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

https://imagesofvenice.com

Neutron transfer reactions as an indirect approach to (n,γ)

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

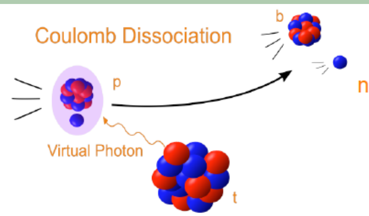
- Bird's eye view of nuclear reactions
- Case study Cs isotopes
  - astrophysical motivation
  - reaction model for (d,p)
  - predictions
- Uncertainties
  - Bayesian optical model calibration
  - uncertainties in Hauser-Feshbach predictions
  - discussion of global approaches
- Opportunities for the future

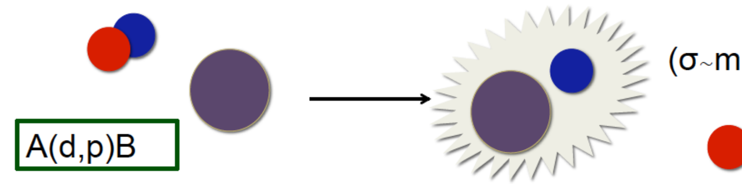
Bird's eye view of nuclear reactions

Probe of neutron capture: breakup and transfer

A+Pb ↦n+B+Pb

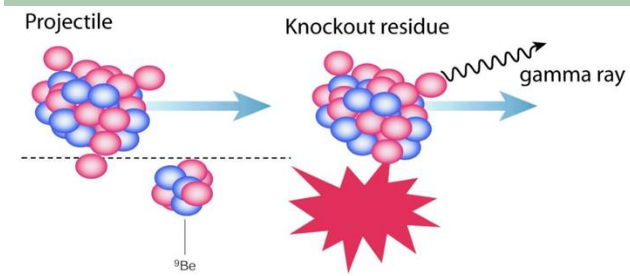
(σ~mb)



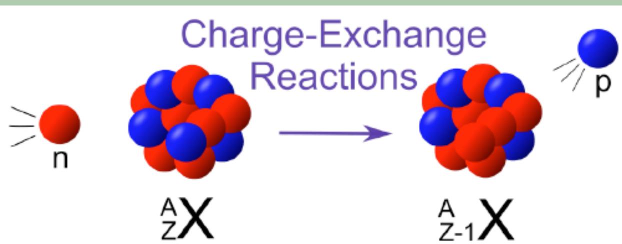


(σ~mb)

Probe of single-particle structure: knockout



Probe of electron capture: charge-exchange



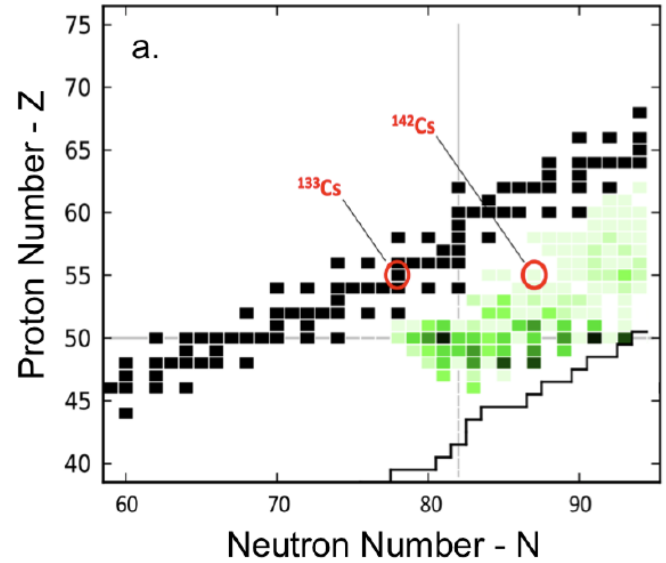
Reactions are the most diverse probes to extract astrophysics and structure information, especially for unstable isotopes…

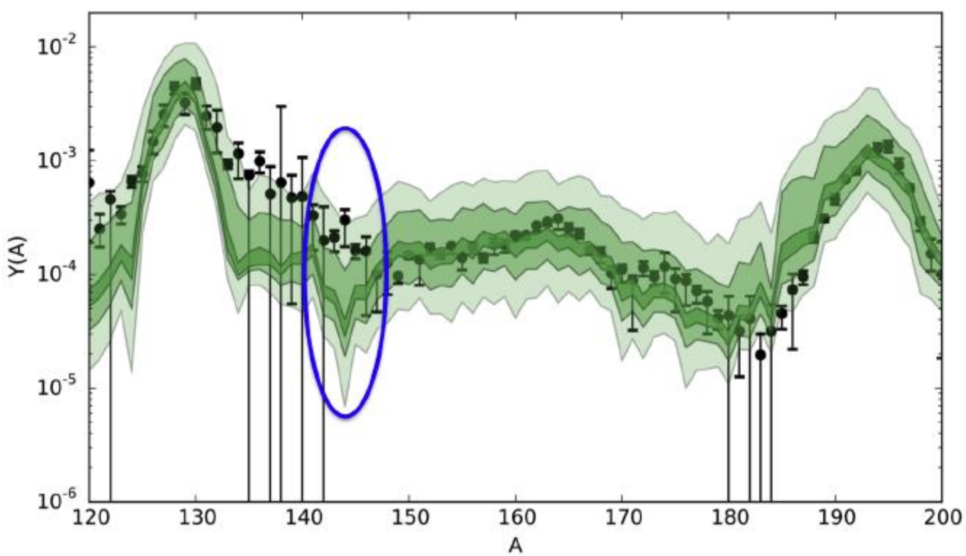
But reaction theory is key for translation!

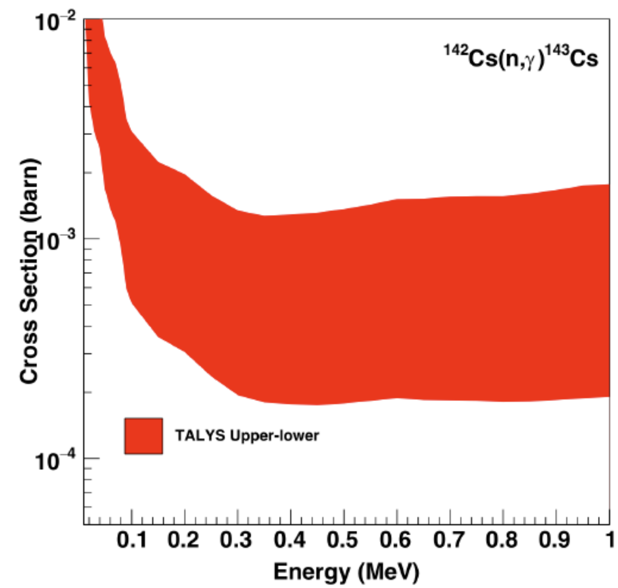
The $^{142}Cs(n,\gamma)$ case study

Constraining neutron capture rates for r-process nuclei in the A=140 region

Muecher, Spyrou, et al., Experiment approved for TRIUMF







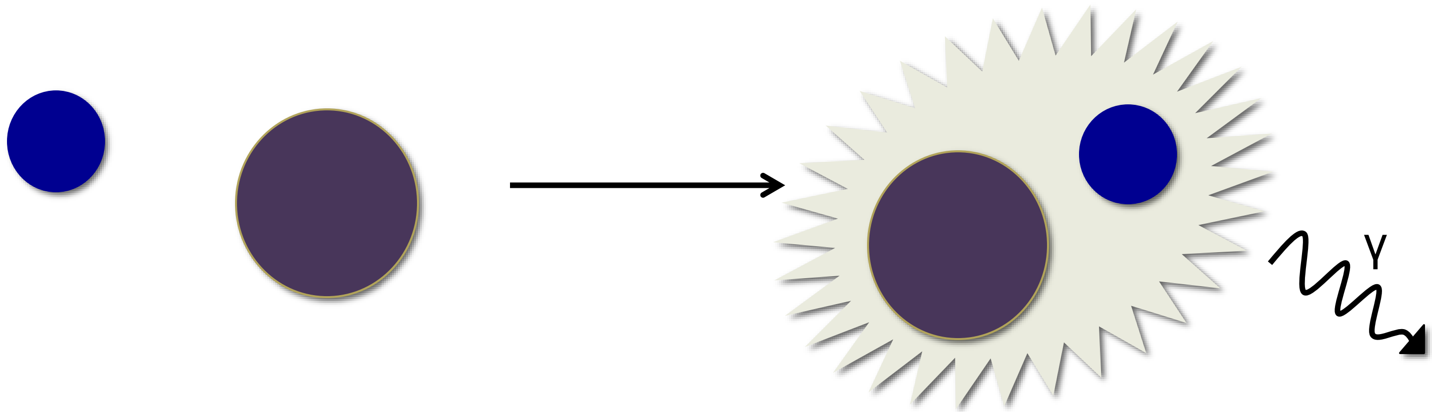
Impact of uncertainties in (n,γ) rates on r-process abundances

