Quantifying uncertainties in nuclear reactions

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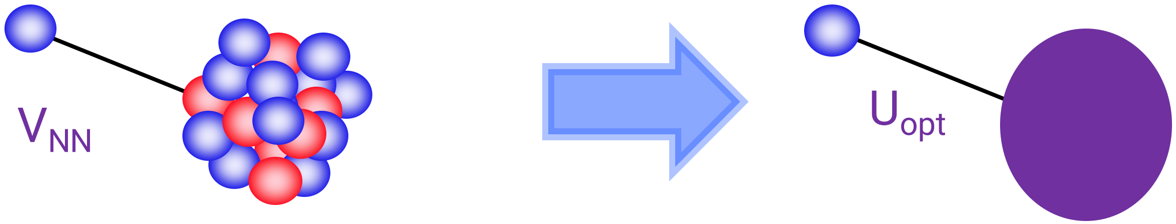
Michigan State University

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 role of optical potentials in reactions
- Bayesian analyses of optical potentials
- Propagation to other observables
  - Transfer
  - Charge-exchange
  - Knockout
- Emulators
  - Application to model for breakup
- Opportunities for the future

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:

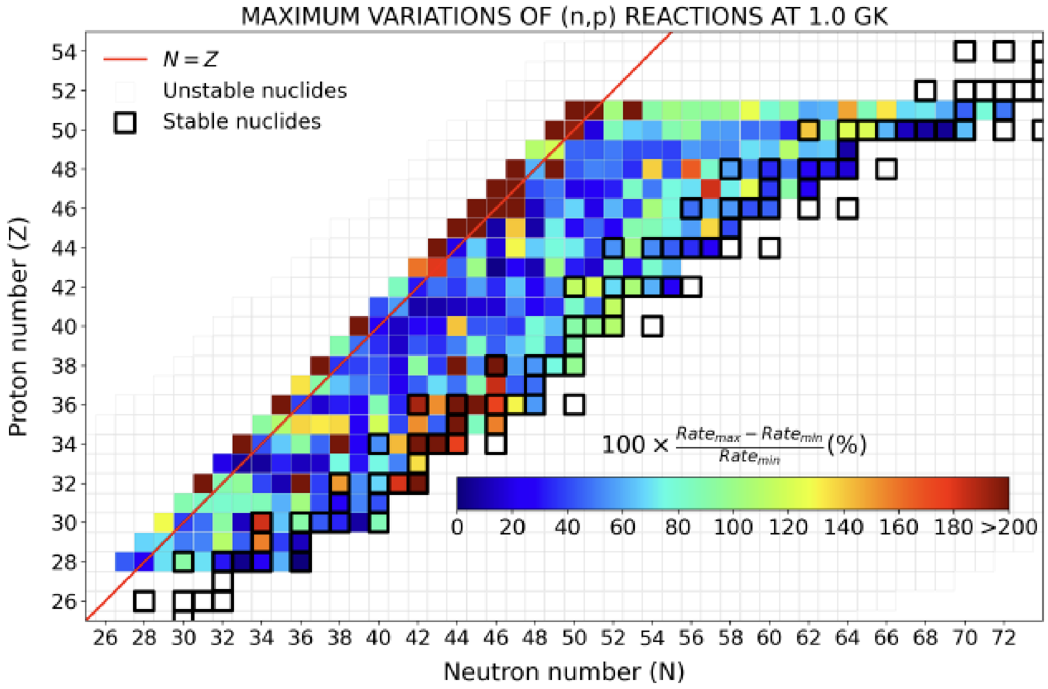
$$V_{\rm opt} = \mathcal{V}_{00} + \sum_{j,k\neq 0} \mathcal{V}_{0j}\frac{1}{E - H_{jk} + i\eta}\mathcal{V}_{k0}$$

U_{opt}= V(R) + iW (R) can be obtained phenomenologically!

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 the main source of uncertainty

Need uncertainty quantification!

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

OP white paper shows current state of the art

	Mass	Energy	D.	Mic.	UQ
KD	$24 \leq A \leq 209$	$1 \text{ keV} \leq E \leq 200 \text{ MeV}$	✗	✗	✗
KDUQ	$24 \leq A \leq 209$	$1 \text{ keV} \leq E \leq 200 \text{ MeV}$	✗	✗	✓
DOM (STL)	C, O, Ca, Ni, Sn, Pb isotopes	$-\infty < E < 200 \text{ MeV}$	✓	✗	✓
MR	$12 < Z < 83$	$E < 200 \text{ MeV}$	✓	✗	✗
MBR	$12 < Z < 83$	$E < 200 \text{ MeV}$	✓	✗	✗
NSM	^{40}Ca, ^{48}Ca, ^{208}Pb	$E < 40 \text{ MeV}$	✓	✓	✗

phenomenological

Mean field

microscopic

Ab-initio

Nuclear Matter

Semi-phenomenological

Ab-initio optical potentials are limited:
- methods specific to restricted energy regimes
- methods specific to restricted mass regions

Very challenging for ab-initio:
- theory needs to get thresholds exactly right
- theory needs to get the size exactly right
- theory needs to include absorption to cluster channels
- OP need to be uncertainty quantified

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

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Bayesian statistics

Thomas Bayes (1701–1761)

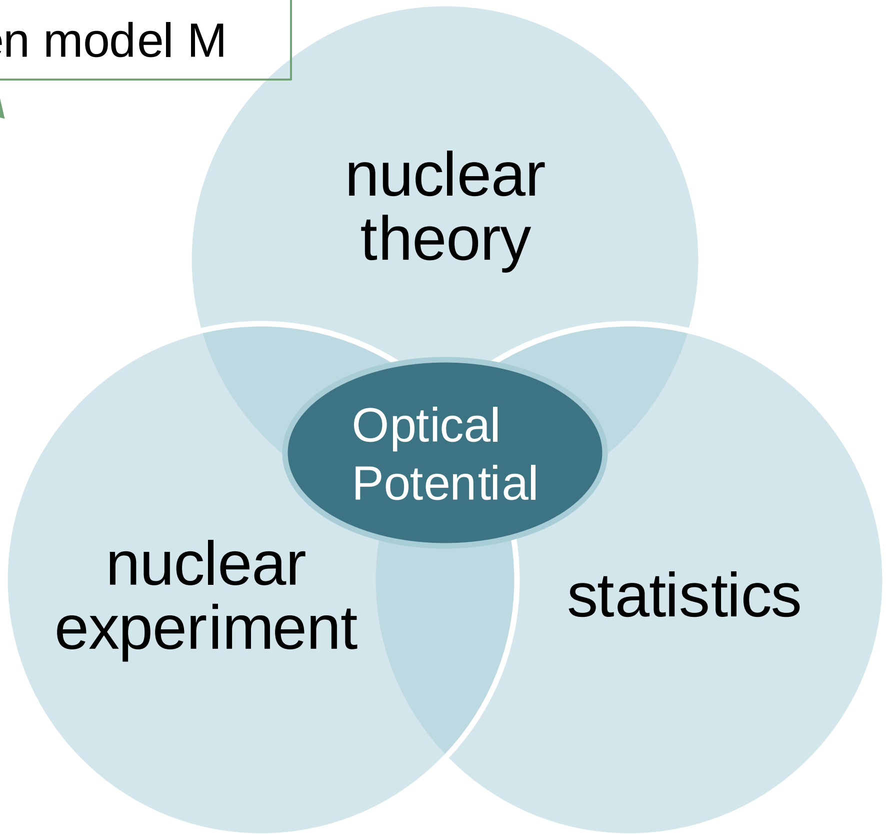
likelihood: assess the probability of observing D given model M

prior distribution of parameters H given model M

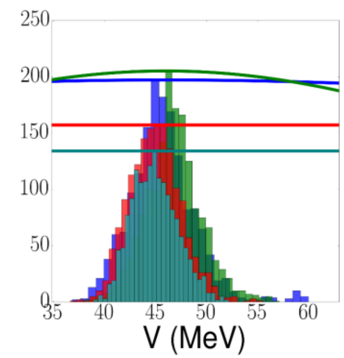
$$p(H|D, M) = \frac{p(D|H, M)p(H|M)}{p(D|M)}$$

Bayesian evidence

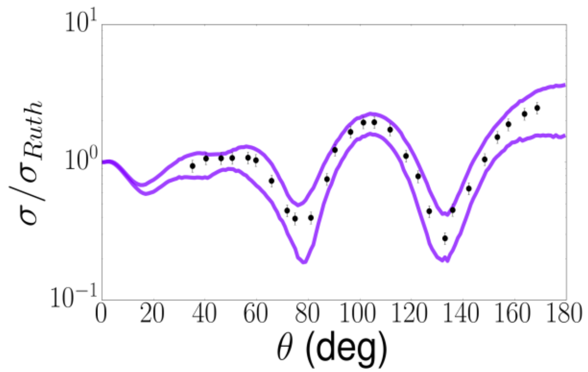
posterior distributions: information updated after seeing data D



Bayesian analysis



- Calibration of the model M
  (parameter posterior distributions)

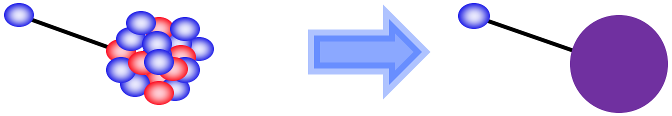


- Estimation of uncertainty in predictions
  (credible intervals on observables)

- Model assessment
  (comparison between models and with data)
- Model mixing
  (admixture between models with different strengths)
- Experimental design
  (What is the optimum measurement
  that adds information?)

Amy Lovell (LANL)

Physical model: optical model



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

The model has a set of parameters

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

We use previous OP parameterizations to set the priors
(typically wide priors to allow process to be data driven)

- use MCMC to sample parameter space

Amy Lovell (LANL)

Statistical model

Data: elastic scattering angular distributions/polarizations/total xs
- real exp data with evaluated errors
- mock data calculated using KD with 10% errors

Likelihood:
- No correlations and errors normally distributed

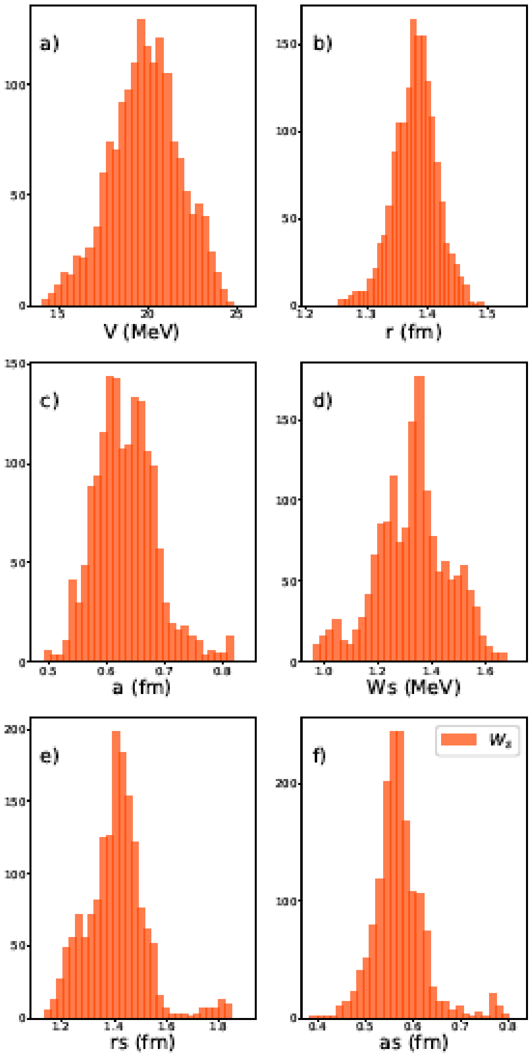
$$p(D|H,M) = \exp[-\chi^2/2]$$

- Include correlations effectively by dividing by the number of data points N (equivalent to inflating errors)

