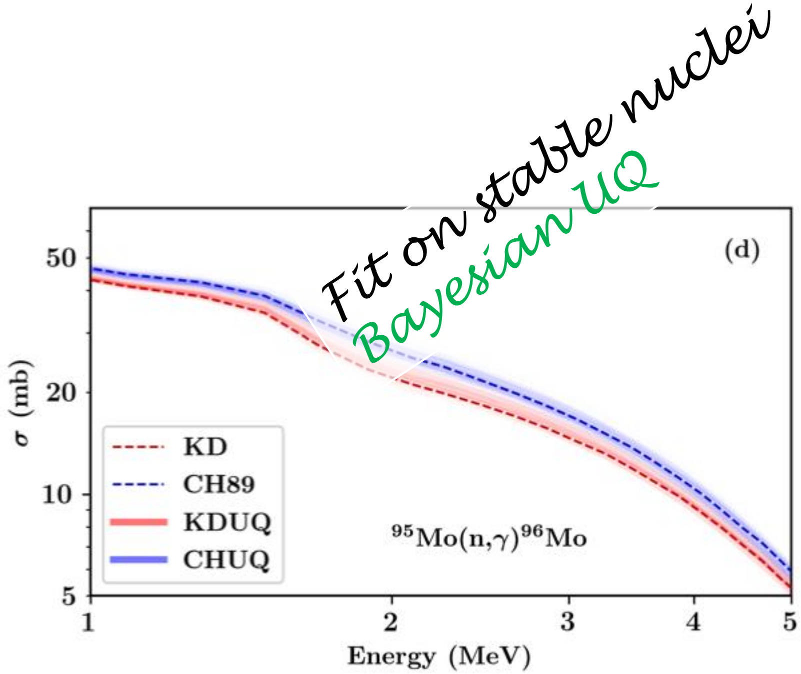
Ekstrom talk:
UQ important for decision-making and model assessment

Lovell, Nunes, Catacora-Rios, King, JPG (2020)

Uncertainty quantified **global** optical potential (CHUQ and KDUQ)

Bayesian analysis using the same experimental protocol as in the original CH89 and KD2003 parameterizations



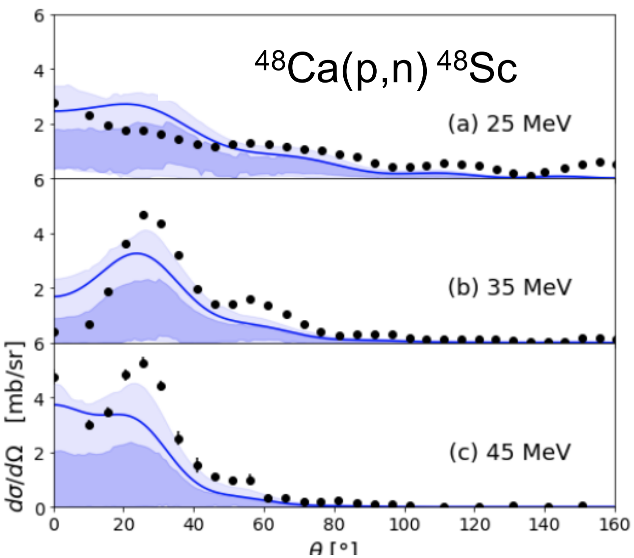


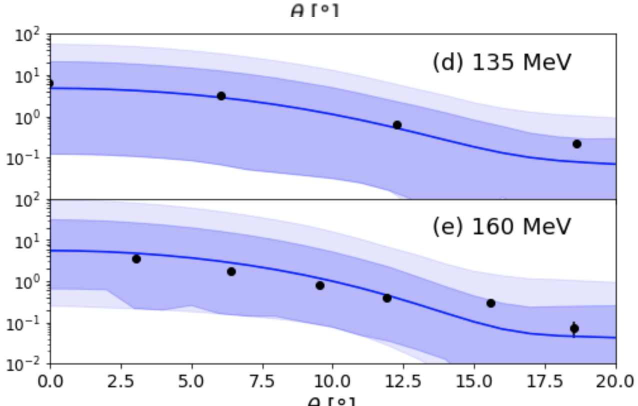
Pruitt et al., Phys. Rev. C 107, 014602 (2023)

OP uncertainties in charge exchange to IAS

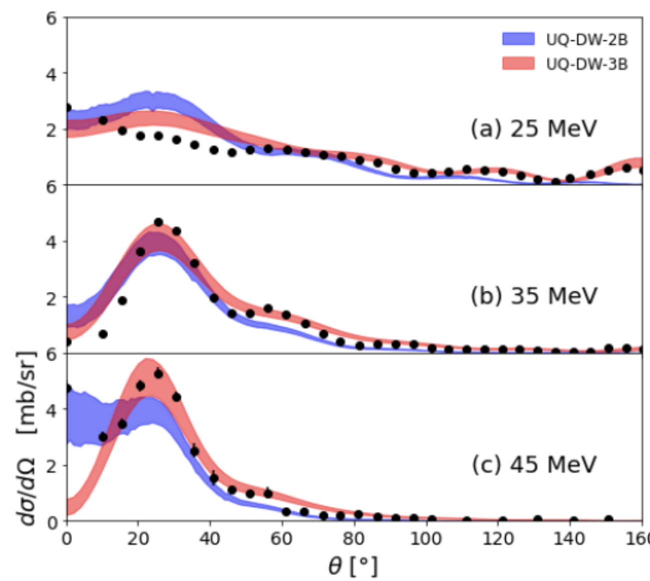
- DWBA formalism
- Using parameter posterior from KDUQ

Dark shade (68% ci)
Light shade (95% ci)