large uncertainties in cross sections for $^{142}Cs(n,\gamma)$

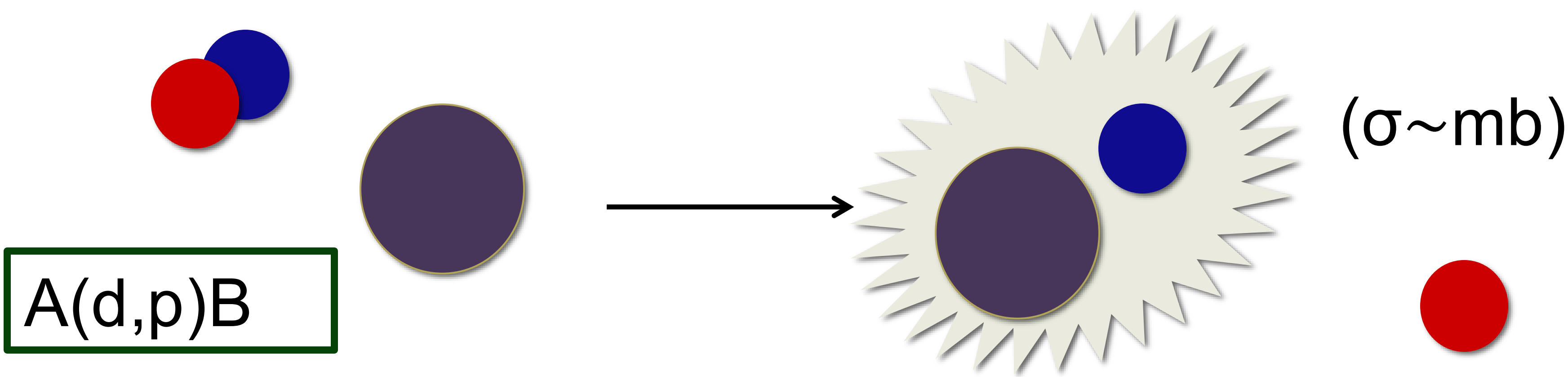
Liddick et al., Phys. Rev.Lett., 116:242502, 2016

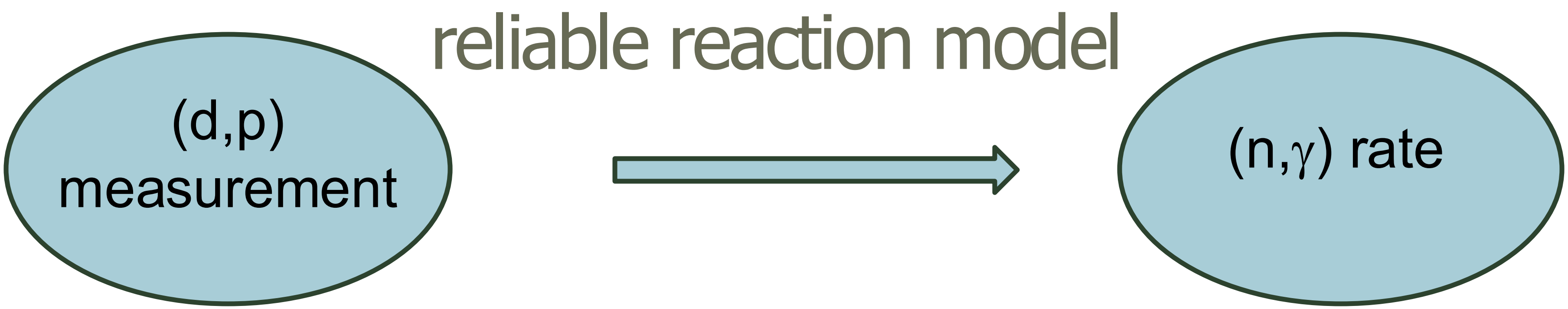
r-process: how do we measure neutron capture on unstable nuclei?

✧ (n,g) cross sections on unstable nuclei: **Currently Impossible!**



✧ (d,p) cross section offers an indirect measurement!





Compound nucleus (d,pγ) is determined through:

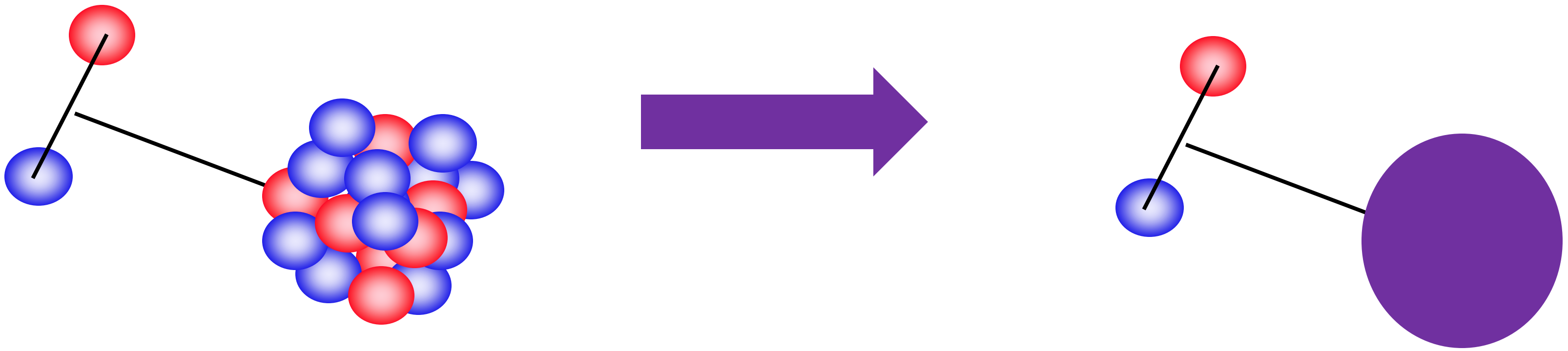
$$P_{\delta\chi}(E_{ex},\theta_p) = \sum_{J,\pi} F_{\delta}^{\mathrm{CN}}(E_{ex},J,\pi,\theta_p)\, G_{\chi}^{\mathrm{CN}}(E_{ex},J,\pi)$$

Entrance channel   compound decay

L-distributions in (d,p) are different from those in (n,γ)

reaction theory provides essential input

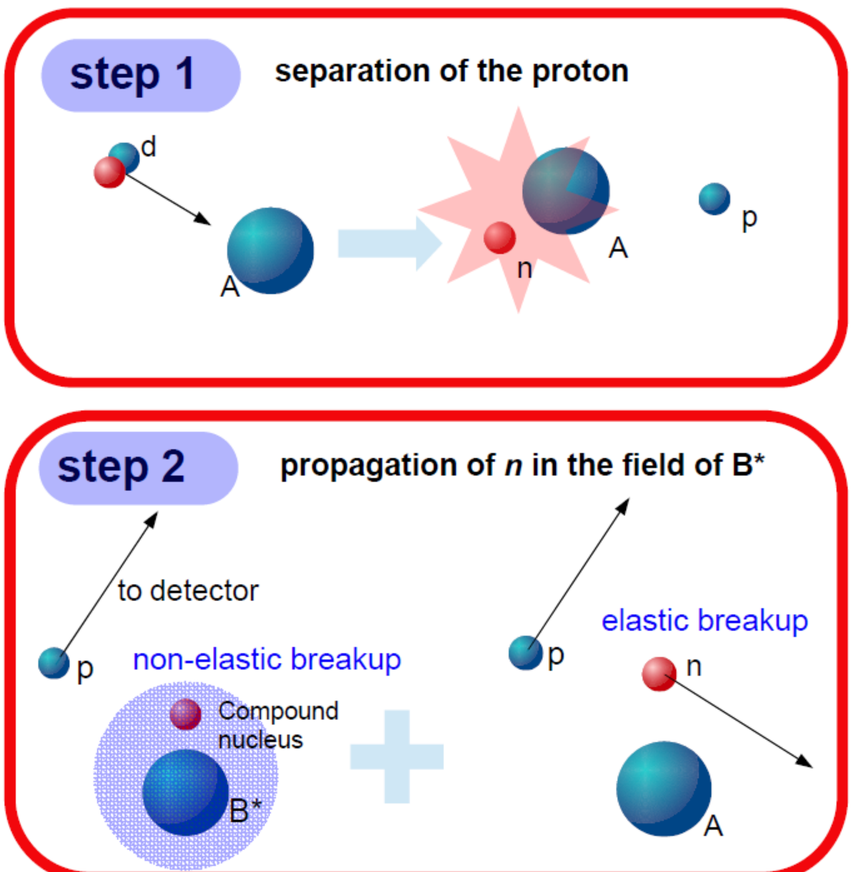
Reaction theory maps the many-body into a few-body problem