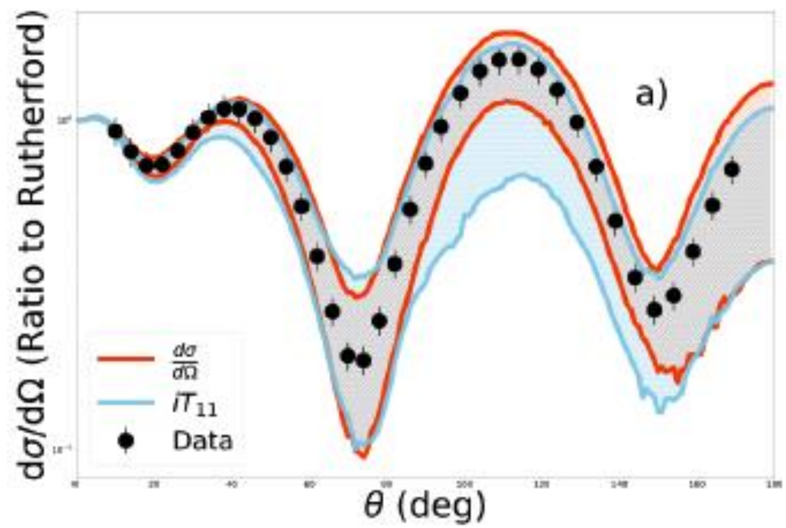
$$p(D|H,M) = \exp[-\chi^2/(2N)]$$

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

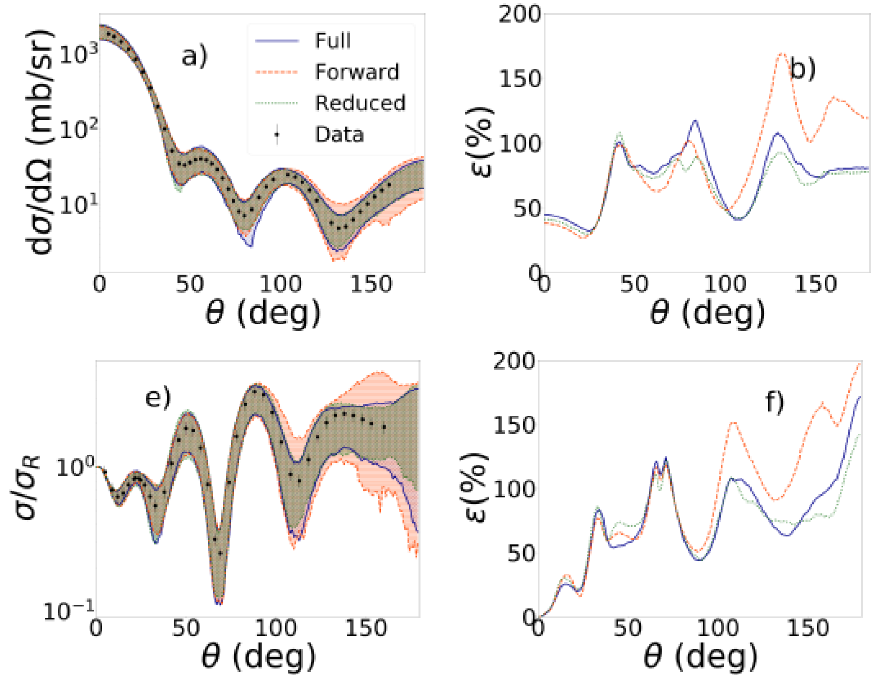
Bayesian: parameter posterior distributions



Create 95% confidence intervals for observable



What angular information needed?



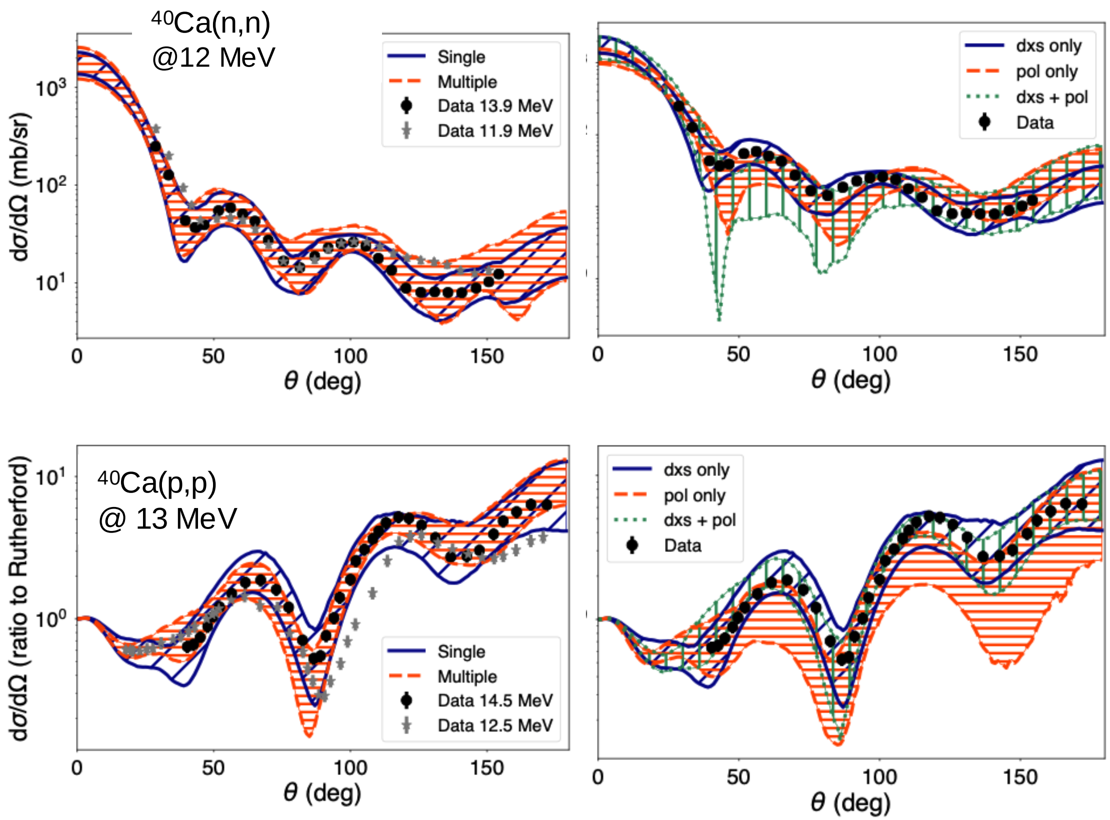
^{48}Ca(n,n)^{48}Ca at 12 MeV

^{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

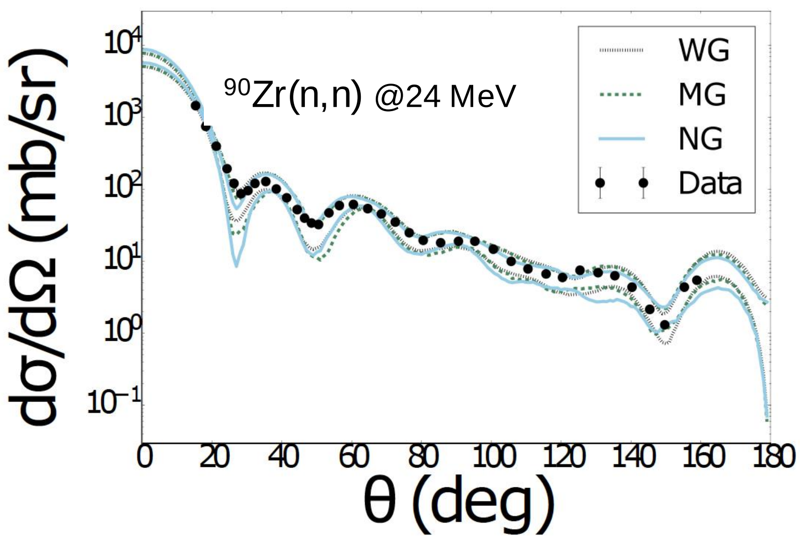


King, Lovell, Neufcourt, Nunes PRL (2019)
Catacora-Rios et al. PRC 100, 064615 (2019)
Lovell, Nunes, Catacora-Rios, King, JPG (2020)
Catacora-Rios et al. PRC 104, 064611 (2021)

What prior to use?

Priors encapsulate our prior knowledge
(e.g. a previous global parameterization)

Use gaussian distributions on parameters
How wide should these be?



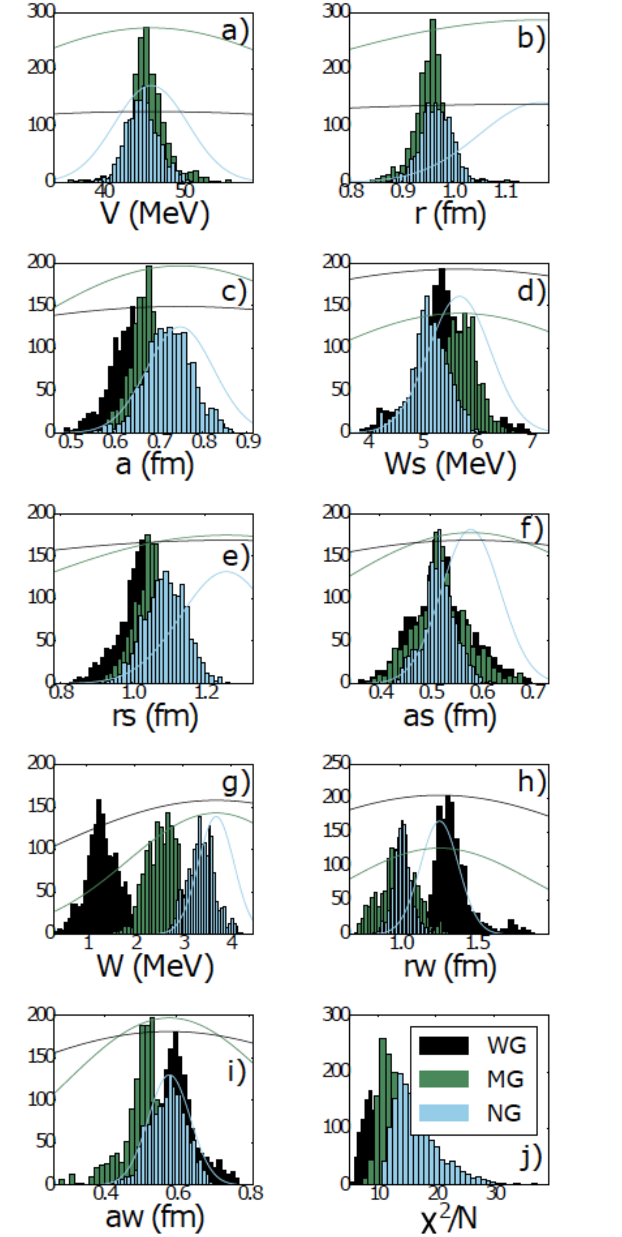


FIG. 2: (Color online) Comparison of the posterior distributions (histograms) resulting from various prior distributions (corresponding solid lines) for a wide Gaussian (WG), medium Gaussian (MG), and narrow Gaussian (NG) as defined in Table II for ^{90}Zr(n,n)^{90}Zr at 24.0 MeV.

Lovell and Nunes PRC (2018)

Which likelihood to use?

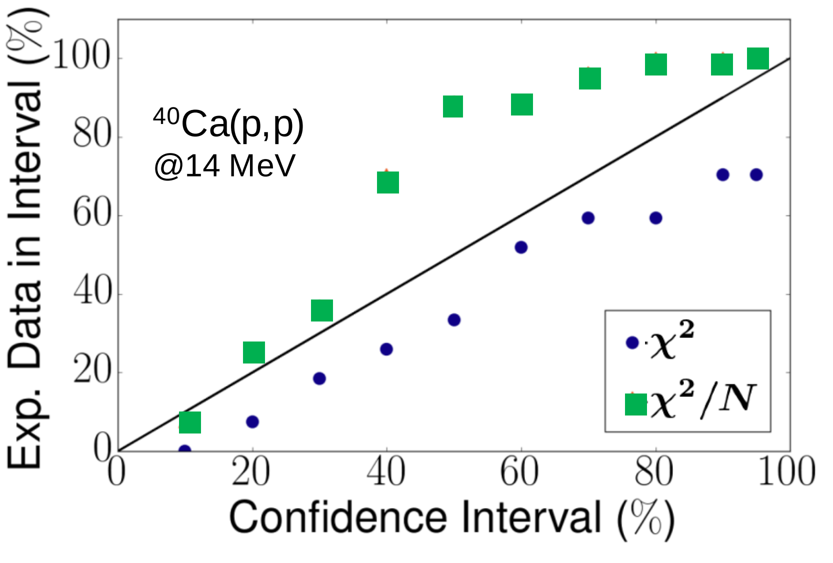
Complications:

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

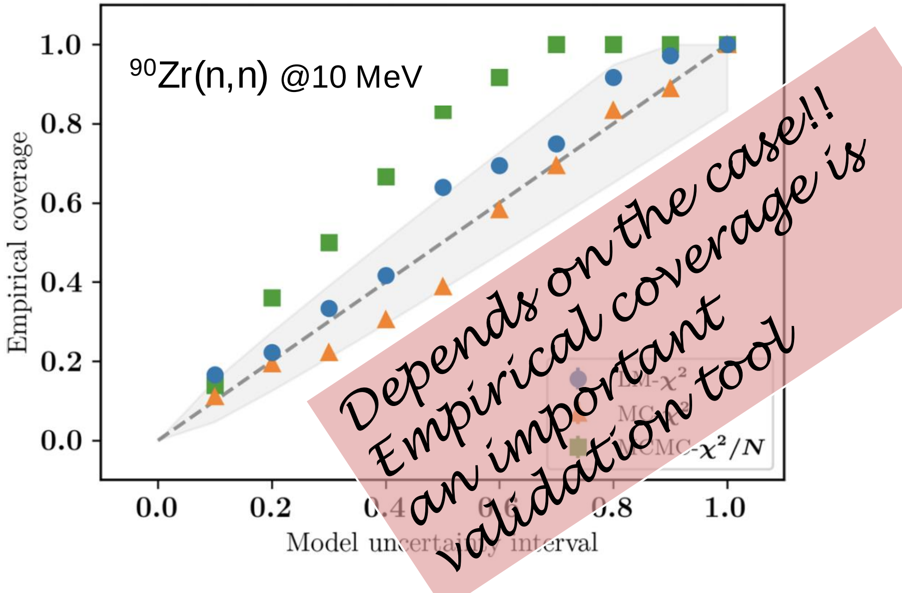
How to combine sets of angular distributions?