Comparing two-body and three-body models for charge exchange

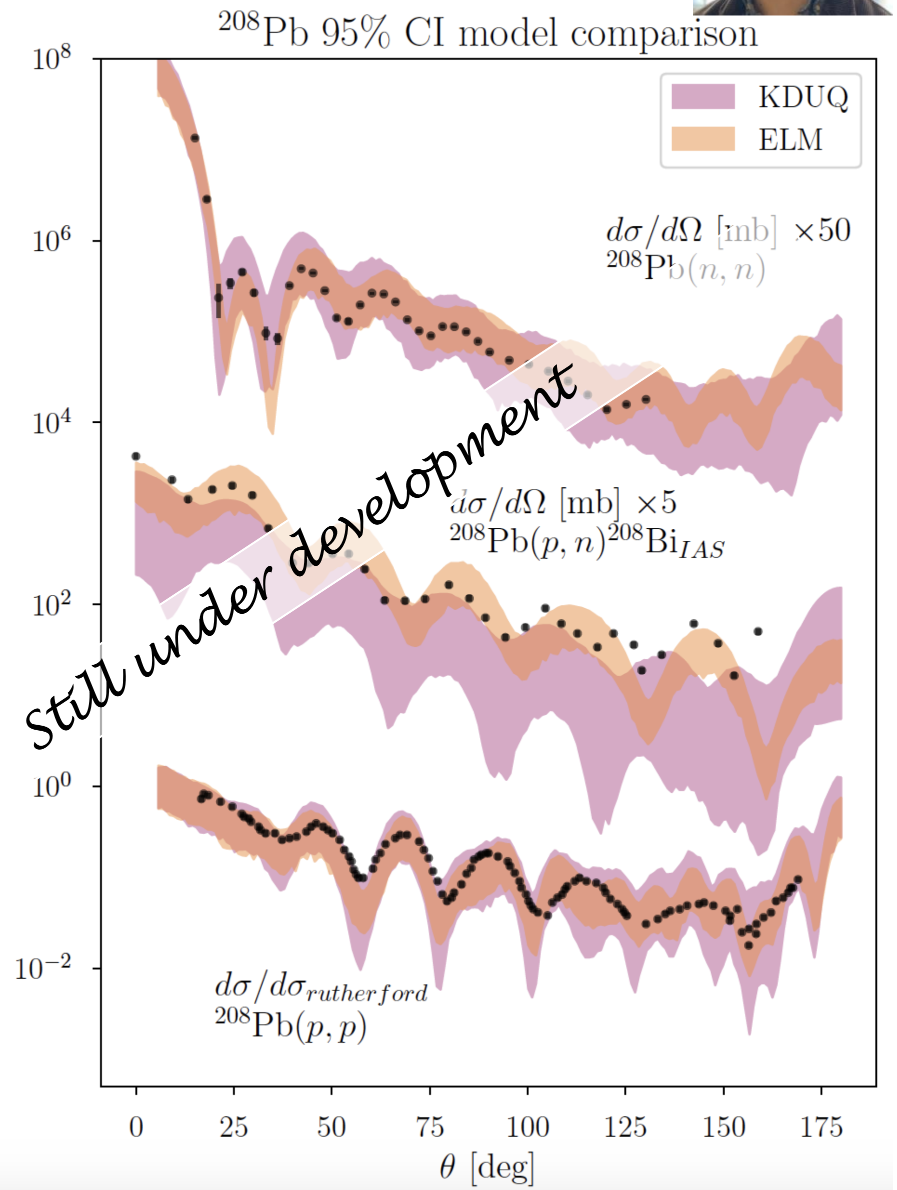


Smith, Hebborn, Nunes, Zegers, PRC **110**, 034602 (2024)

Uncertainty quantified **global** optical potential (East Lansing Model)