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

Theory for deuteron induced transfer: populating compound states in continuum

assume a two-step process



Source term generates flux from breakup

$$S = (\chi_p | (U_{\mathrm{Ap}} - U_{\mathrm{Ad}} + U_{\mathrm{An}}) | \chi_d \phi_d \rangle$$

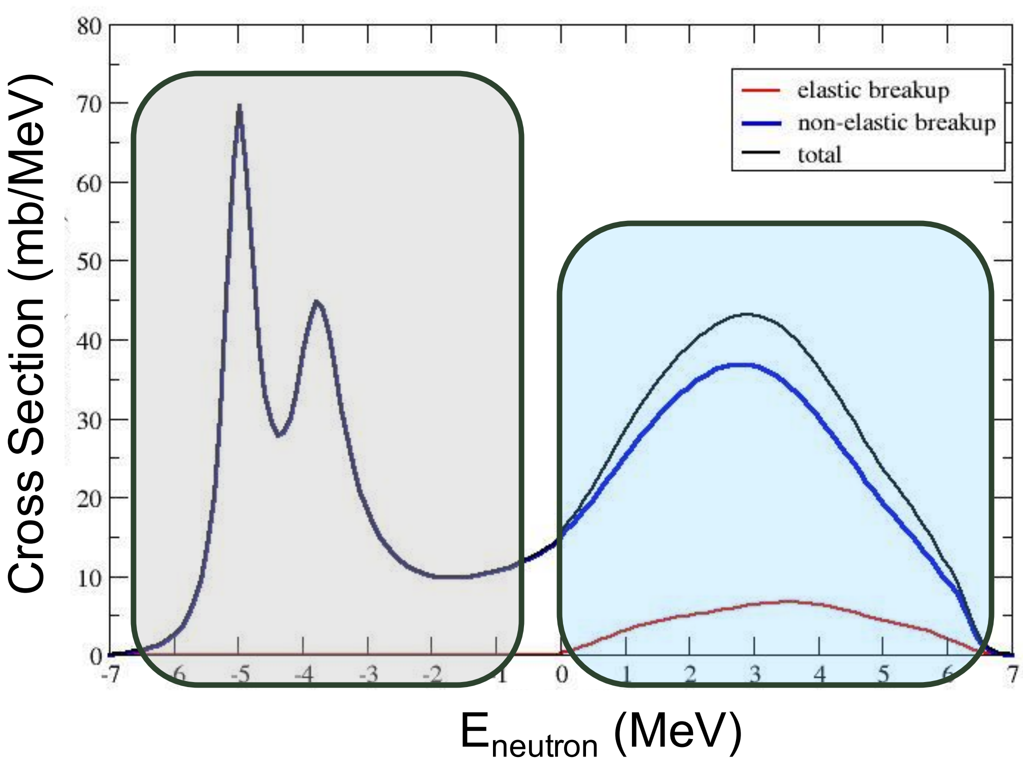
Neutron in the field of the target after breakup

$$\Phi_n = G_B^{\mathrm{opt}} S$$

Potel, Nunes, Thompson, PRC92 (2015) 034611

Predictions for ^{142}Cs(d,p) ^{143}Cs* at 12 MeV

Comparing elastic and non-elastic breakup



transfer to bound states

transfer to neutron unbound states

Input Optical Potentials:
d-Cs: Lohr-Haeberly
p-Cs: KD
n-Cs E>0: KD
N-Cs E<0: Re(KD)