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

$$p(D|H,M) = \exp\left[-\chi^2/2\right]$$ **?**



King et al., PRL 2019



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

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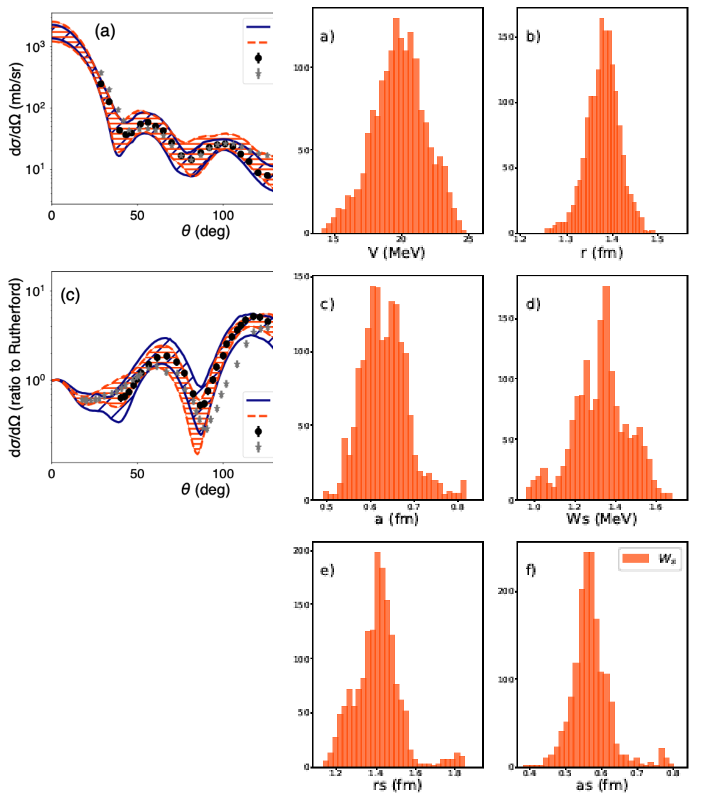
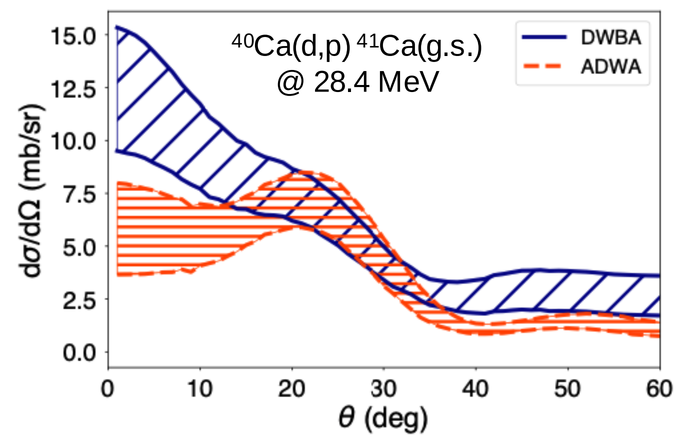
Propagating uncertainties to transfer

OP constrained with elastic scattering to obtain posterior distributions for parameters



Propagate to other reaction observables

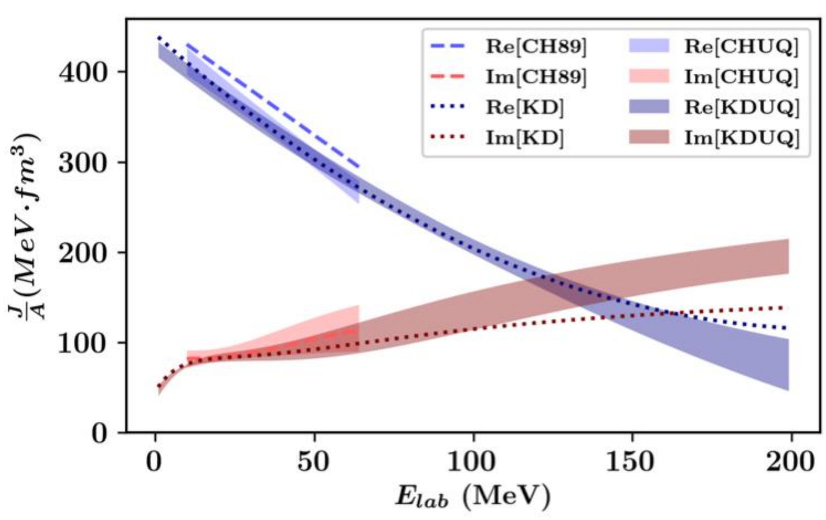


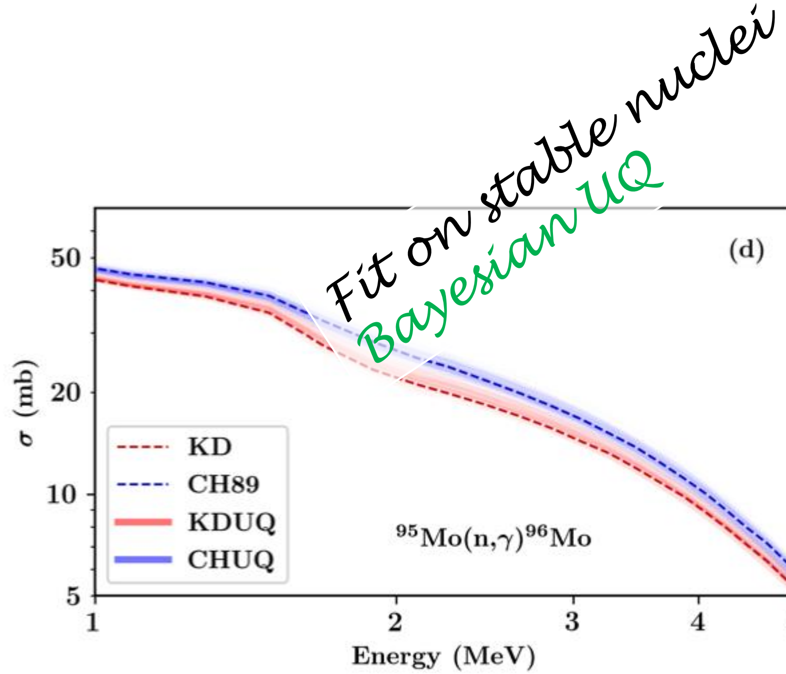
Ekstrom talk:
UQ important for decision-making and model assessment

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





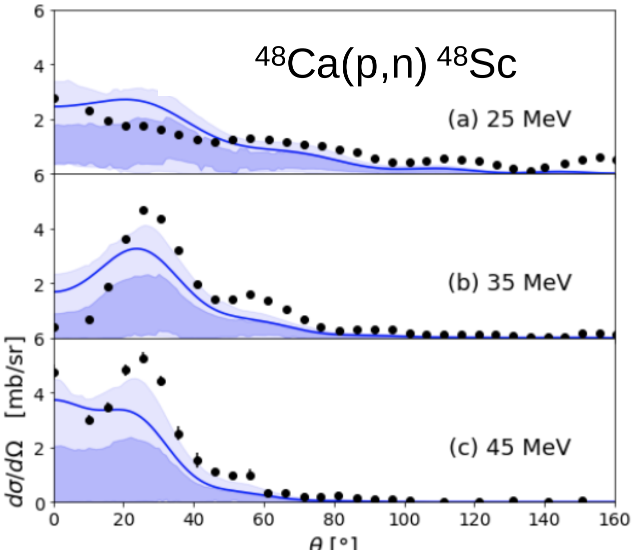
Pruitt et al., Phys. Rev. C 107, 014602 (2023)

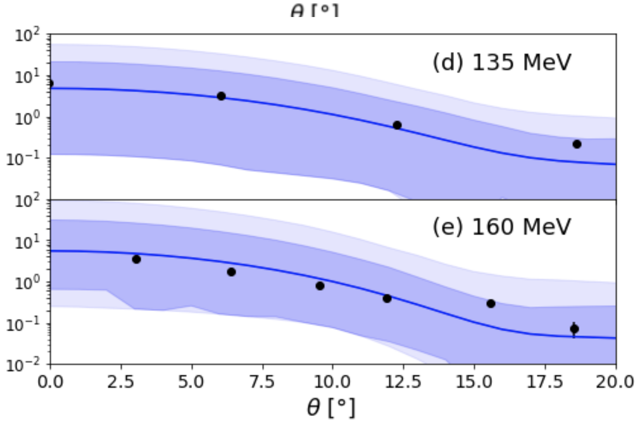
Andy Smith

OP uncertainties in charge exchange to IAS

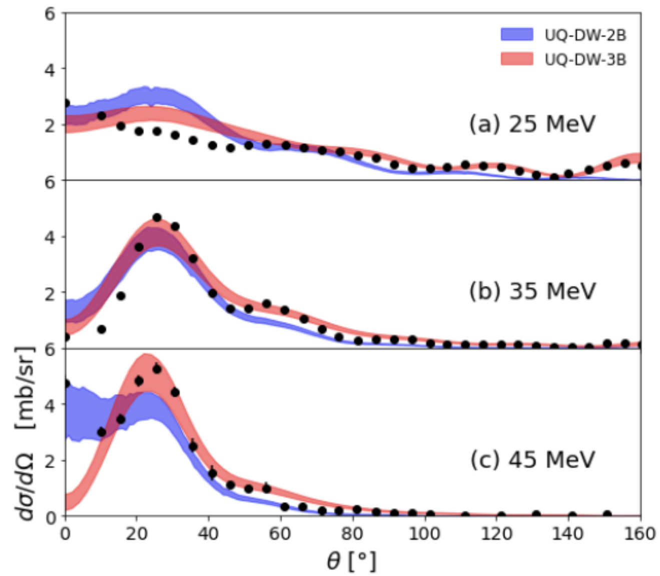
- DWBA formalism
- Using parameter posterior from KDUQ