ELM uses a much smaller set of data compared to KDUQ

Includes charge-exchange to IAS for key isotopes

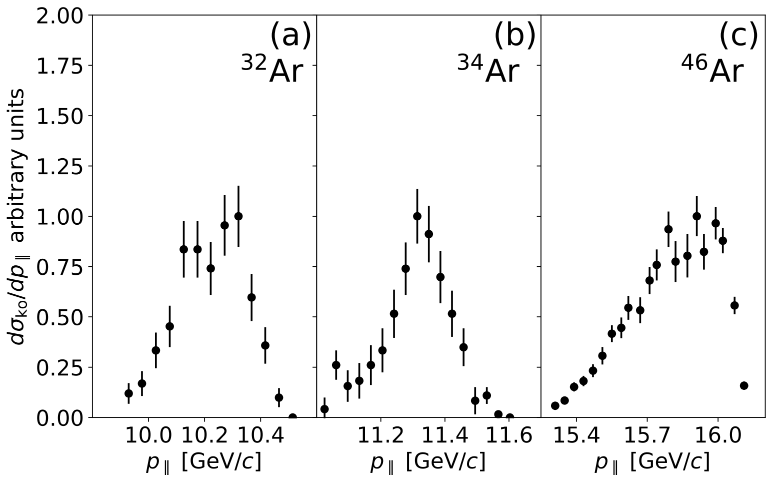


Beyer and Nunes, in preparation

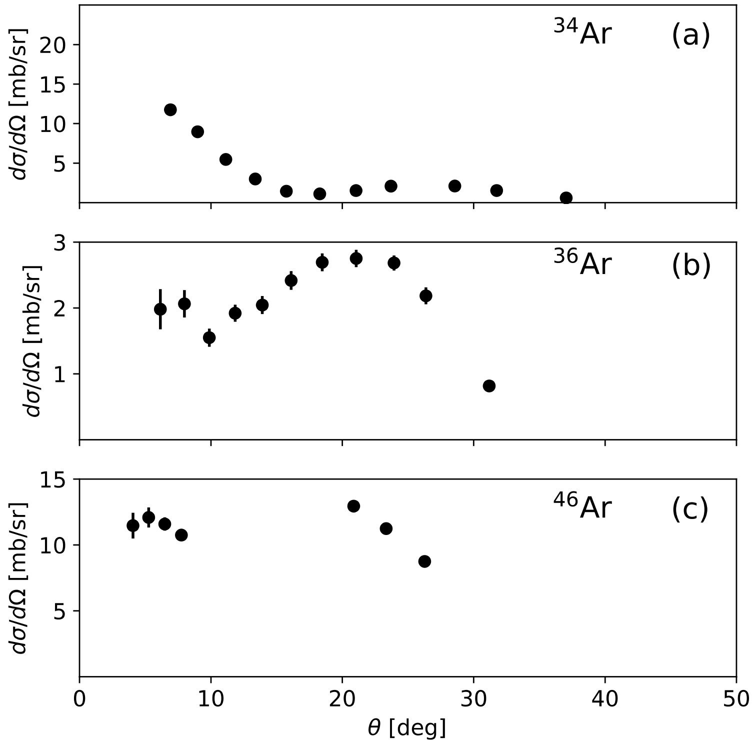
Propagating uncertainties to knockout

- Eikonal model
- Using parameter posterior from KDUQ

^{32,34,46}Ar on ^{9}Be @ ~70 MeV A



compare with a consistent ADWA study of transfer ^{34,26,46}Ar(p,d)

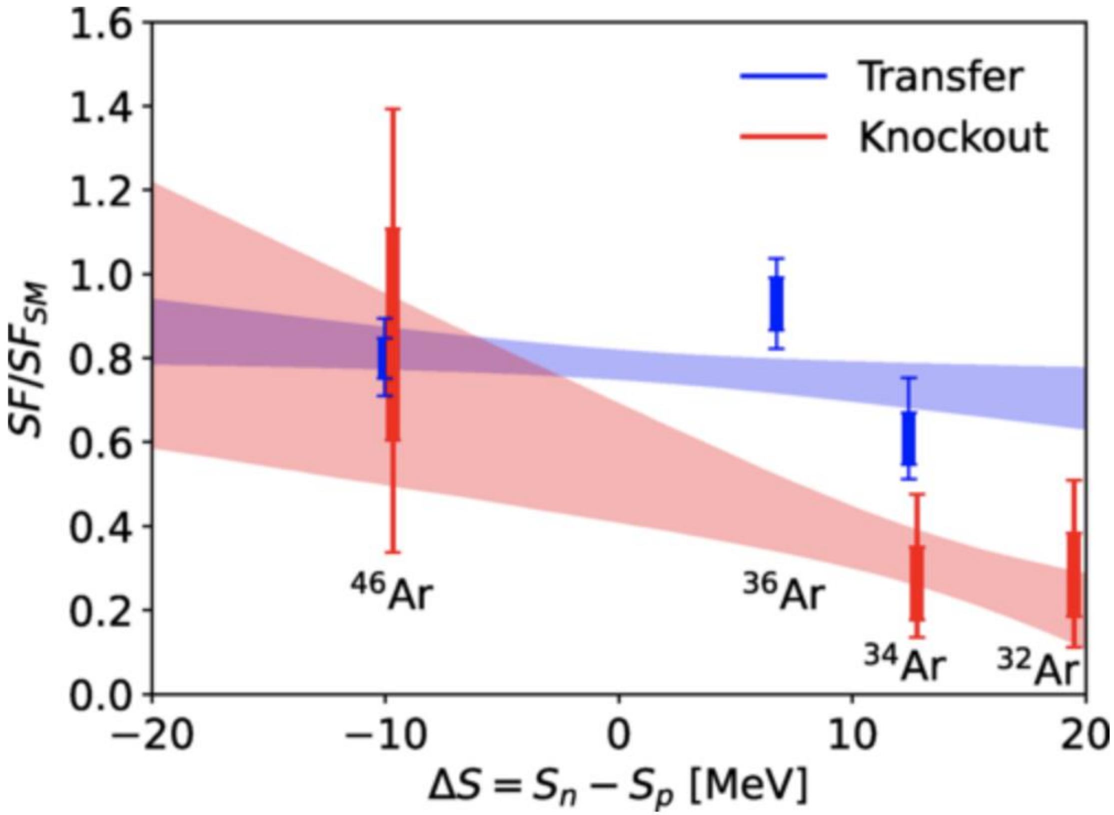


dark (light) shade:
68% (95%) credible intervals

Hebborn, Nunes, Lovell, PRL 131, 212503(2023)

Comparing knockout and transfer: linear fit

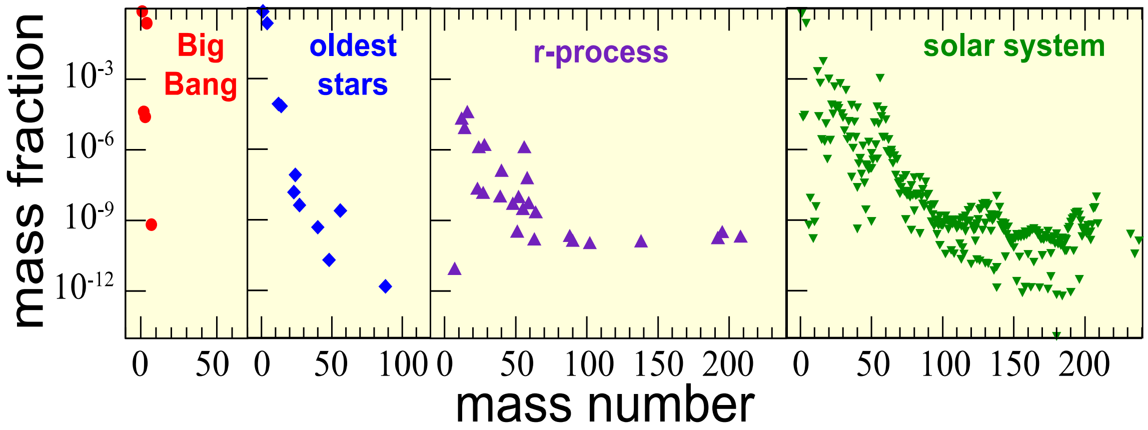
$$\mathcal{R}(\Delta S) = a\Delta S + b$$