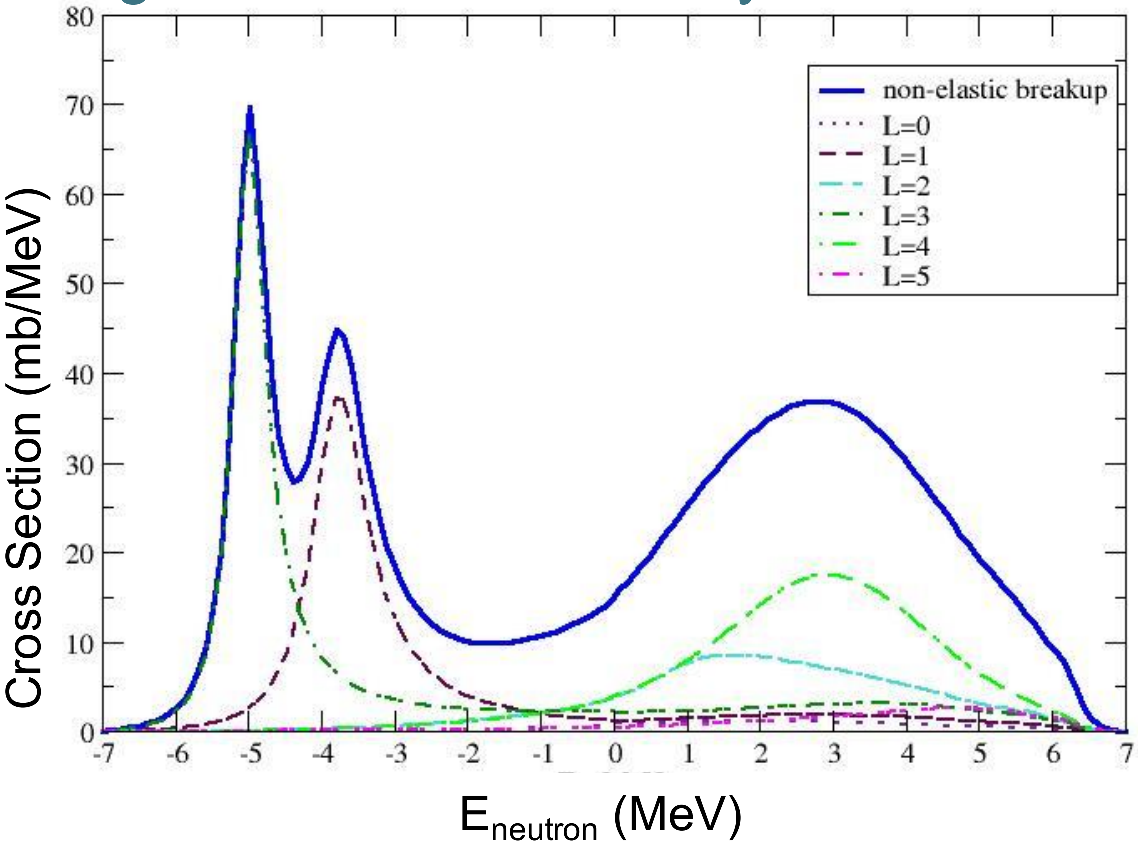
elastic breakup not negligible

non-elastic breakup corresponds to neutron capture part

Potel, greefeter code

Predictions for ^{142}Cs(d,p) ^{143}Cs* at 12 MeV

Angular momentum analysis



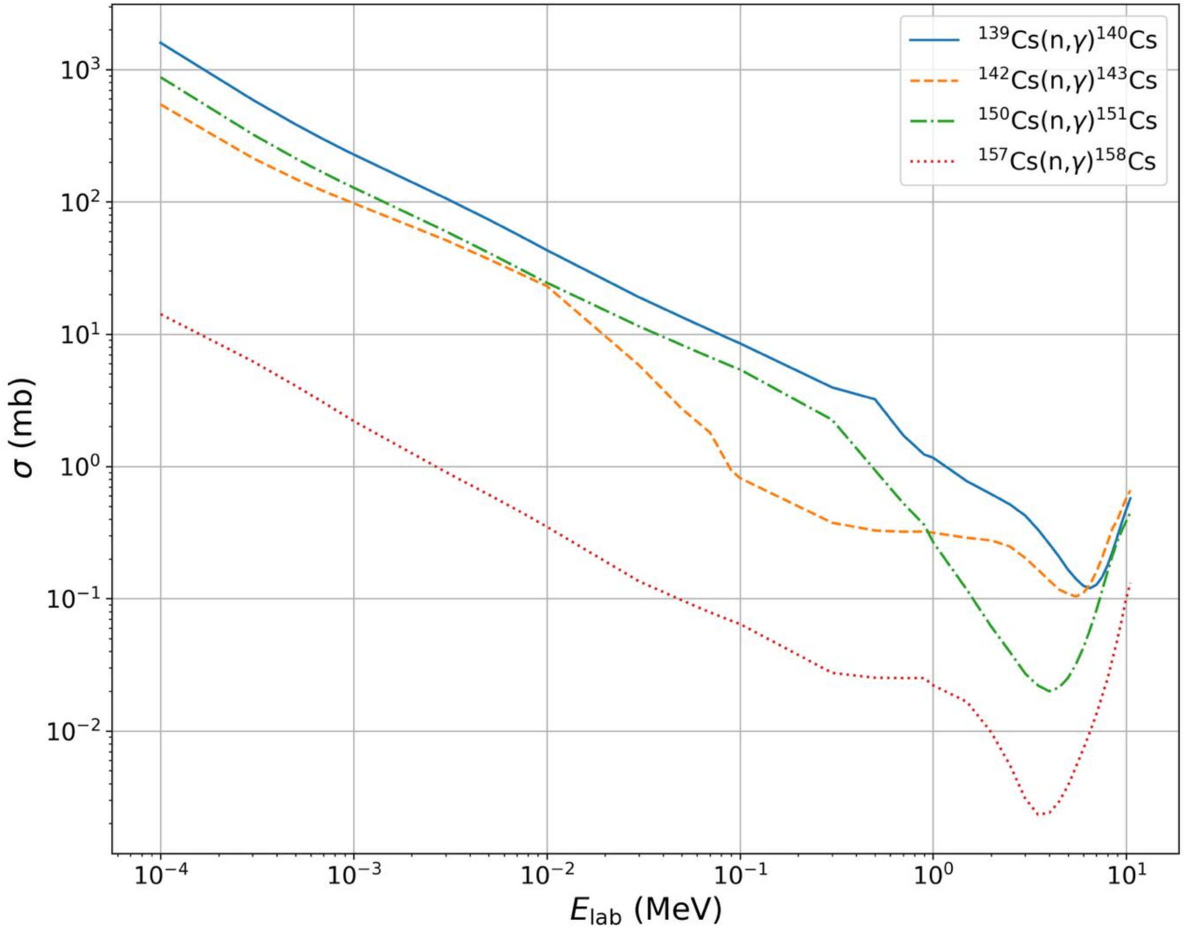
need L dependence to integrate the capture component with compound de-excitation

Potel, greefeter code

What do the Cs(n,γ) cross sections look like?

no Cs(n,γ) data for A>137
A=157 is the predicted dripline!

Cs(n,γ) cross sections are large, well beyond A=137



Lifetimes:
^{139}Cs 9 min
^{142}Cs 1.7 s
^{150}Cs 81 ms

Samuel Sullivan, TALYS

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- Uncertainties
  - Bayesian optical model calibration
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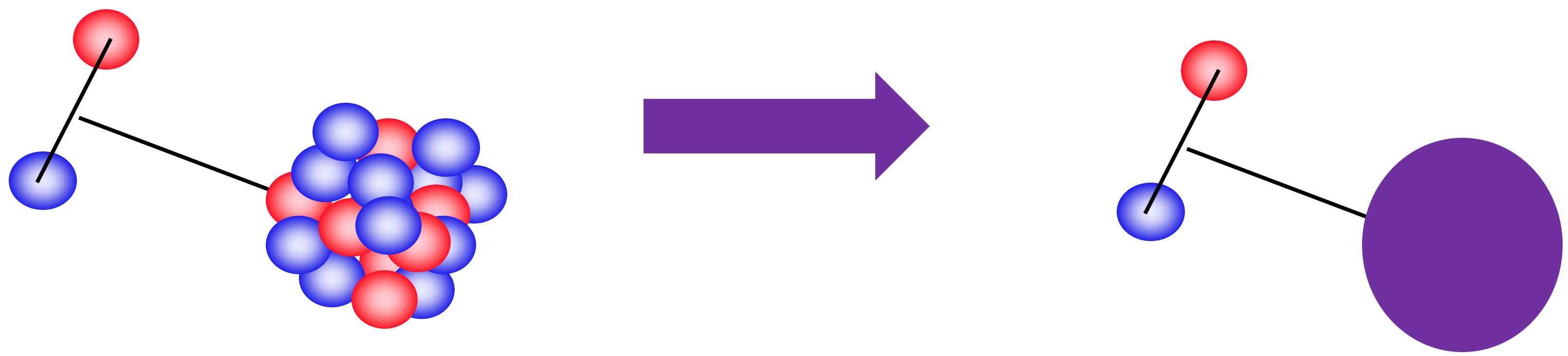
Reaction theory maps the many-body into a few-body problem

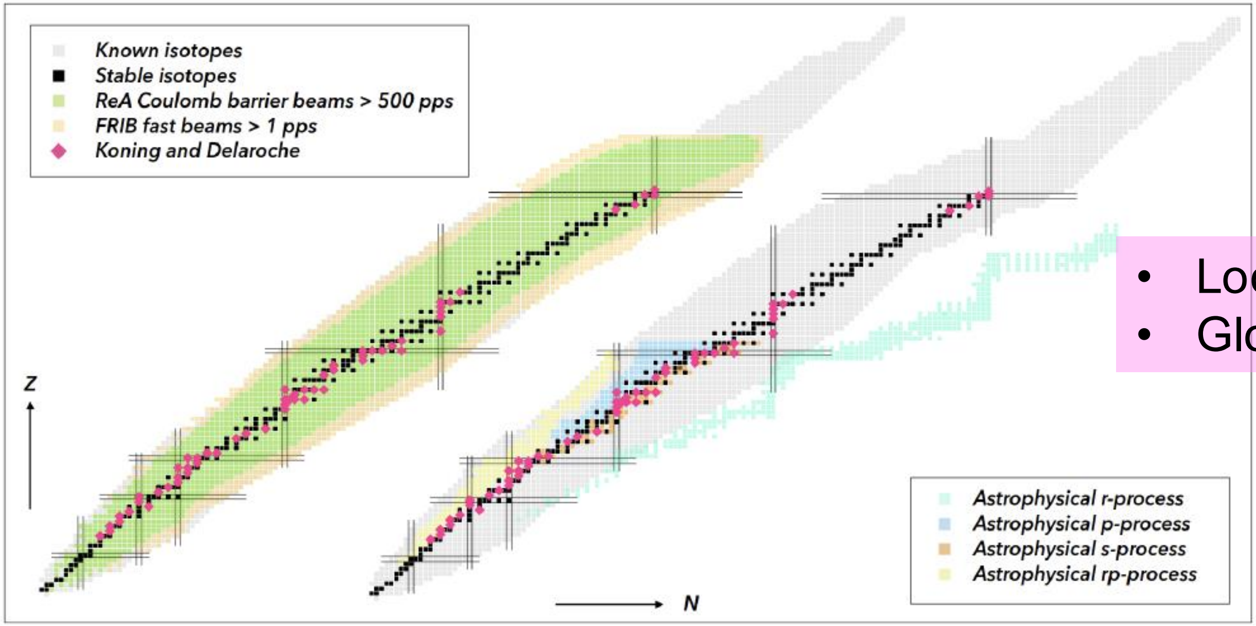


- ❑ isolating the important degrees of freedom in a reaction
- ❑ solve the **few-body dynamics** exactly
- ❑ effective nucleon-nucleus interactions (or nucleus-nucleus) usually referred to as **optical potentials**