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



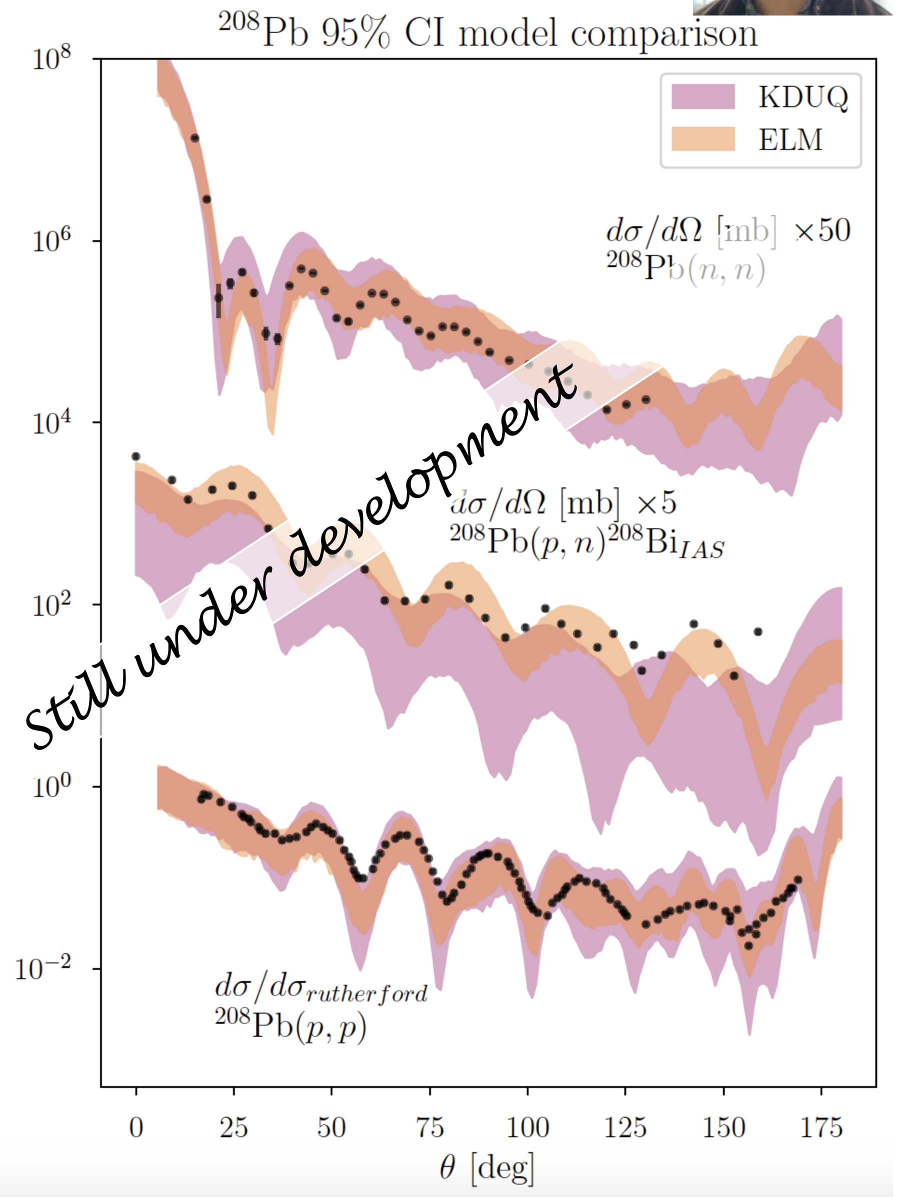


Comparing two-body and three-body models for charge exchange



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

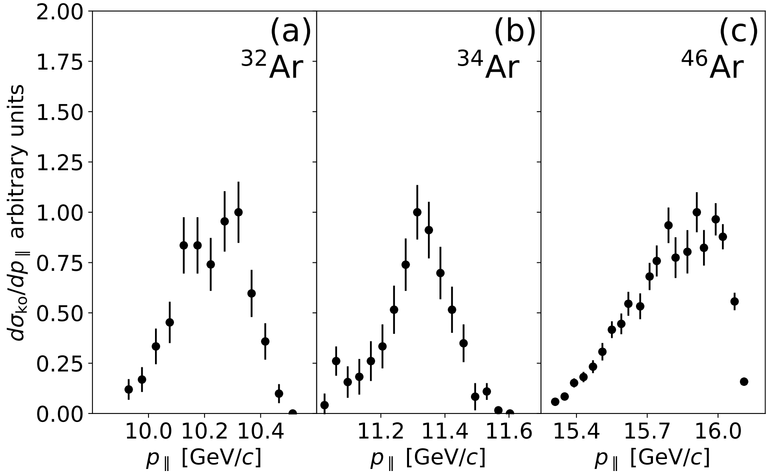
Includes charge-exchange to IAS for key isotopes

Beyer and Nunes, in preparation

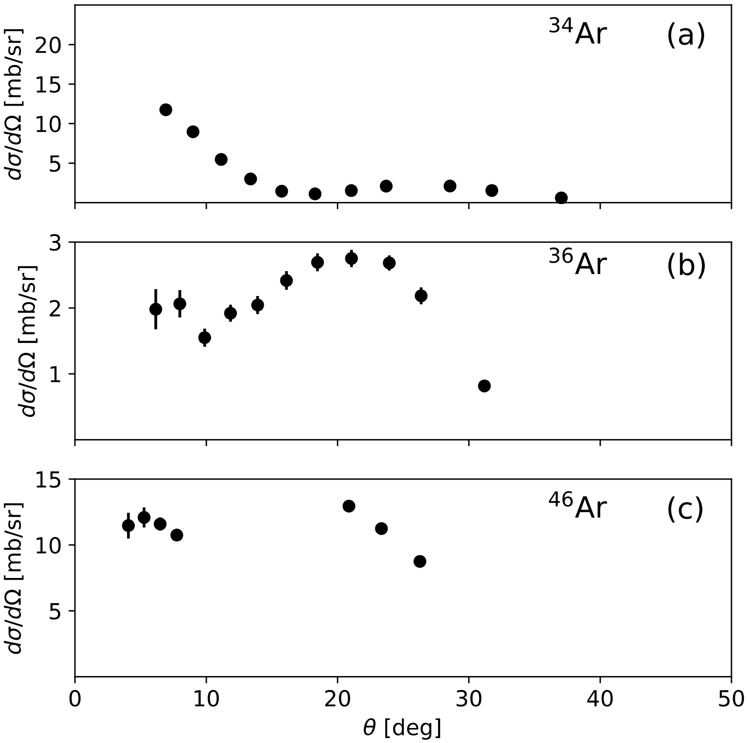
Propagating uncertainties to knockout

- 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)

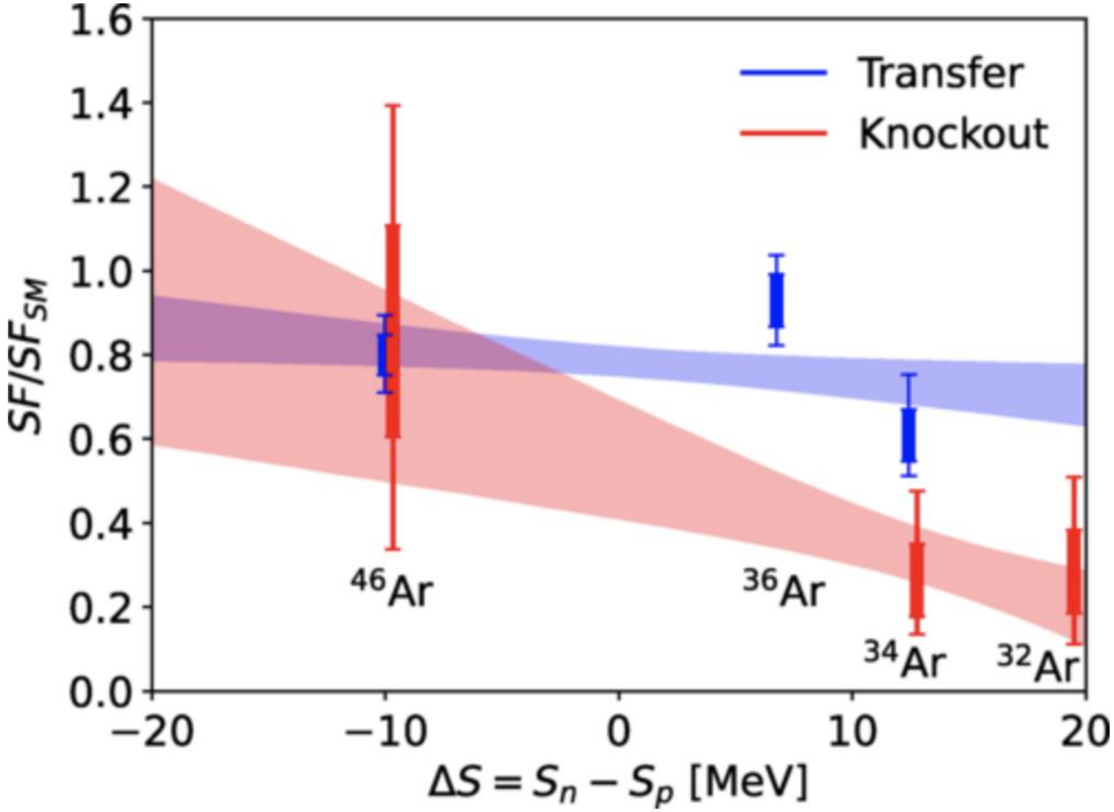


dark (light) shade:
68% (95%) credible intervals

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)

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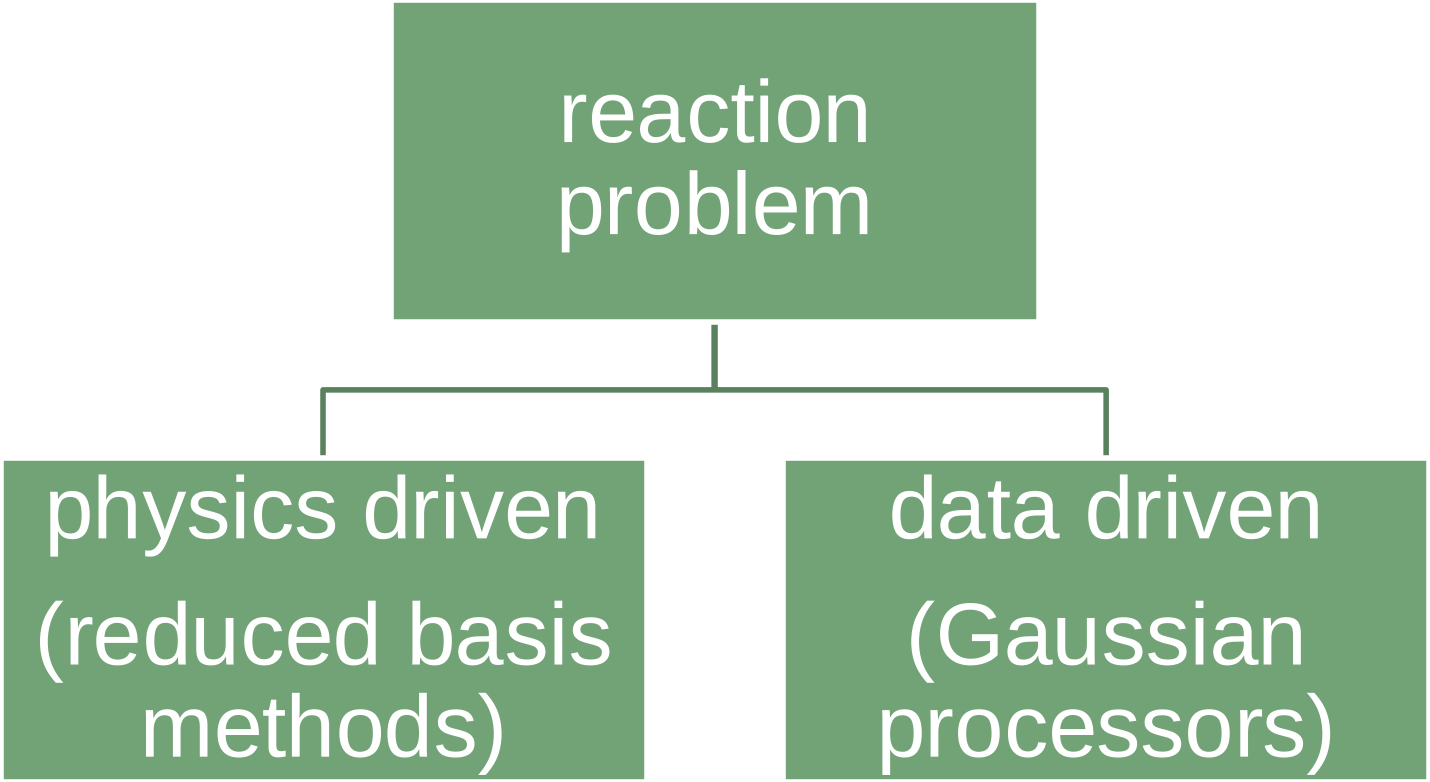
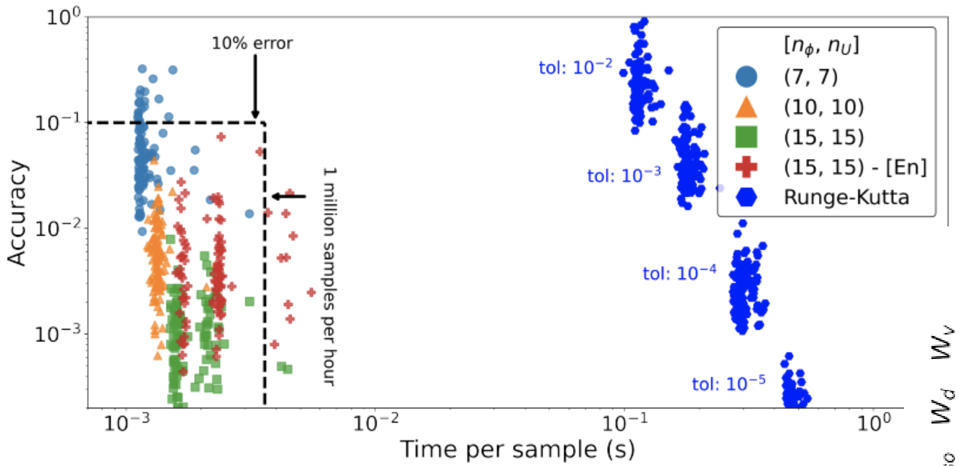
Emulators for nuclear reactions