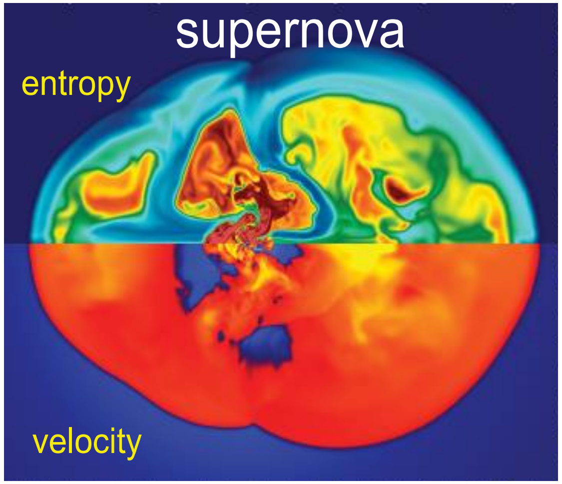


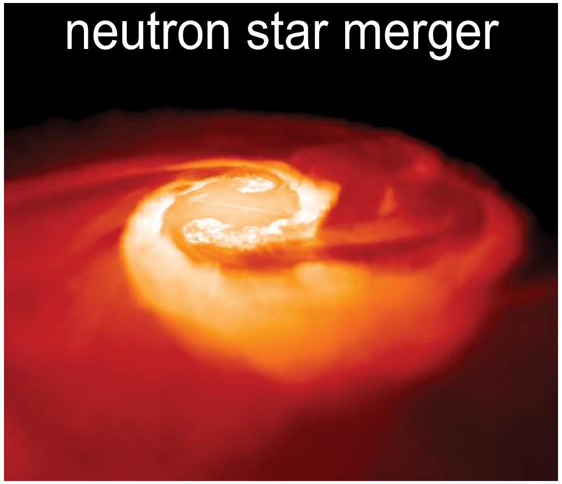
68% (95%) credible intervals

Hebborn, Nunes, Lovell, PRL 131, 212503(2023)

Bird's eye view of nuclear reactions







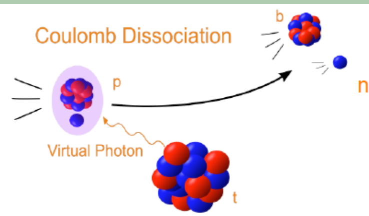
Nuclear reactions got us from the lightest elements all the way to the wide range of elements found in our solar system!

Bird’s eye view of nuclear reactions

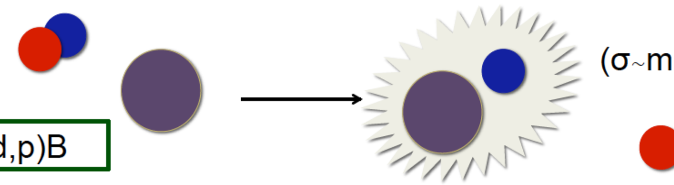
Probe of neutron capture: breakup and transfer

A+Pb ↦n+B+Pb

(σ~mb)

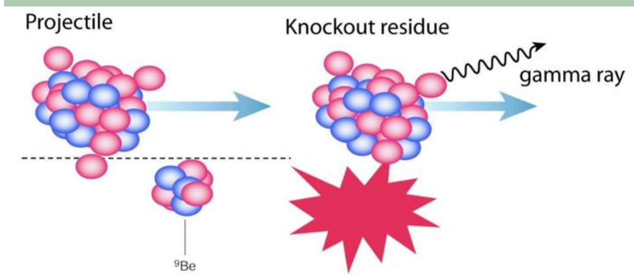


A(d,p)B

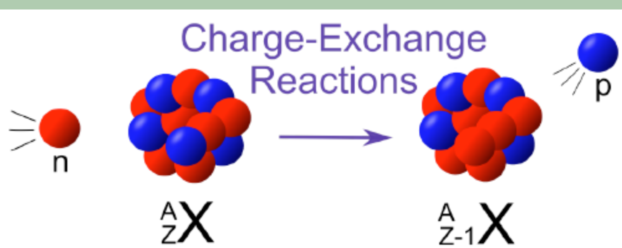


(σ~mb)

Probe of single-particle structure: knockout



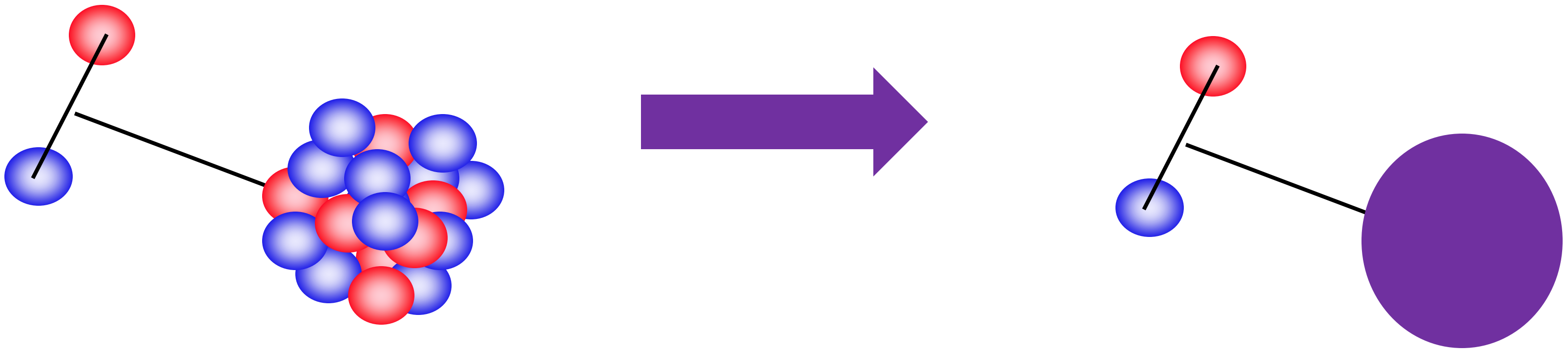
Probe of electron capture: charge-exchange