main cause of uncertainty

Optical potentials are pervasive in reaction models

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



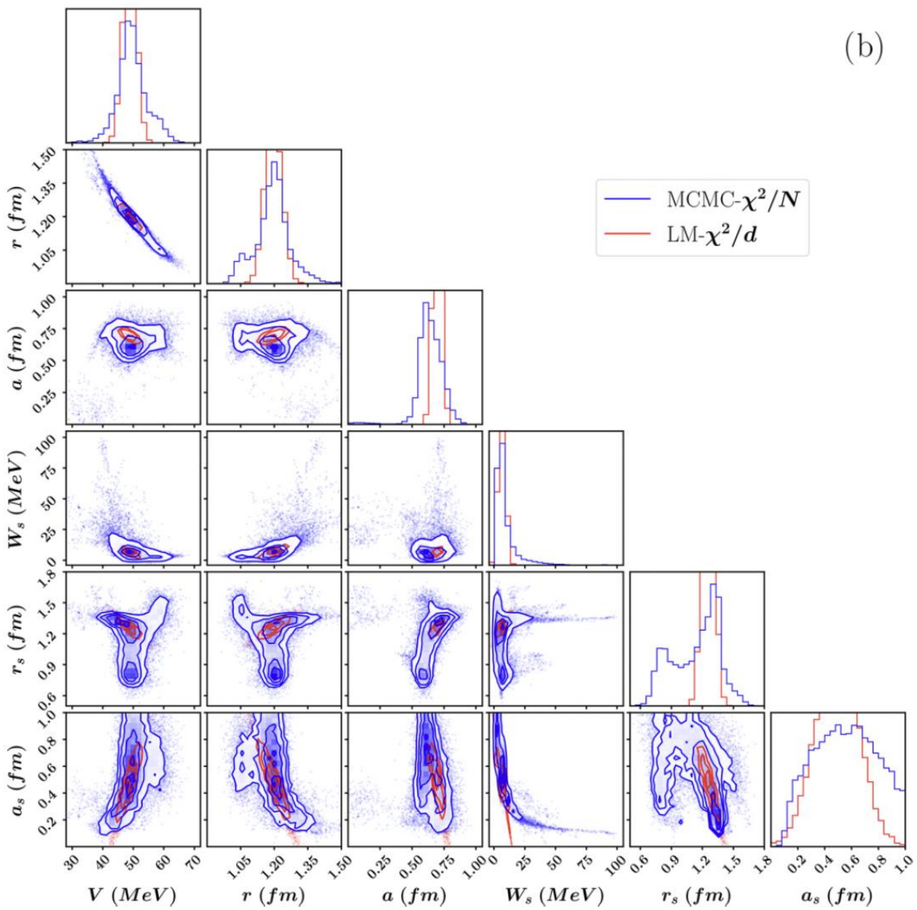
- Local calibrations
- Global calibrations

Reaction observables are very sensitive to details of the optical potential.
For r-process, these are needed away from stability

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

Bayesian approach versus normal distributions?

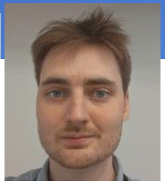
When doing Uncertainty Quantification: statistical model + physics model + evidence



The more complex the model and the parameter space, the less likely that the normal distribution assumption is valid

Parameters are correlated
UQ is not determined by varying them independently

Pruitt, Nunes, et al., PRC 110 (2024) 064606

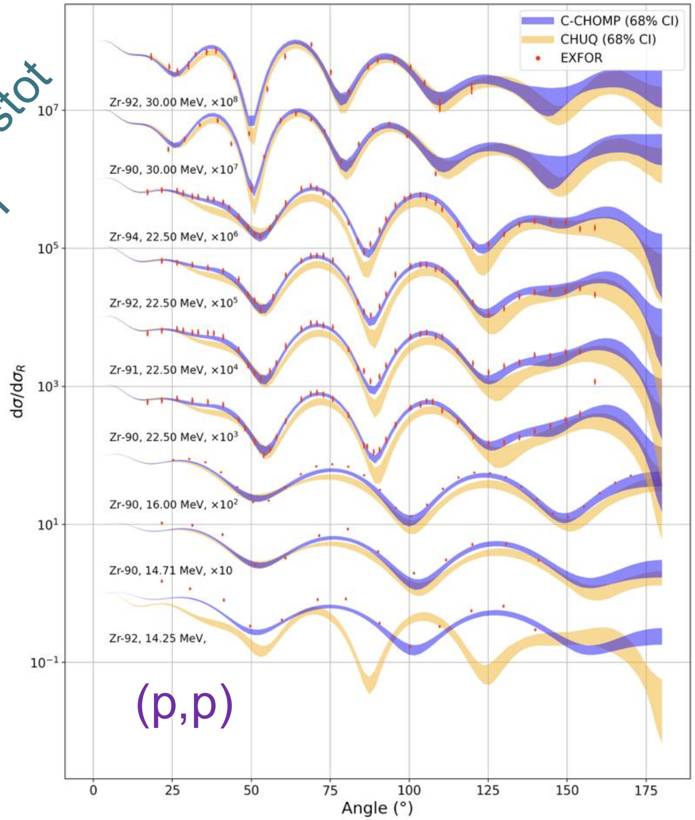


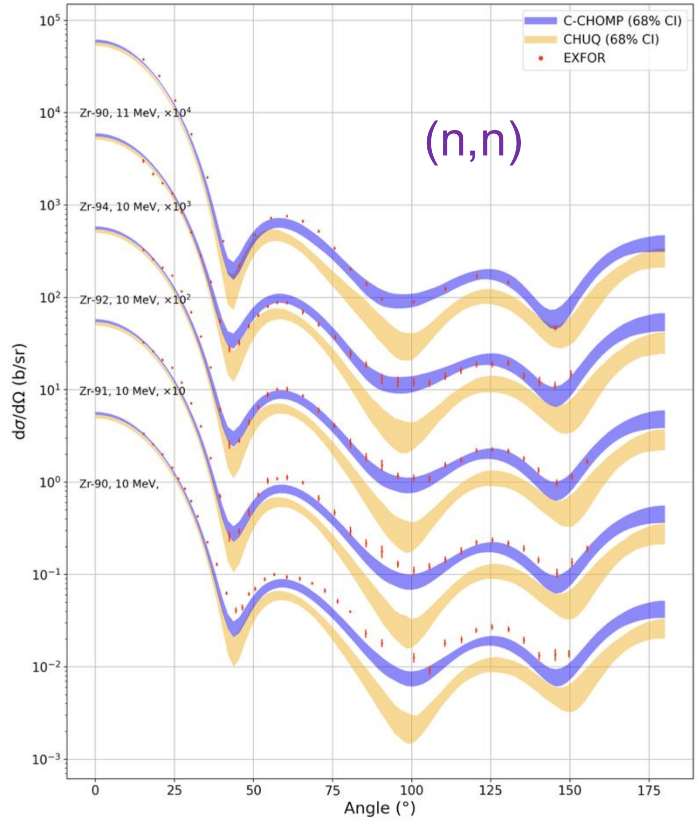
Local calibrations of the optical potential

Bayesian Analysis of optical potential – isotopic chain approach $^{90\text{-}94}$Zr

Exploring the energy dependence using data from 10-30 MeV

Prior – chapel hill (CH)
Evidence – elastic dxs, Ay, xstot
Physical model – local CH