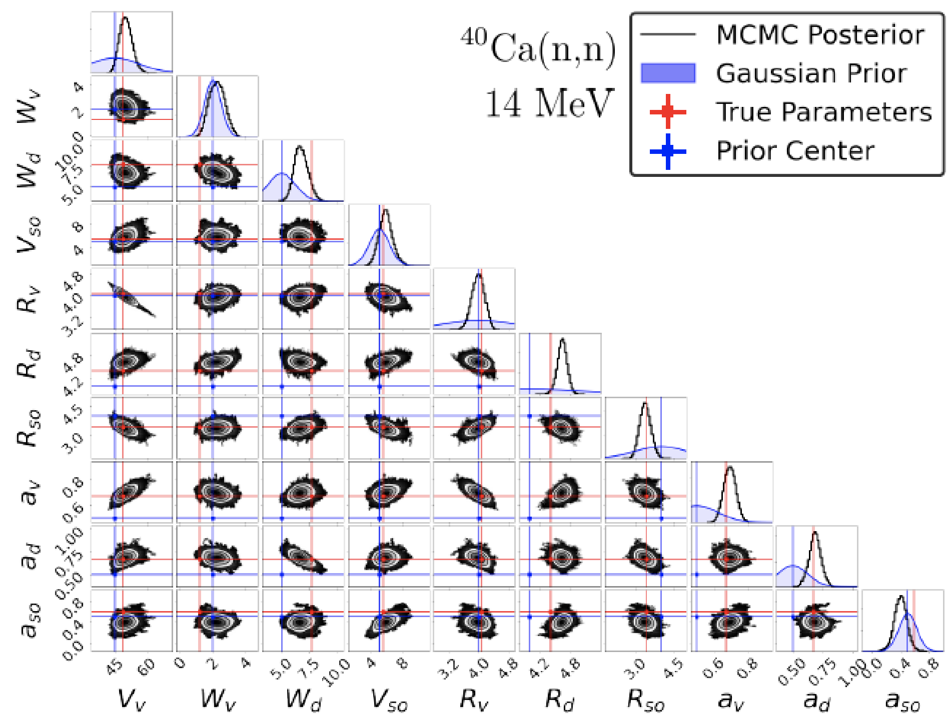
An emulator is a fast and efficient replacement for a complex physics model



Physics Driven Emulator
ROSE: Reduced Order Scattering Emulator



New software ROSE is 3 orders of magnitude faster than standard finite differences integration methods



Extension to coupled channels in development!

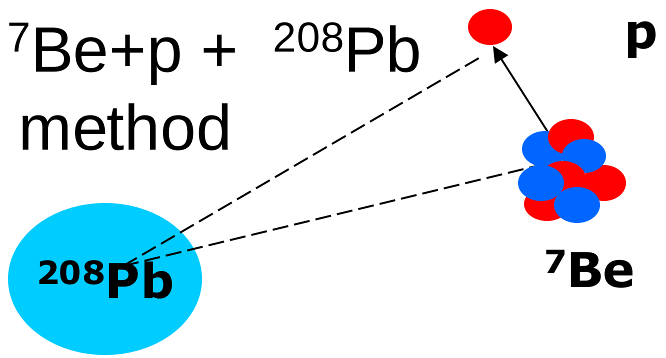
Odel et al., Phys. Rev. C **109**, 044612 (2024)

Data driven emulator
Breakup cross sections needed for astrophysics

Example:
^{7}Be(p,γ)^{8}B reaction
relevant for solar fusion

^{8}B+ ^{208}Pb —» ^{7}Be+p + ^{208}Pb

Indirect method



Working horse for modeling these reactions:
Continuum Discretized Coupled Channel (CDCC)

Large scale (large memory requirements)
Long runs (many hours to days)

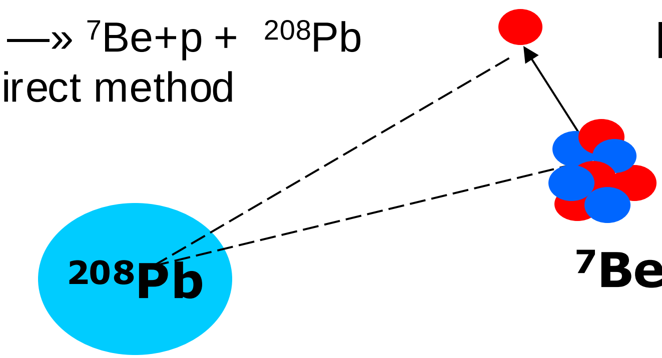
Impossible to do Bayesian analysis directly with CDCC!

Predictions: Angular distributions and energy distributions of fragments

Emulators for breakup cross sections

$^{7}Be(p,\gamma)^{8}B$
reaction relevant for
solar fusion

$^{8}B + ^{208}Pb$ —» $^{7}Be + p + ^{208}Pb$
Indirect method



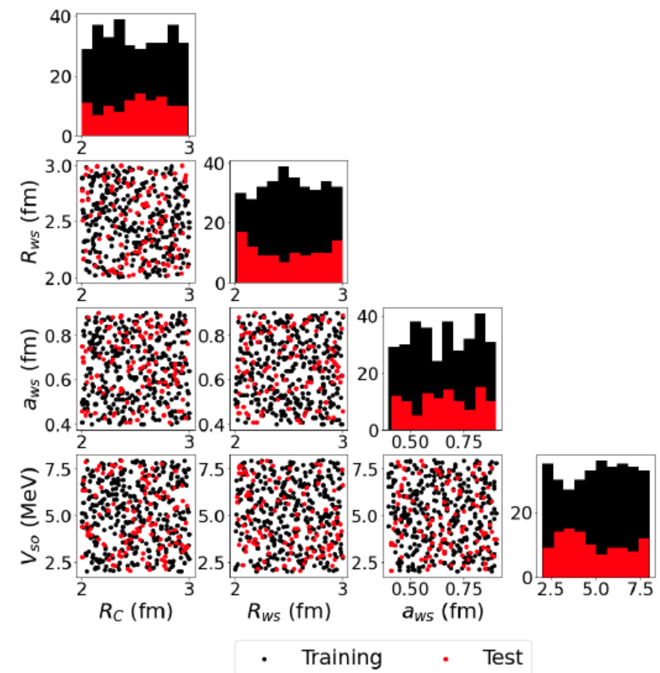
Continuum Discretized Coupled Channel
Gaussian-processors emulator for breakup:
Angular distribution and energy distribution

uncertainty from $^{7}Be+p$ interaction

mock data generated for set of interactions from
G. Goldstein et al., Phys. Rev. C 76, 024608 (2007)

TABLE I: Model parameters and their ranges.

Parameter	Label	Range $[\underline{\rho_i}, \overline{\rho_i}]$
R_C	ρ_1	[2, 3] (fm)
R_{ws}	ρ_2	[2, 3] (fm)
a_{ws}	ρ_3	[0.4, 0.9] (fm)
V_{so}	ρ_4	[2, 8] (MeV)

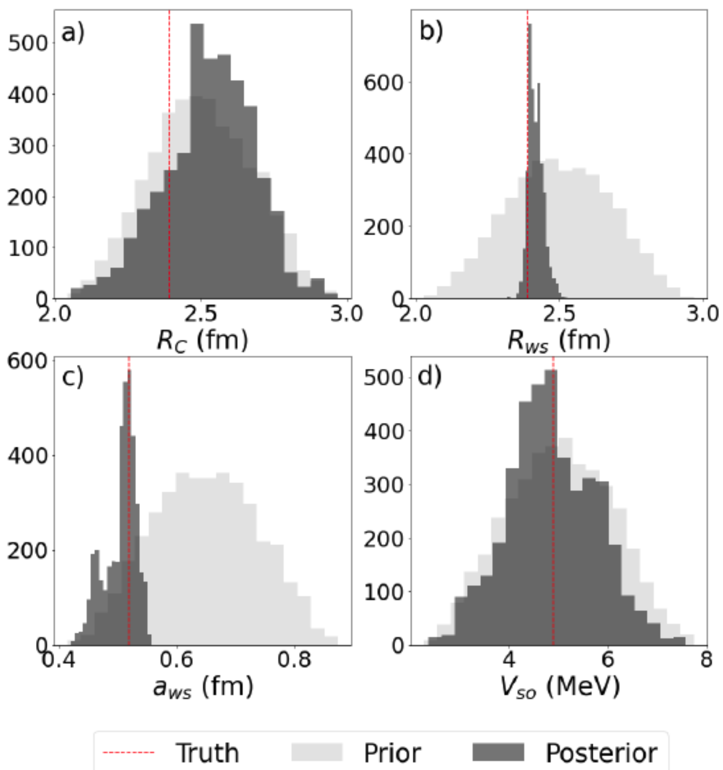


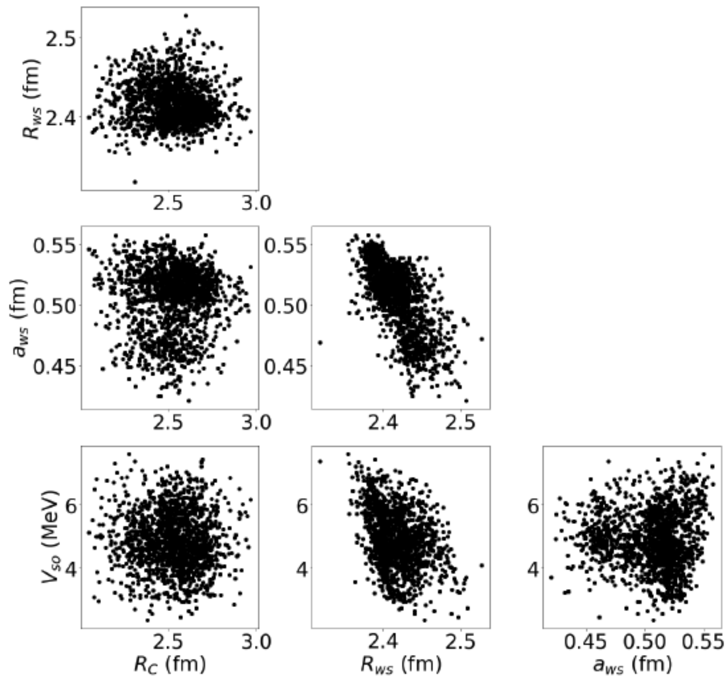
Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Bayesian Analysis of Nuclear Dynamics

Emulators for breakup cross sections

Posterior distributions and correlation plots

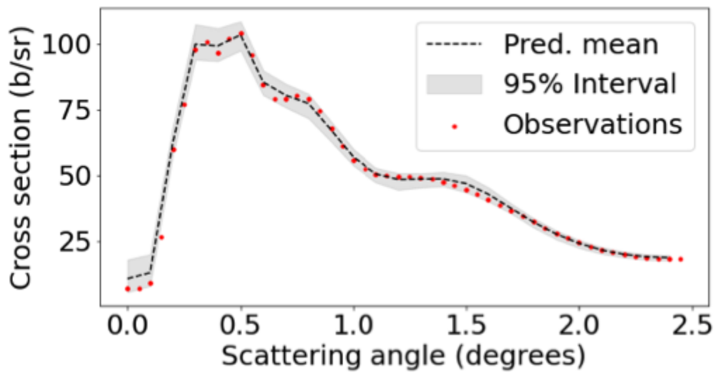




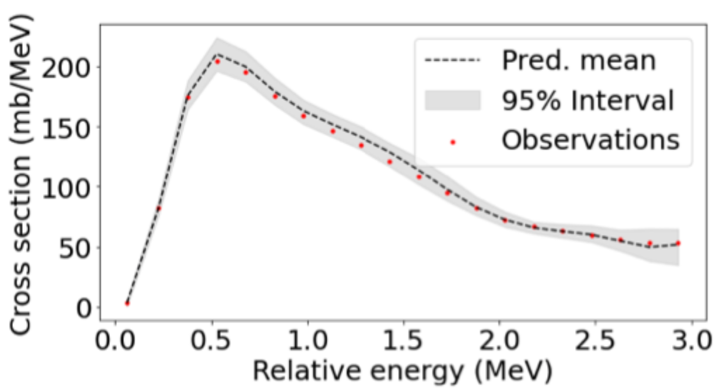
Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Emulators for breakup cross sections

$^{8}B + {}^{208}Pb \mapsto {}^{7}Be + p + {}^{208}Pb$ 80 MeV.A



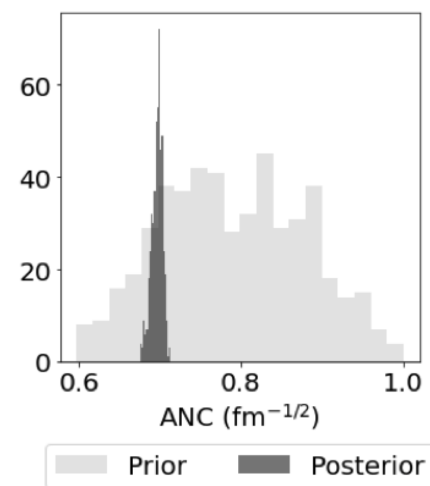
(a) Angular distribution.