Reactions are the most diverse probes to extract astrophysics and structure information, especially for unstable isotopes…

But reaction theory is key for translation!

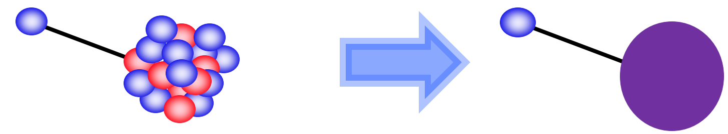
Reaction theory maps the many-body into a few-body problem

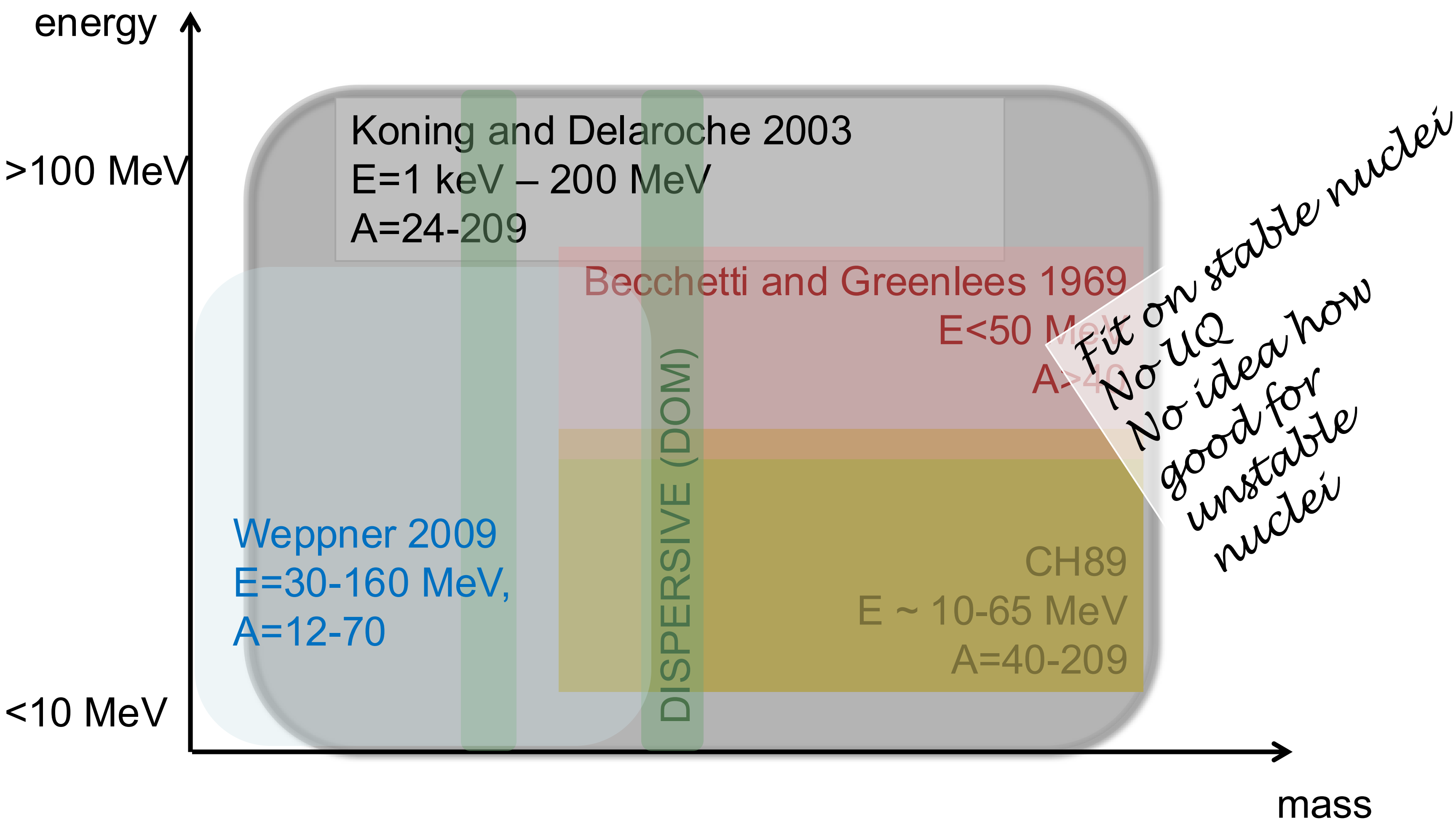


- ❑ isolating the important degrees of freedom in a reaction
- ❑ effective nucleon-nucleus interactions (or nucleus-nucleus) usually referred to as **optical potentials**