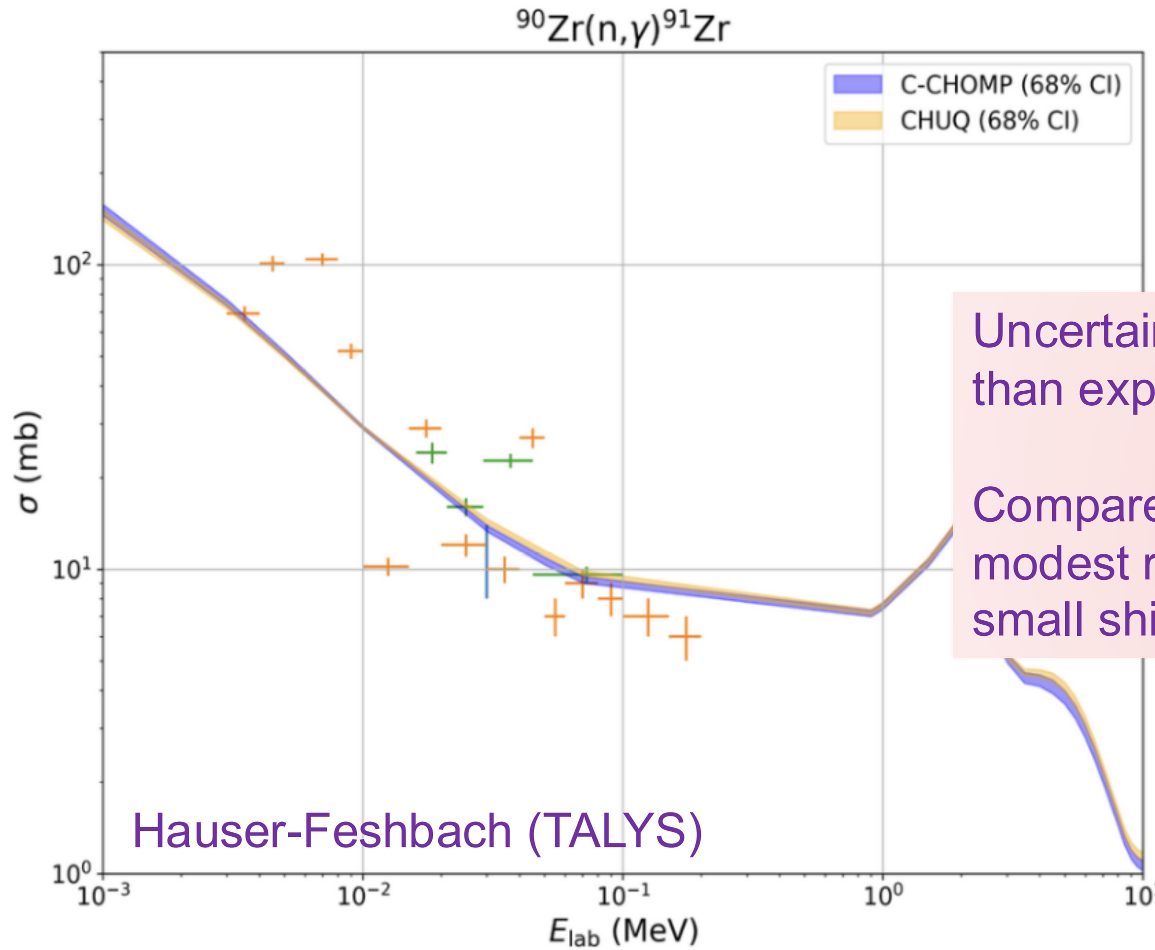


CHOMP potential has Lane form (appropriate isospin dependence) critical for extrapolating away from stability

Sullivan, Beyer, Nunes, in preparation

Uncertainties in neutron capture for Zr

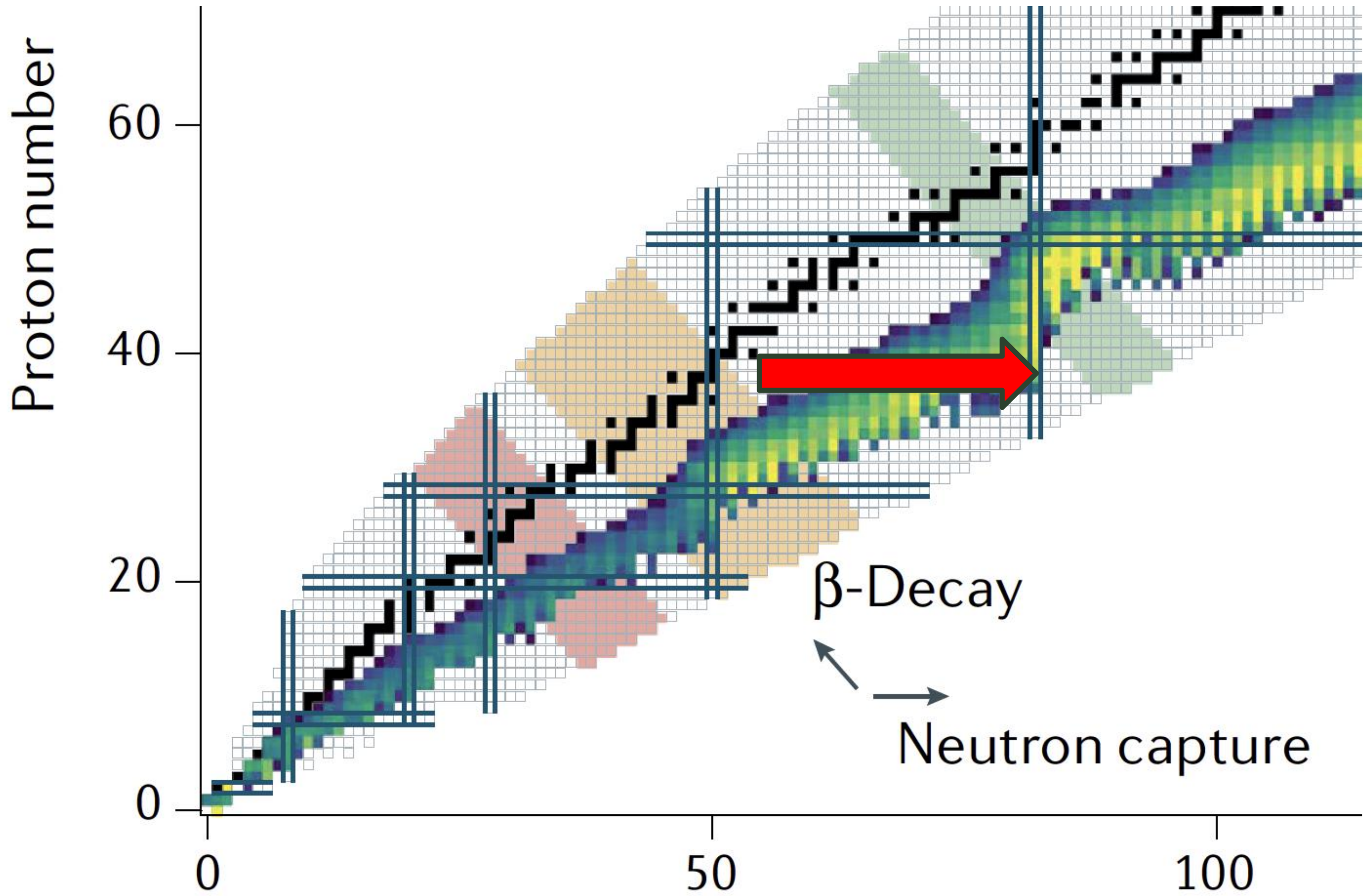
Bayesian Analysis of optical potential – isotopic chain approach $^{90\text{-}94}$Zr



Uncertainties in predictions smaller than experimental error reported

Compared to CHUQ:
modest reduction of uncertainties
small shift to lower (n,γ) xs

Sullivan, Beyer, Nunes, in preparation



Extrapolate away from stability?

Seigel, Nature Phys. May 2022

East Lansing Model (ELM)
Global Lane-consistent optical potential including (p,n)

- Incorporated into the optical potential by Lane[4]

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

- Previous Bayesian analysis of global optical potential [5]: scattering on stable isotopes poorly constrains U_1
- hence, large uncertainties for (p,n)[6] and for reactions on highly asymmetric isotopes [7]

Goal: construct a Lane-consistent, uncertainty-quantified global optical potential including $(p,n)_{IAS}$ as a constraint

Beyer, Nunes, in preparation

Bayesian Calibration of ELM

Evidence: data curation

- balance model fidelity: for now, even-even 0^+ isotopes only
- $40 \leq A \leq 208$
- $10\ \mathrm{MeV} < \mathrm{E_{lab}} < 200\ \mathrm{MeV}$
- $d\sigma/d\Omega$ and A_y from elastic (p,p), (n,n)
- $d\sigma/d\Omega$ with clean $\Delta J^\pi = 0^+$ from $(p,n)_{IAS}$
- over 100 EXFOR entries

github.com/beykyle/exfor_tools

Statistical model: likelihood

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

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

$$\Sigma_{ij}(\alpha) = \delta_{ij}\left(\sigma^2_{exp,i} + \sigma^2_{UFU,i}\right)$$

- $\mathbf{\Sigma}$ approximated as diagonal
- unaccounted-for-uncertainty is a free parameter

$$\sigma_{UFU,i} \equiv \frac{1}{2}\epsilon(y_{\mathcal{M}}(x_i, \alpha) + y_i)$$

- no re-scaling of covariance or likelihood!