(b) Energy distribution.

Continuum Discretized Coupled Channel
Gaussian-processors emulator for breakup:
Angular distribution and energy distribution

uncertainty from $^{7}Be+p$ interaction



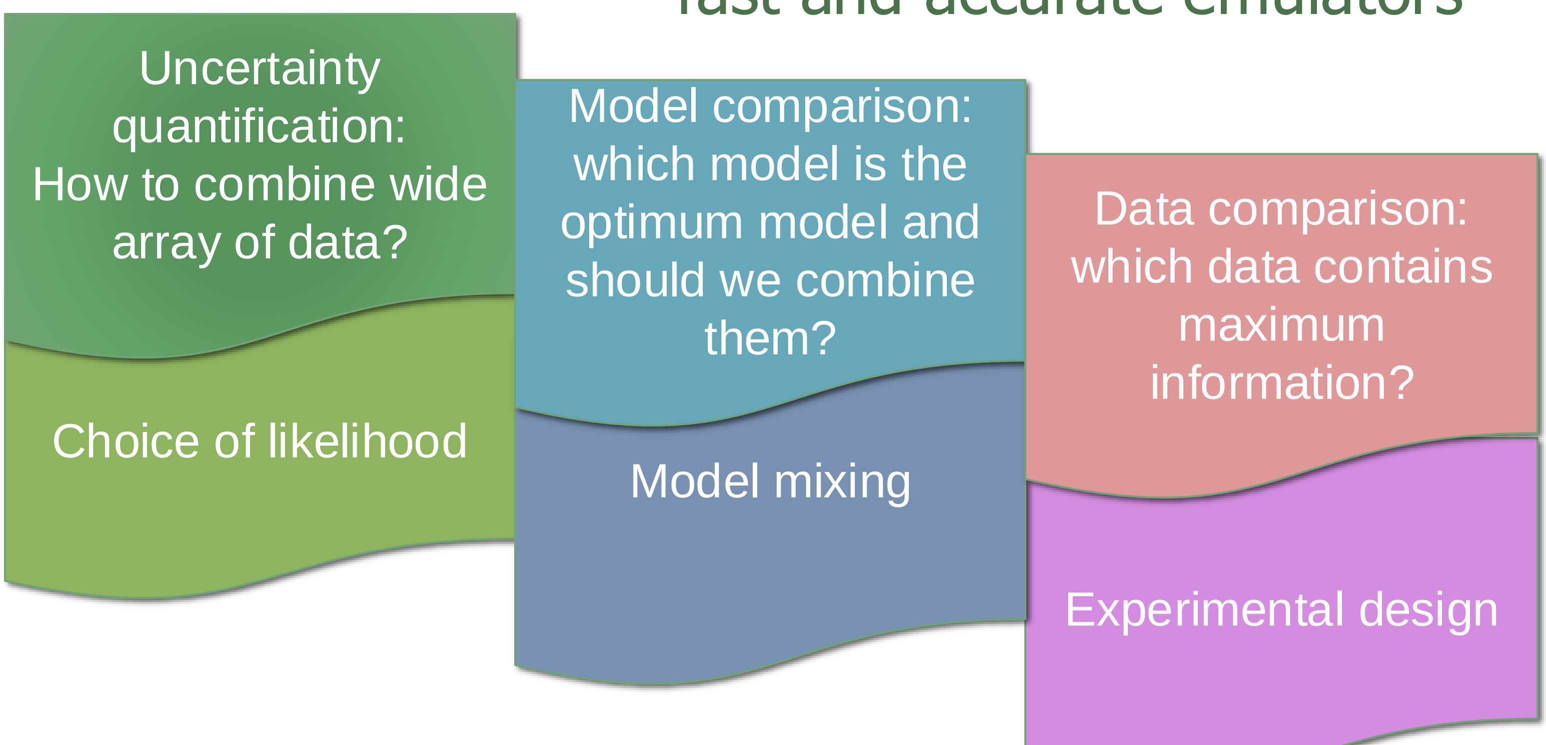
Excellent constraint on S_{17}

Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Opportunities for the future

- Optical potential validated for rare isotopes:
  - nucleon global optical potential with UQ informed by (p,n); ab-initio priors; extension to heavy-ions…
- Bayesian analysis for complex reactions models:

fast and accurate emulators



Opportunities for the future

most important of all are the people!

Filomena Nunes

Chloë Hebborn

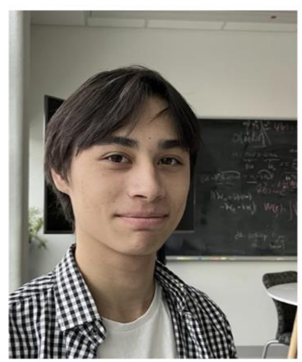
Kyle Beyer

Patrick McGlynn

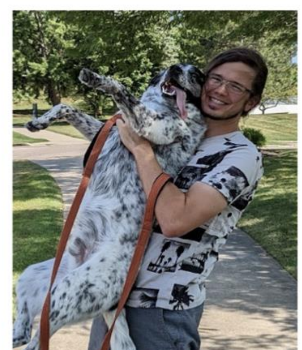
Cate Beckman

Manuel Catacora Rios

Andy Smith



Daniel Shiu



Pablo Giuliani

Grigor Sargsyan

few-body reaction group@MSU, summer 2024

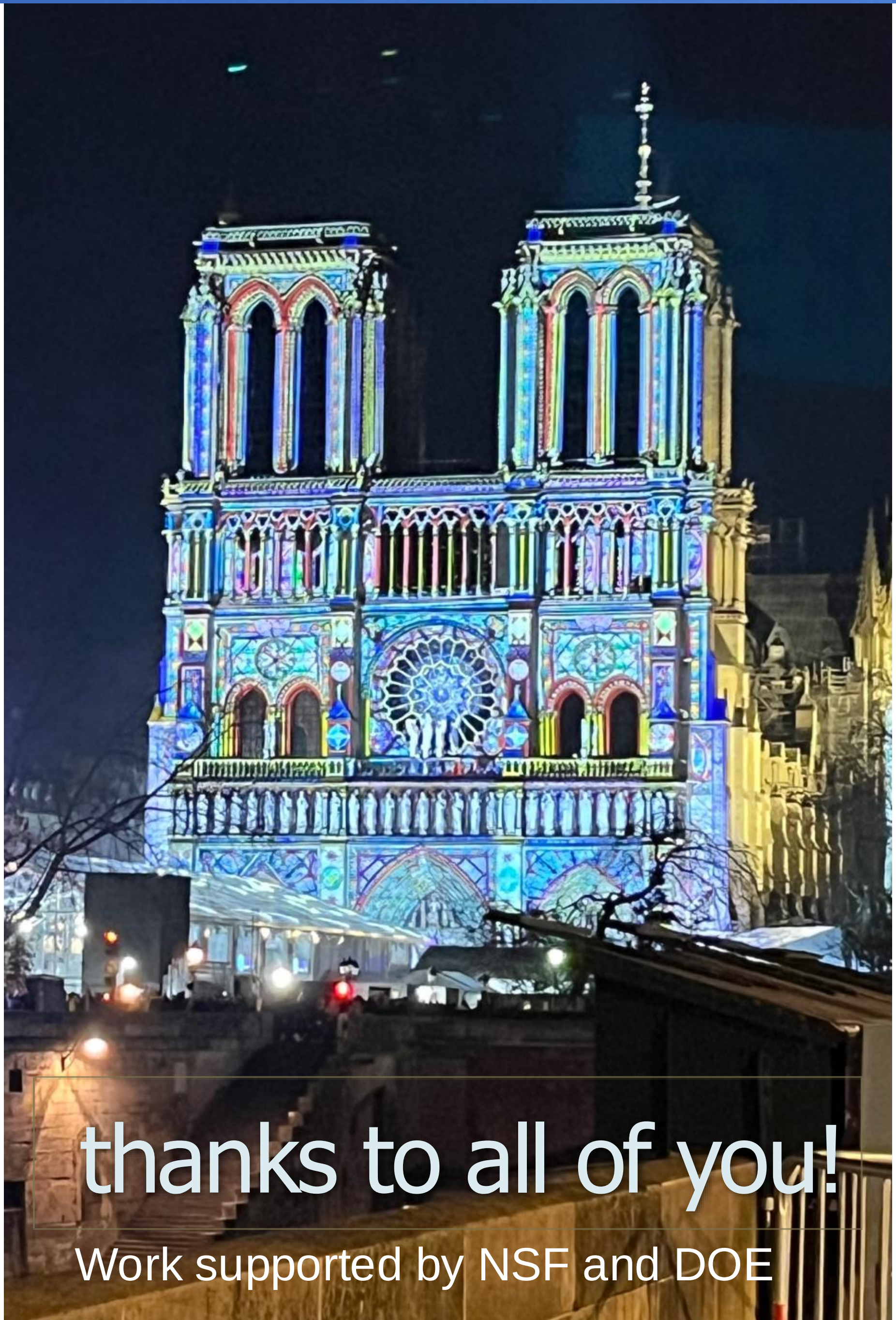
Collaborators:

Bayesian Analysis:
Amy Lovell (LANL)
Chloe Hebborn (MSU)
Garrett King (WashU)
Manuel Catacora-Rios (MSU)
Cole Pruitt (LLNL)

Charge Exchange:
Terri Poxon-Pearson (NNSA)
Gregory Potel (LLNL)
Andy Smith (MSU)
Chloe Hebborn
Remco Zegers

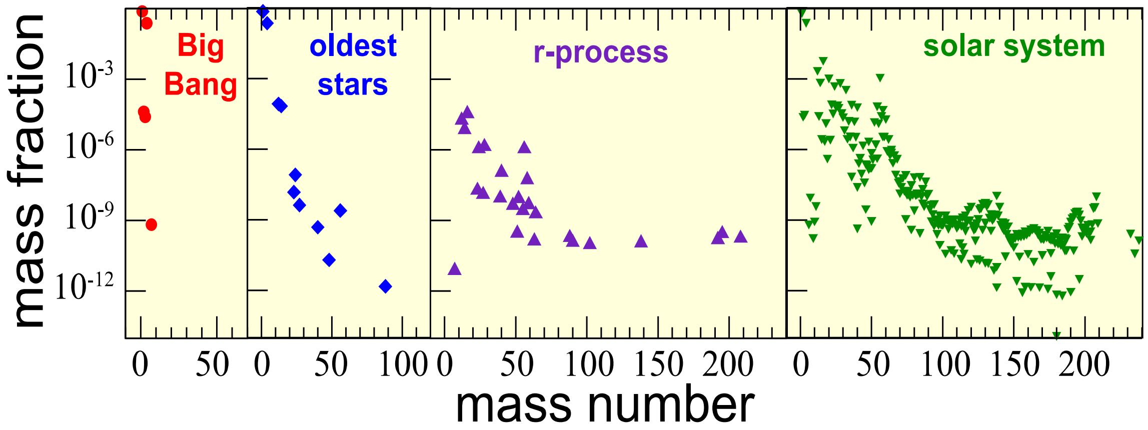
Knockout:
Chloe Hebborn
Amy Lovell

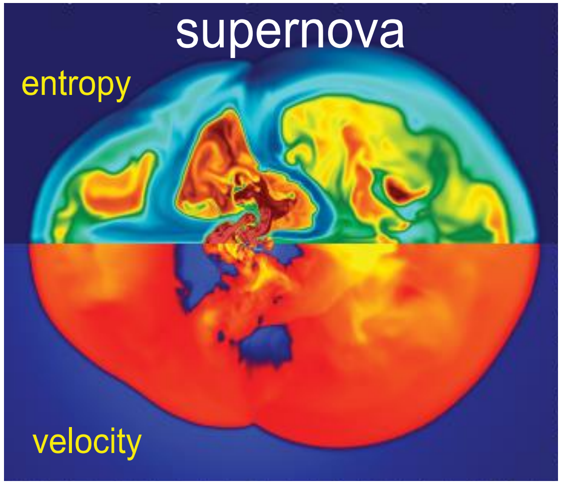
Emulators:
BAND collaboration

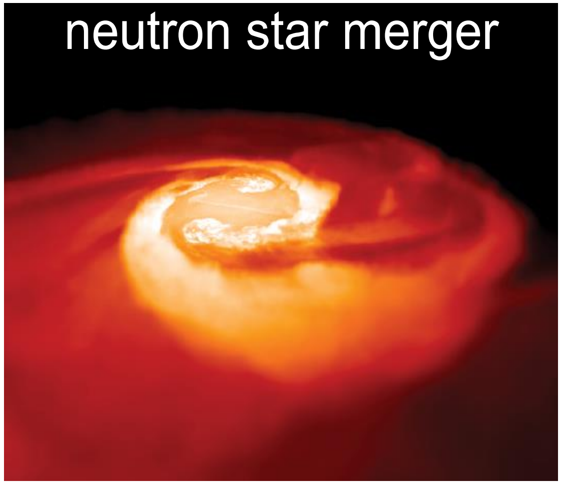


BACKUP

Bird's eye view of nuclear reactions







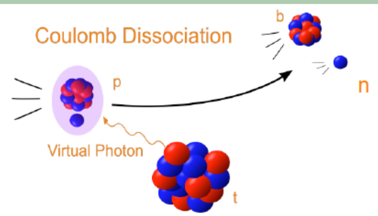
Nuclear reactions got us from the lightest elements all the way to the wide range of elements found in our solar system!