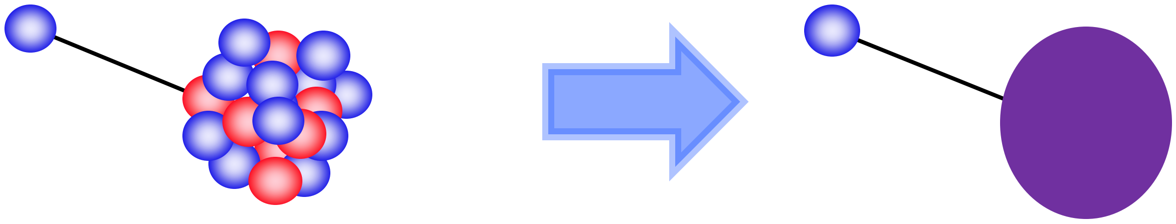
main cause of uncertainty

Landscape of global optical potentials





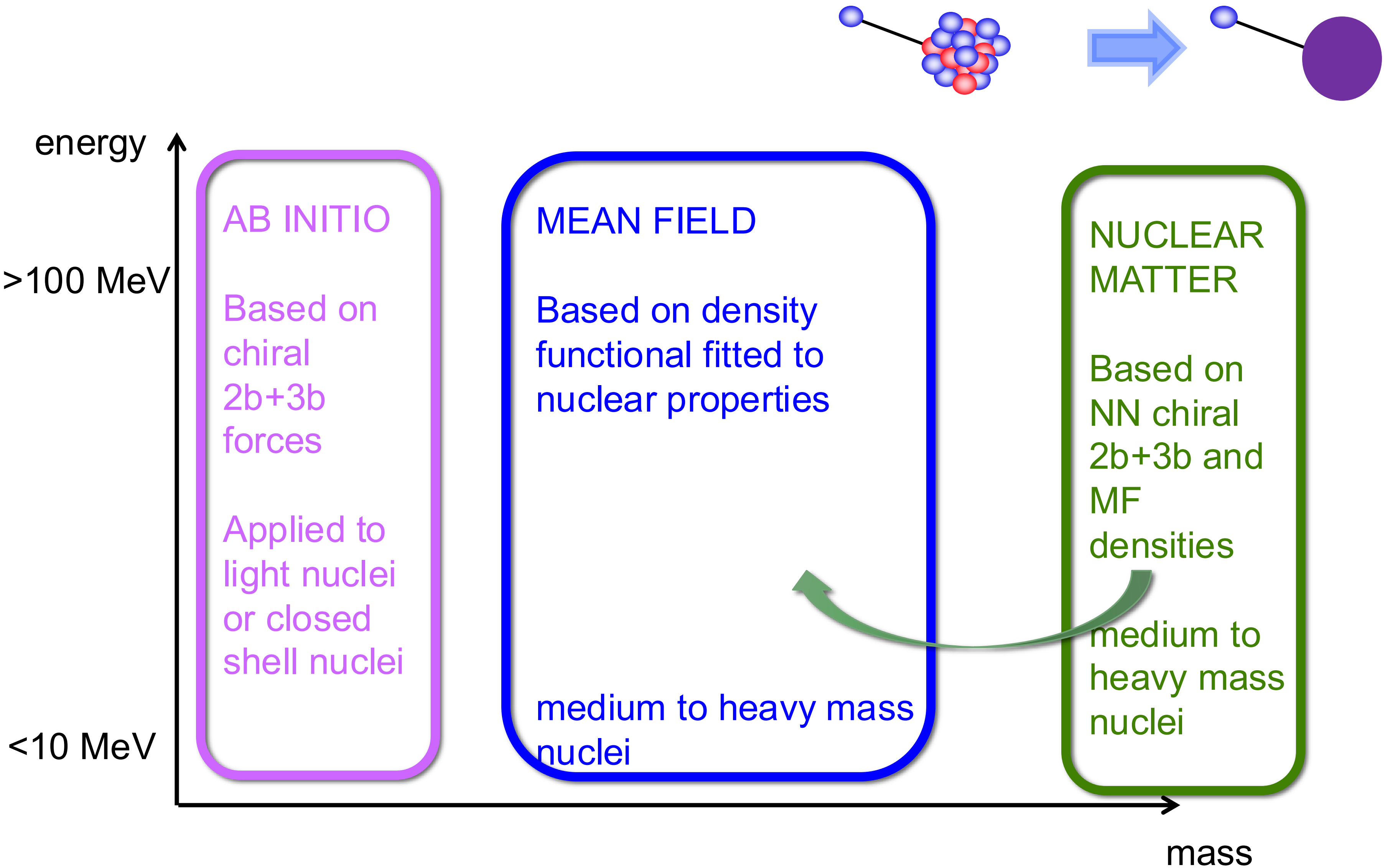
Optical potentials from theory



Microscopic optical potential:

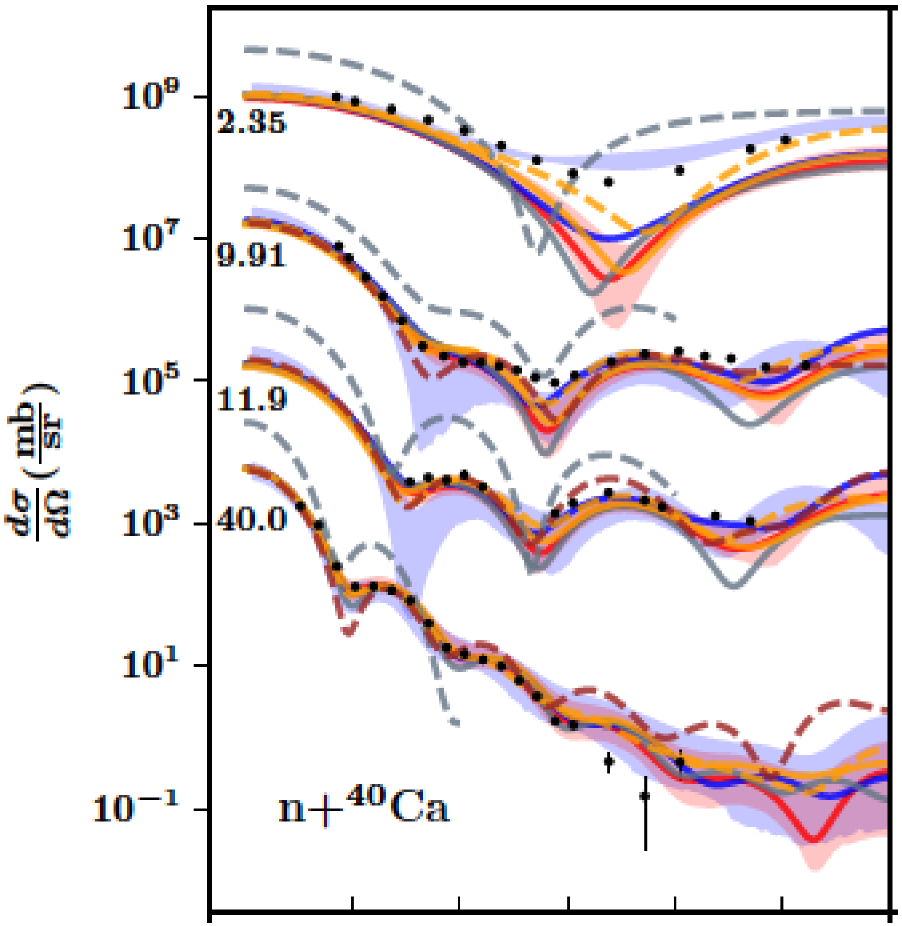
- Non-local, typically not global, no simple general form
- depends on the EFT: cutoffs, regularizations, etc.
- agreement with data is variable…

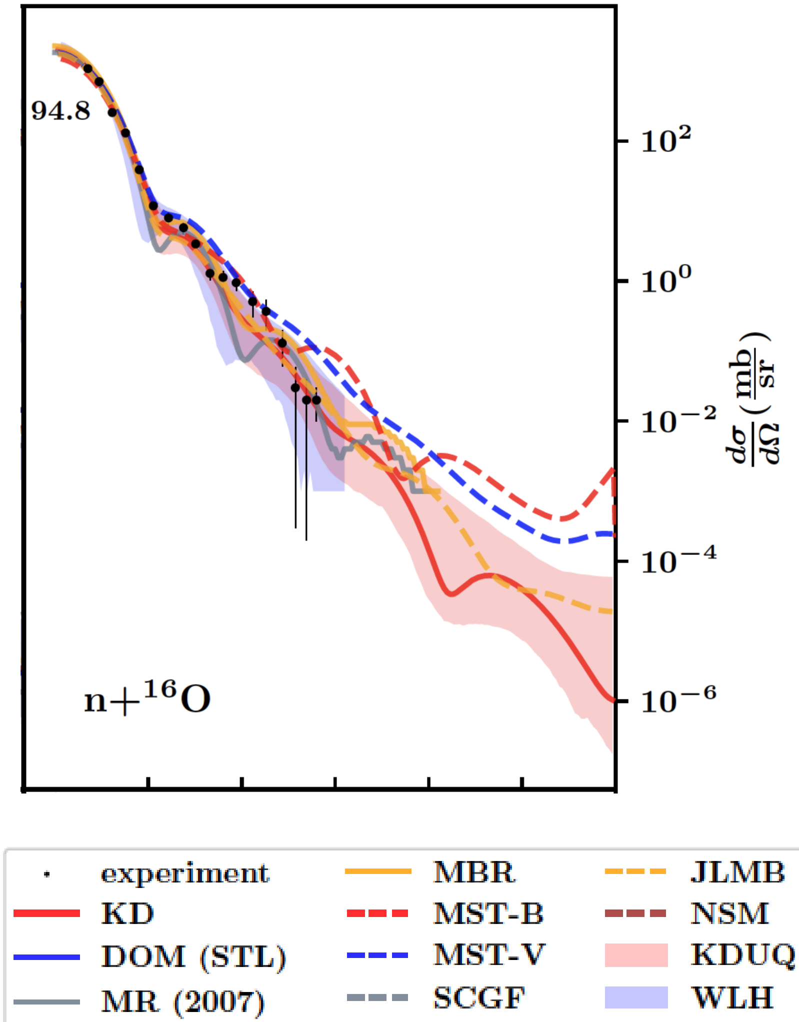
Landscape of microscopic optical potentials



How do optical models compare?

Cross section: Angular distributions
(shaded - 95% credible intervals)