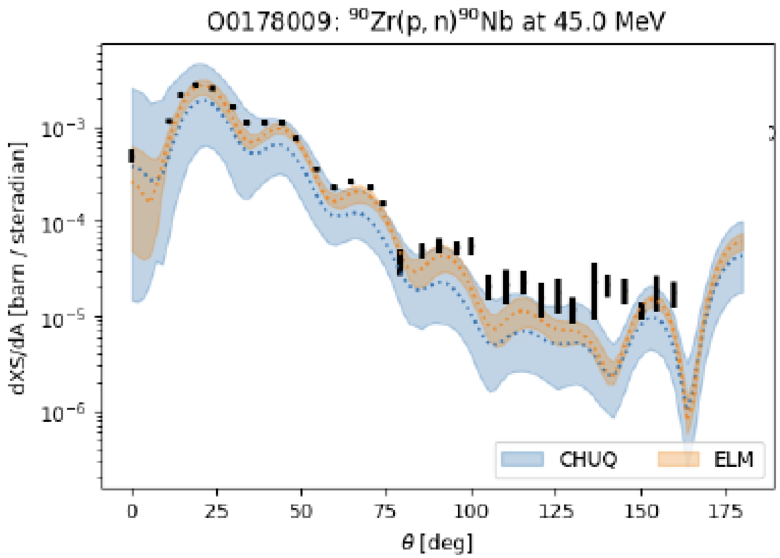
github.com/beykyle/rxmc

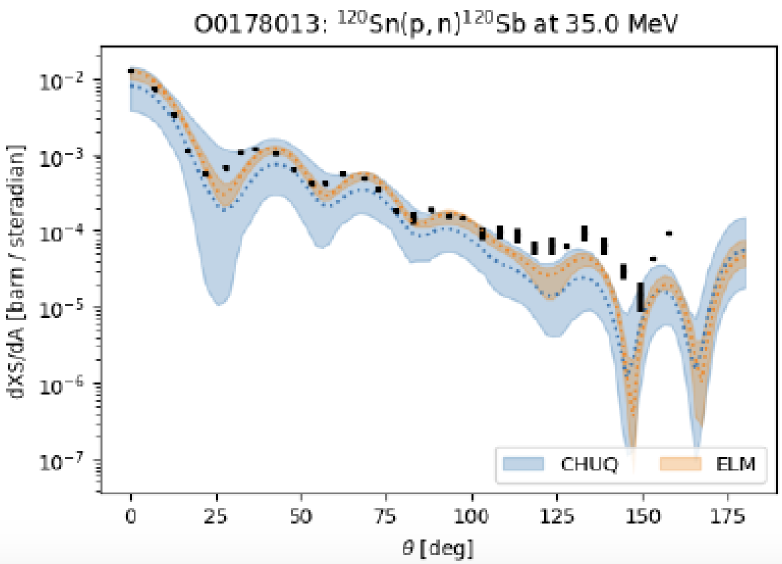
Physical model:

form inspired by Chapel Hill but separate geometries for isoscalar and isovector

Beyer, Nunes, in preparation

ELM results: credible intervals for stable isotopes





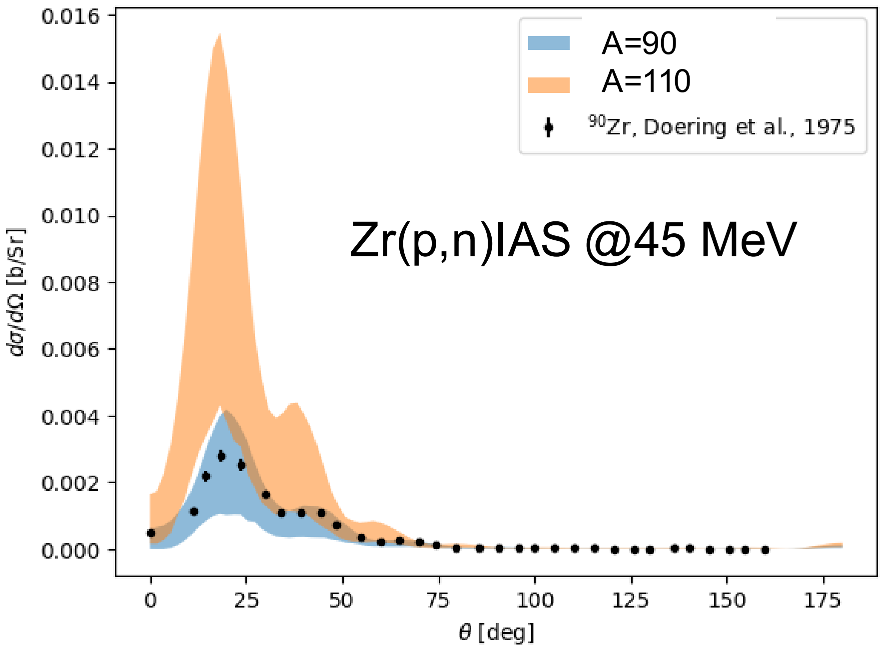
Inner 90% credible intervals of ELM and CHUQ[a]

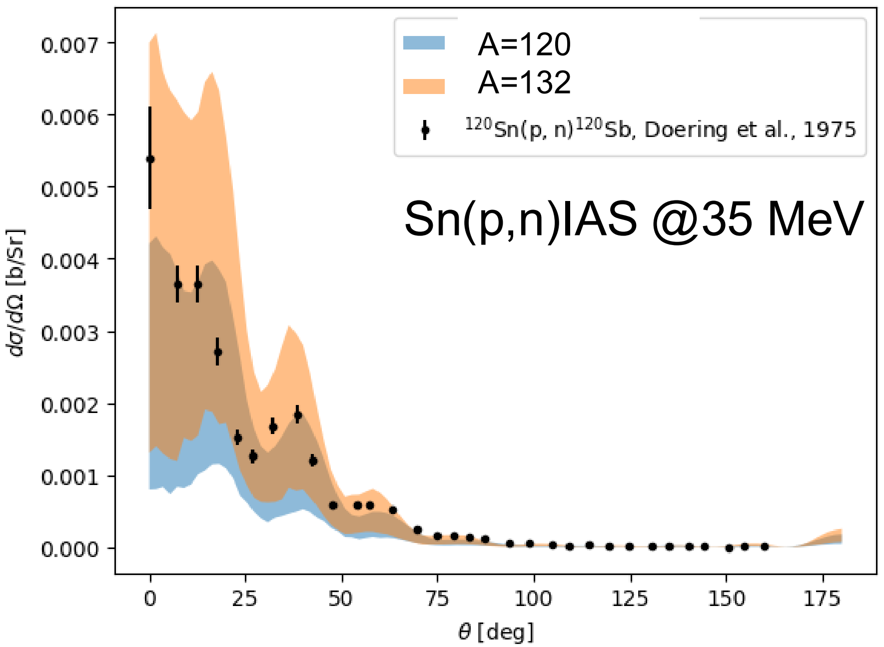
- Good simultaneous description of elastic and $(p, n)_{IAS}$
- isovector potential extends ~ 0.9 fm further than isoscalar, with little A-dependence
- isovector diffuseness stiffer(smaller) than isoscalar
- consistent with interpretation in Danielewicz[b]

[a]Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602
[b]Danielewicz et al. 2017, *Nuclear Physics A* 958, pp. 147–186

Beyer, Nunes, in preparation

ELM: extrapolation to neutron-rich isotopes





Cross section uncertainties dominated by model uncertainties:

grows as (N-Z)/A

Beyer, Nunes, in preparation

Future Opportunities

East Lansing Model:

- need to validate for rare isotopes and connect with EOS
- improvements: dispersion relation to connect bound states and continuum states
- integrate with existing codes like TALYS so it becomes widely available

ELM-UQ propagation to (n,g) and to (d,p) away from stability

Impact in r-process nucleosynthesis?

Future Opportunities

Hauser Feshbach is the working horse:

- couplings between channels introduce corrections
  (direct versus resonant versus compound)

- Often assumption of Gaussian Orthogonal Ensemble
  (very different from Nuclear Shell Model)

Testing these assumptions

Impact for neutron capture?