Bird's eye view of nuclear reactions

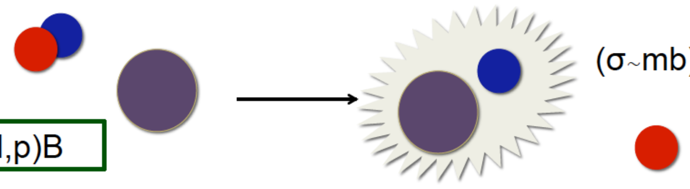
Probe of neutron capture: breakup and transfer

A+Pb ↦n+B+Pb

(σ~mb)

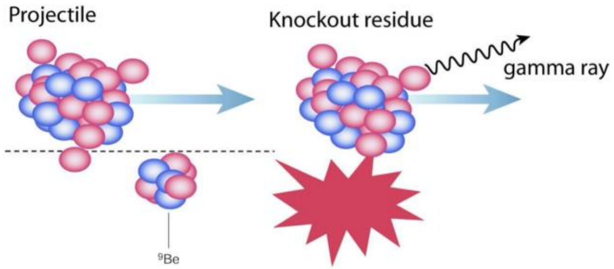


A(d,p)B

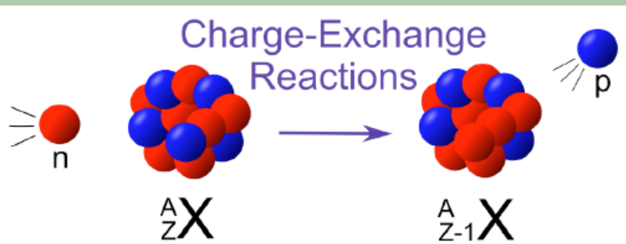


(σ~mb)

Probe of single-particle structure: knockout



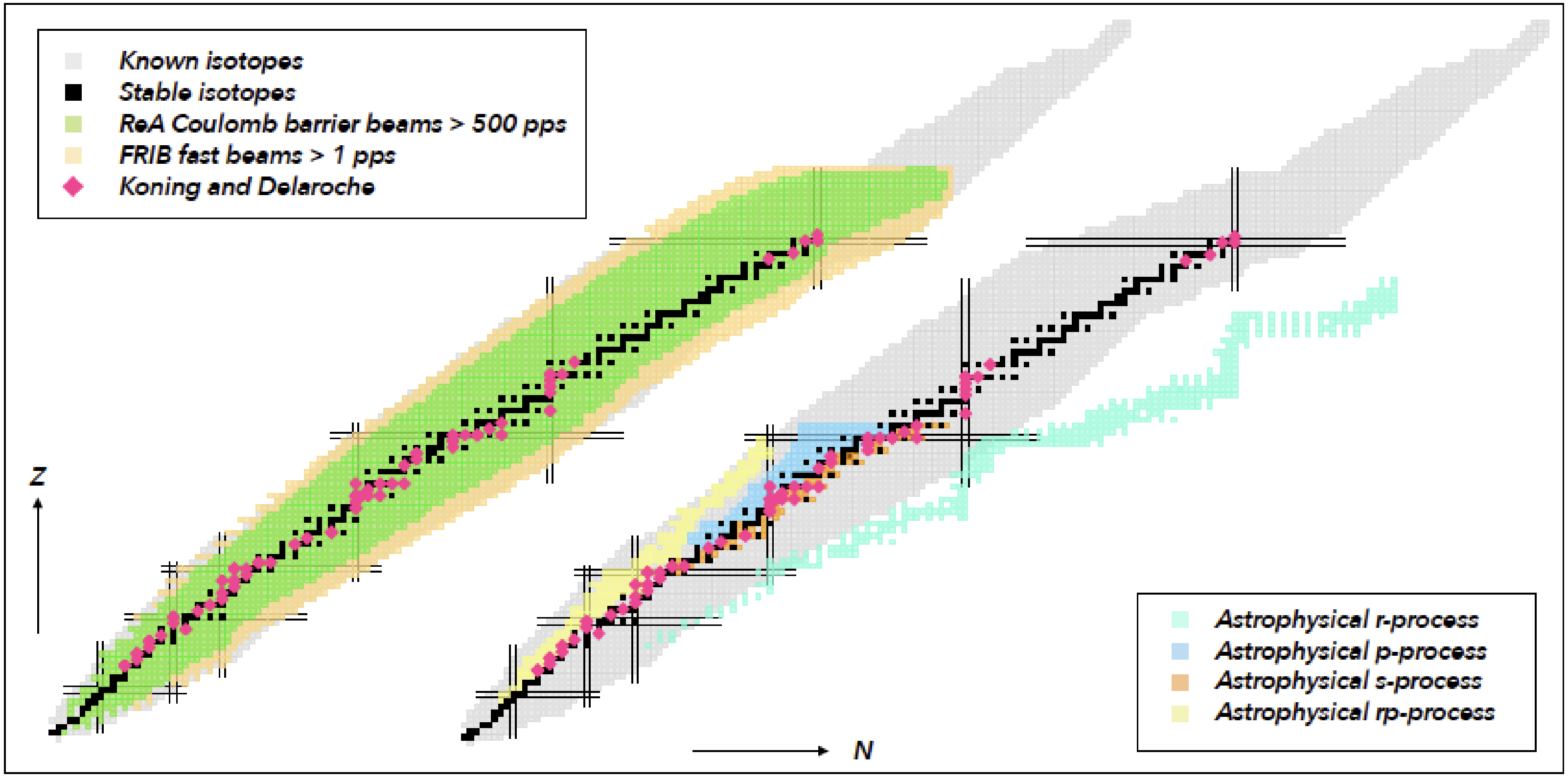
Probe of electron capture: charge-exchange



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

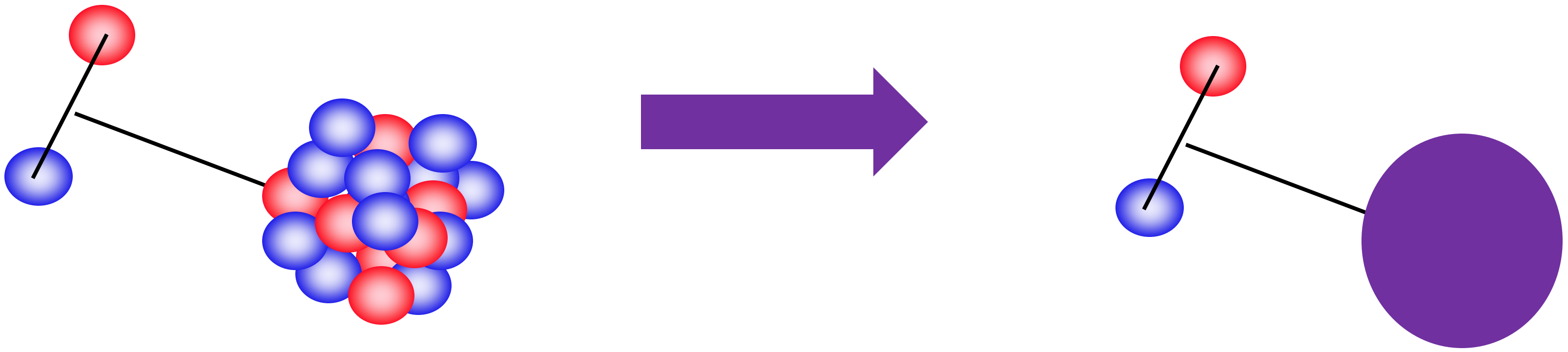
But reaction theory is key for translation!

Phenomenological potentials fitted to stable nuclei

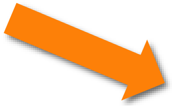


Hebborn, Nunes, et al., JPG 50, 060501 (2023)

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

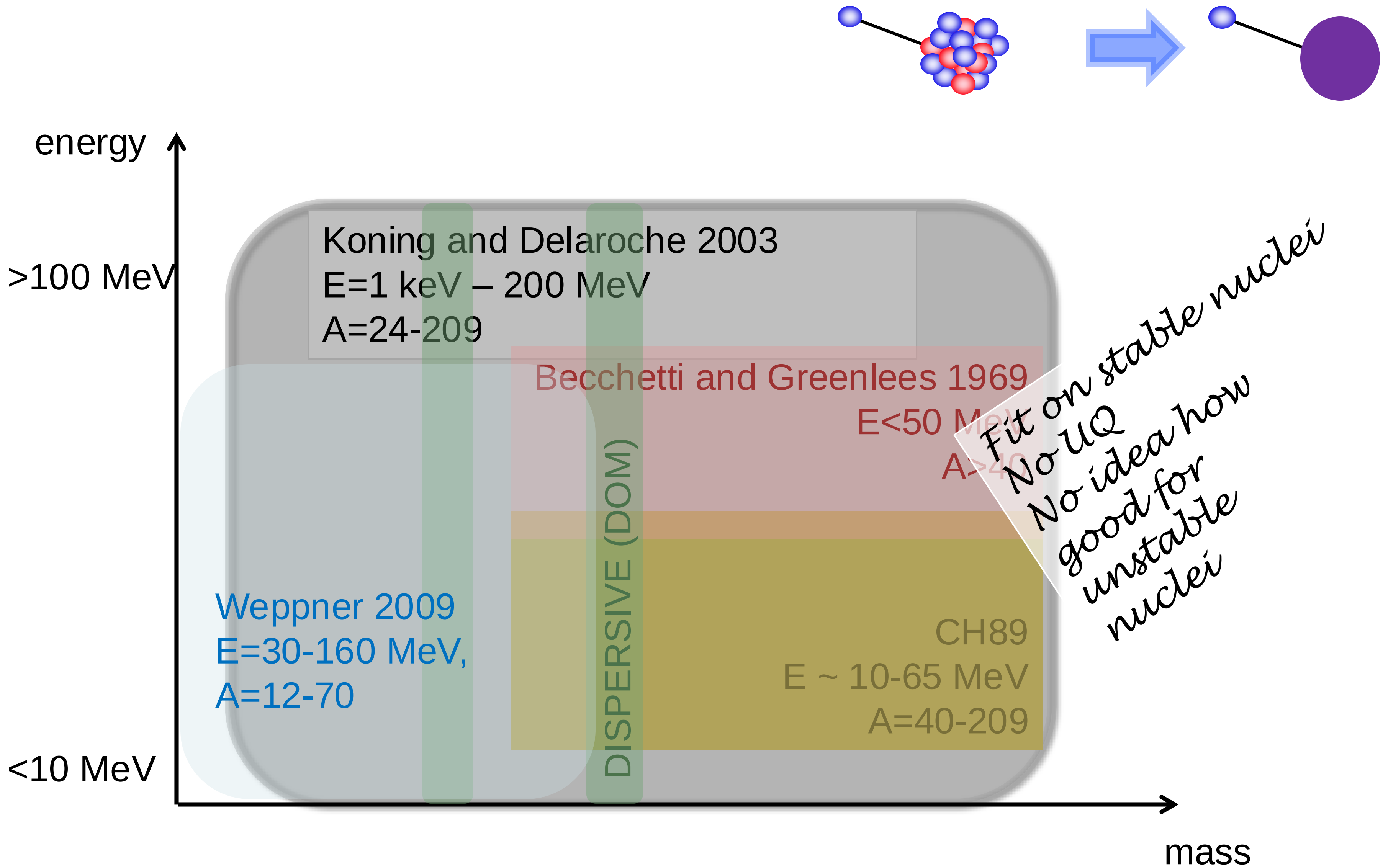


- ❑ isolating the important degrees of freedom in a reaction
- ❑ effective nucleon-nucleus interactions (or nucleus-nucleus) usually referred to as **optical potentials**