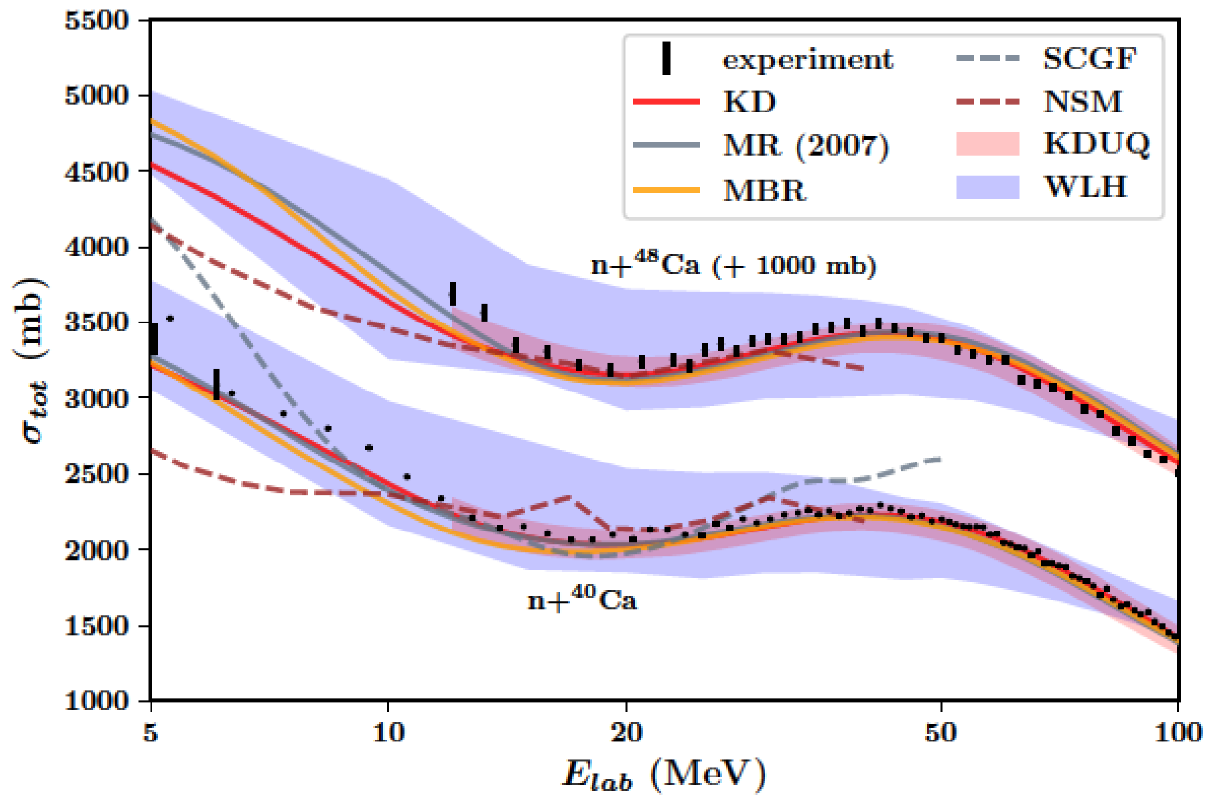


Hebborn, Nunes, et al., JPG 50, 060501 (2023)

How do optical models compare?

95% credible intervals

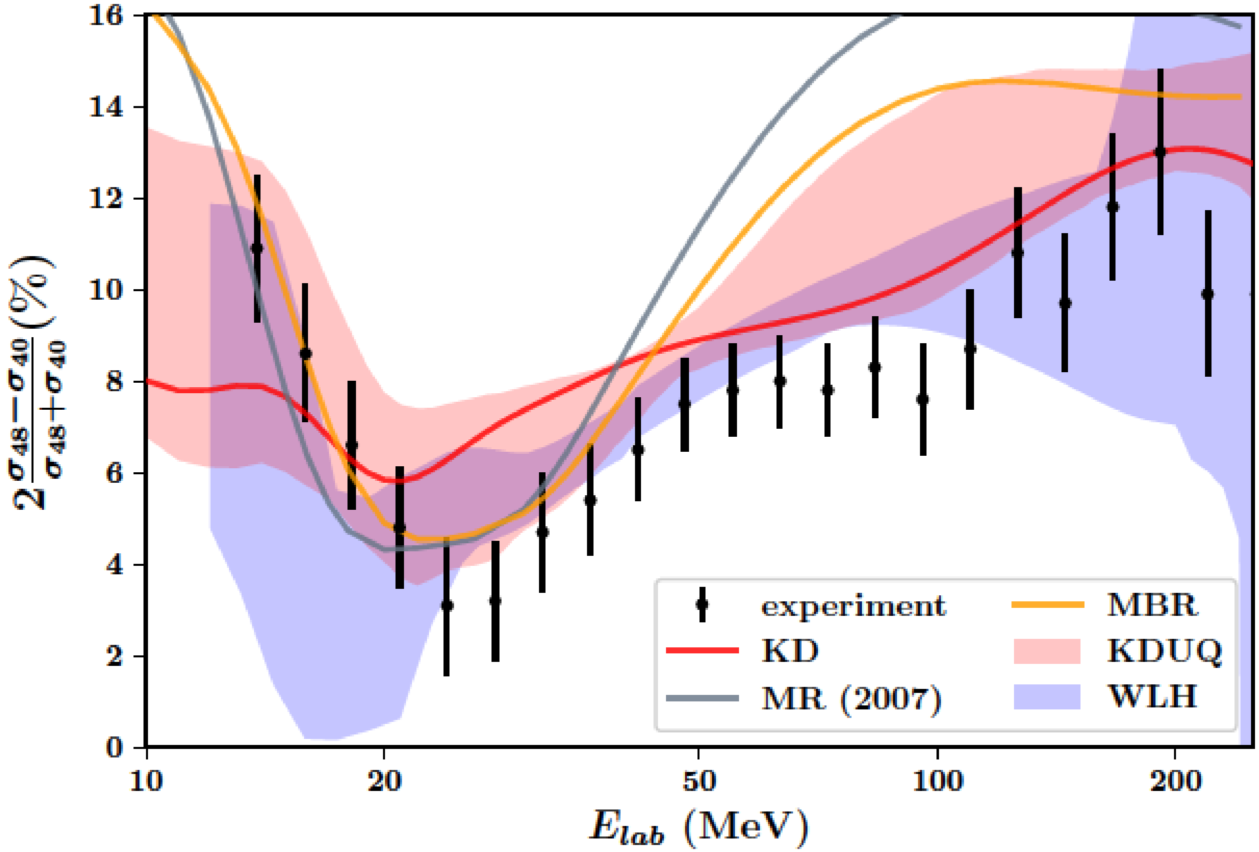
Total cross section as a function of energy



Hebborn, Nunes, et al., JPG 50, 060501 (2023)

How do optical models compare?

Asymmetry of total cross section



95% credible intervals

Hebborn, Nunes, et al., JPG 50, 060501 (2023)