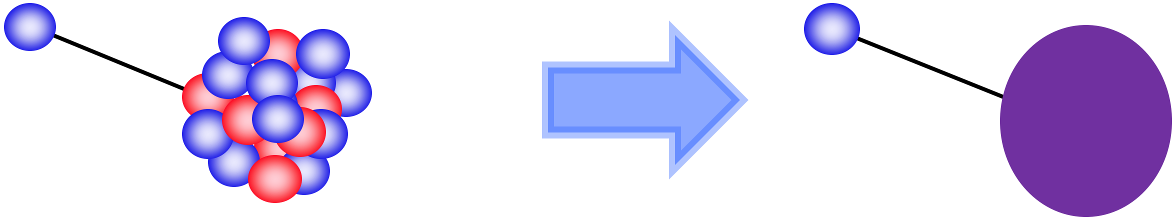


main cause of uncertainty

Landscape of global optical potentials



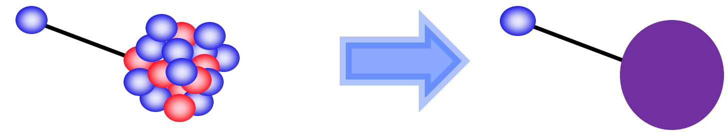
Optical potentials from theory



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



energy

>100 MeV

<10 MeV

AB INITIO

Based on chiral 2b+3b forces

Applied to light nuclei or closed shell nuclei

MEAN FIELD

Based on density functional fitted to nuclear properties

medium to heavy mass nuclei

NUCLEAR MATTER

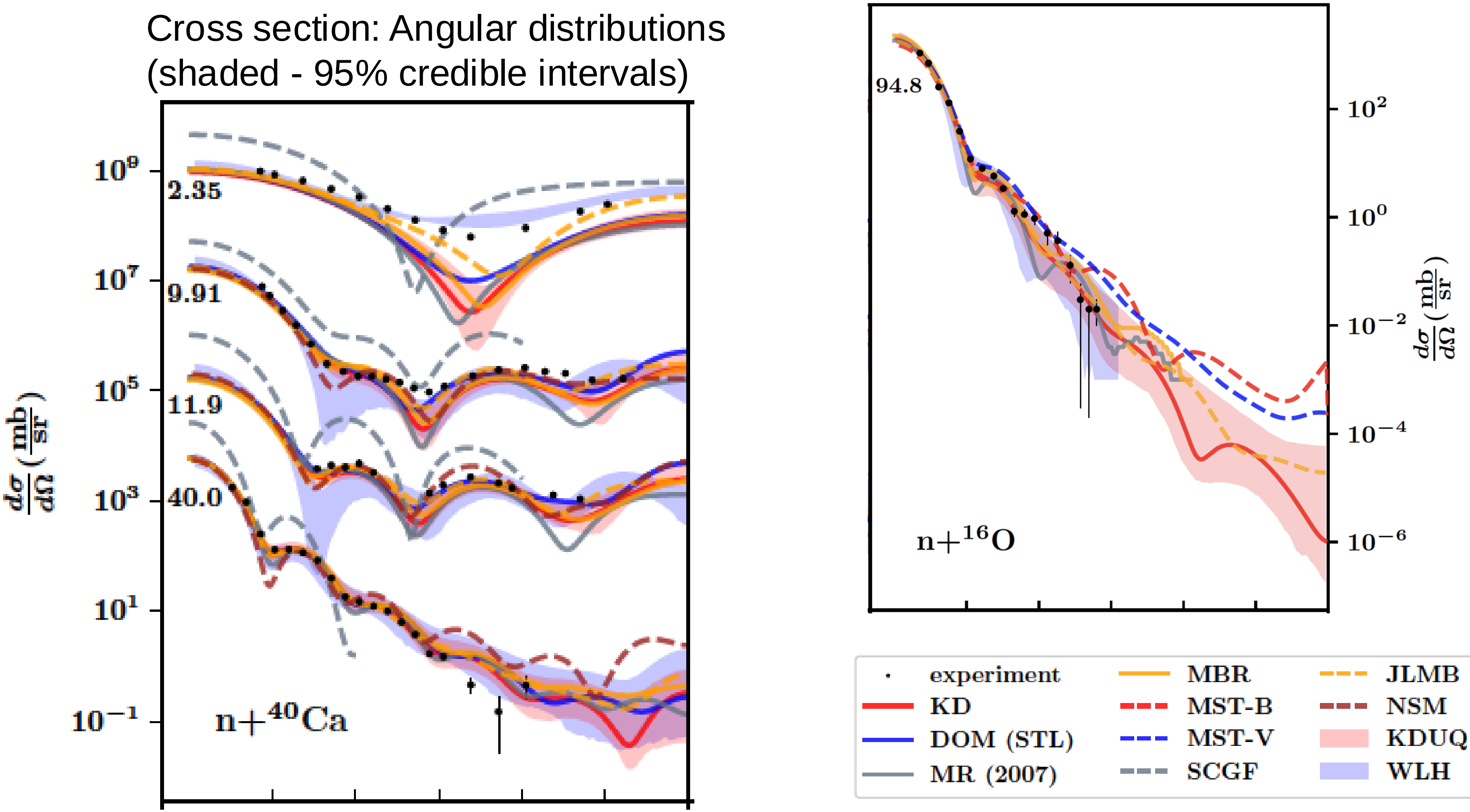
Based on NN chiral 2b+3b and MF densities

medium to heavy mass nuclei

mass

How do optical models compare?

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

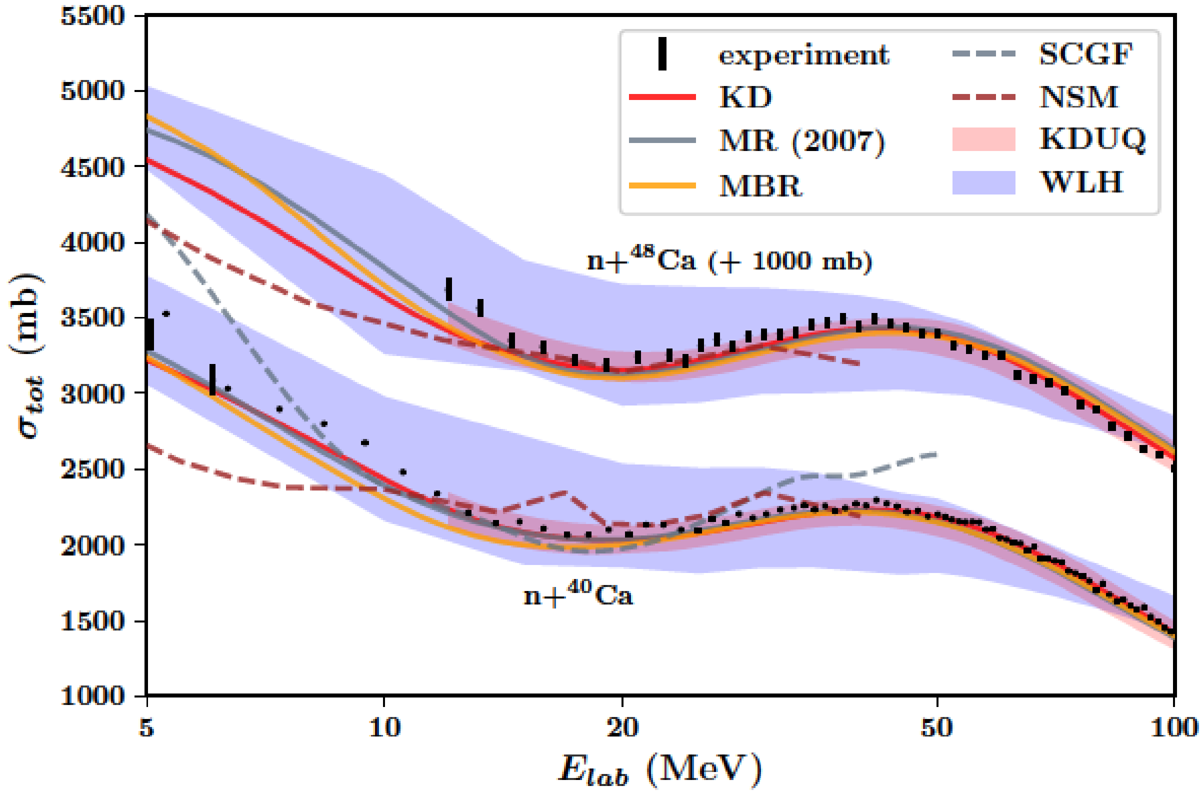


Hebborn, Nunes, et al., JPG 50, 060501 (2023)

How do optical models compare?

95% credible intervals

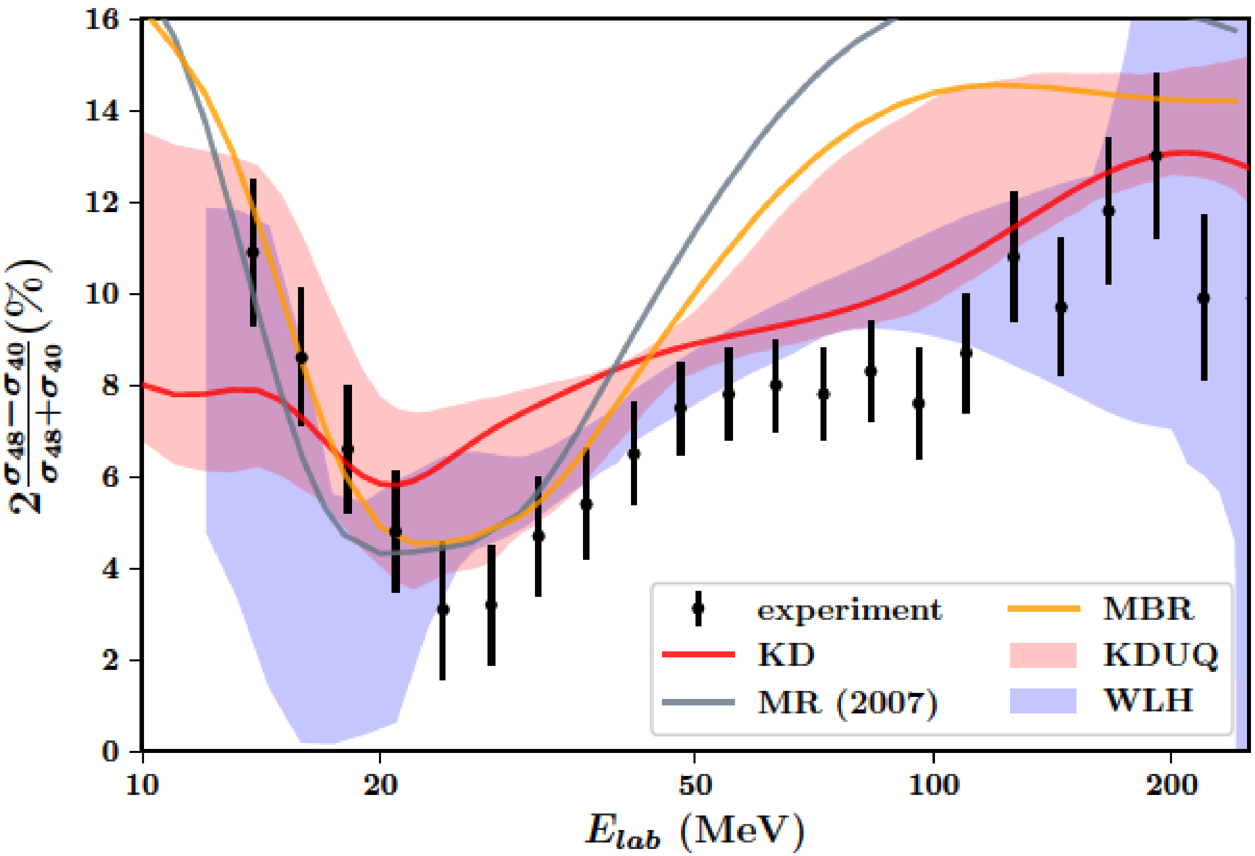
Total cross section as a function of energy



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)

What model encapsulates more information?

Bayesian evidence: provides information contained in a data set.
Integral of the likelihood times the prior over full parameters space

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

Bayesian factor: $$\frac{\bar{p}(d|\mathcal{M})_{(d\sigma/d\Omega)}}{\bar{p}(d|\mathcal{M})_{(iT_{11})}} < 3$$

R	Strength of evidence
1 to 3.2	Not worth more than a bare mention
3.2 to 10	Substantial
10 to 100	Strong
> 100	Decisive

Kass and Raftery,
J. Amer. Stat. Assoc 9 (430) 791

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

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

Catacora-Rios et al. PRC 104, 064611 (2021)