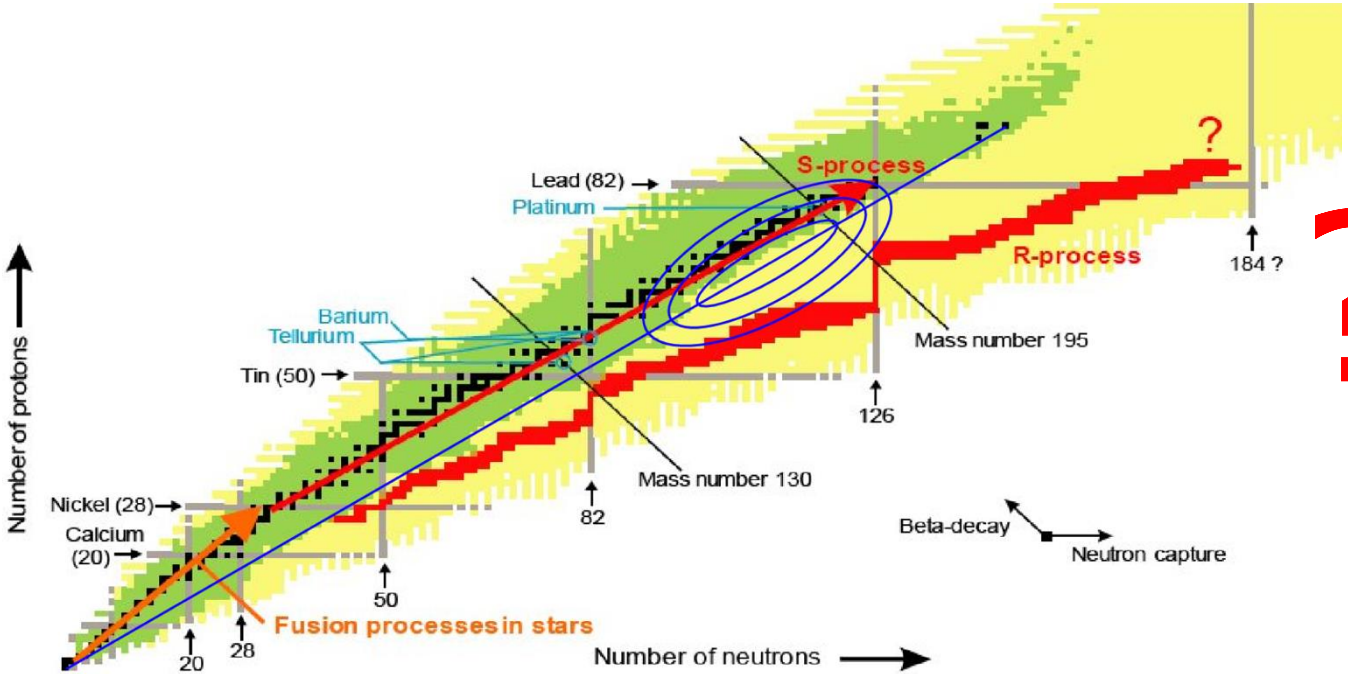
Abduhrraman, Nunes

Future opportunities

Heavy nuclei away from stability are important for r-process

How can we measure (n,γ) on these superheavy rare isotopes?

How to produce them in the laboratory?



??

Paths to superheavy nuclei, Godbey, Nunes et al., JPG 2025

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

The few-body reactions group at FRIB


Filomena Nunes


Chloë Hebborn


Kyle Beyer


Patrick McGlynn

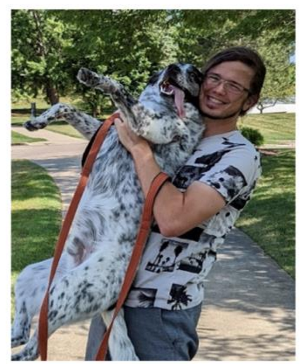

Ibrahim Abdurrahman


Cate Beckman


Manuel Catacora Rios


Andy Smith


Daniel Shiu

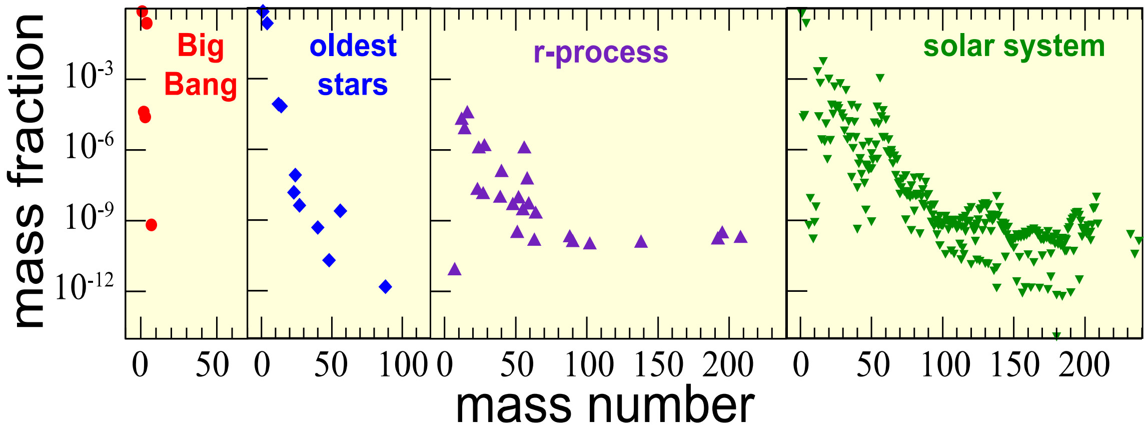

Pablo Giuliani

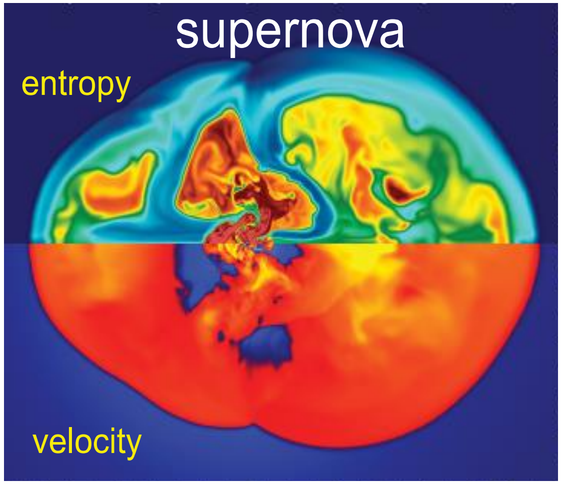

Grigor Sargsyan

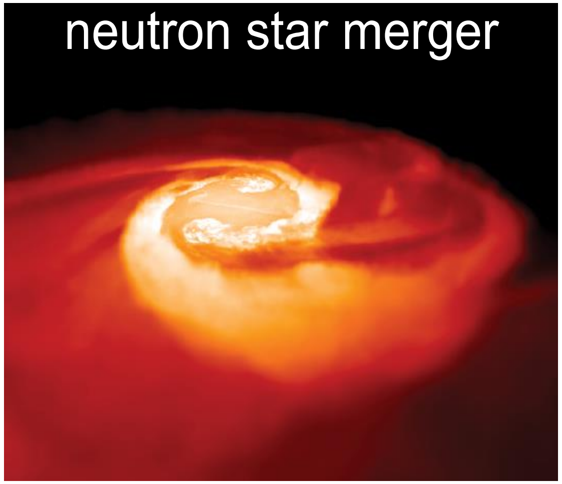

Zetian Ma

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!

Extra slides: ELM physical model

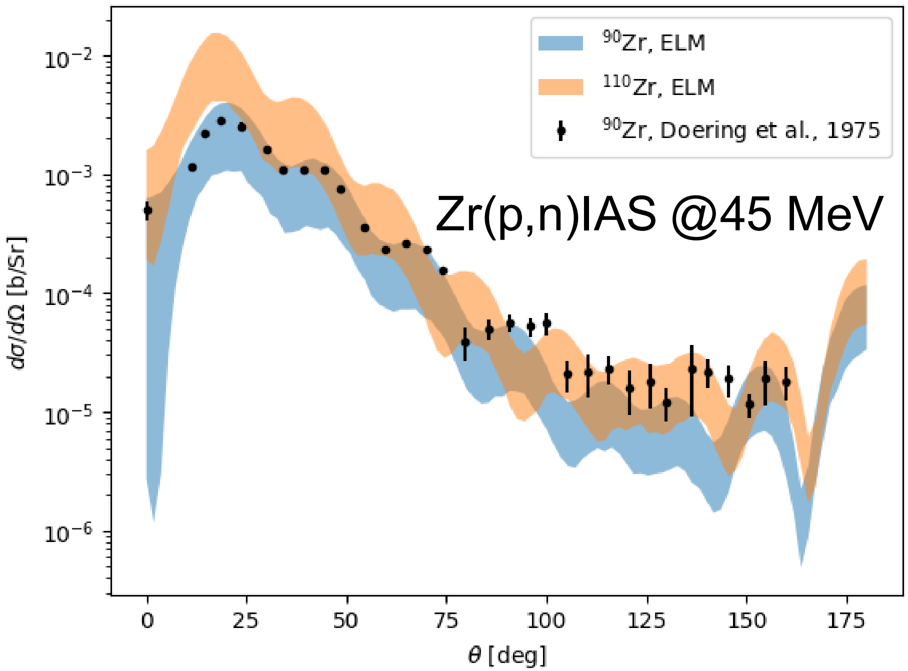
$$U(r,E,A,Z) = U_0(r,E,A) \pm \frac{N-Z}{N+Z} U_1(r,E,A) + V_C$$

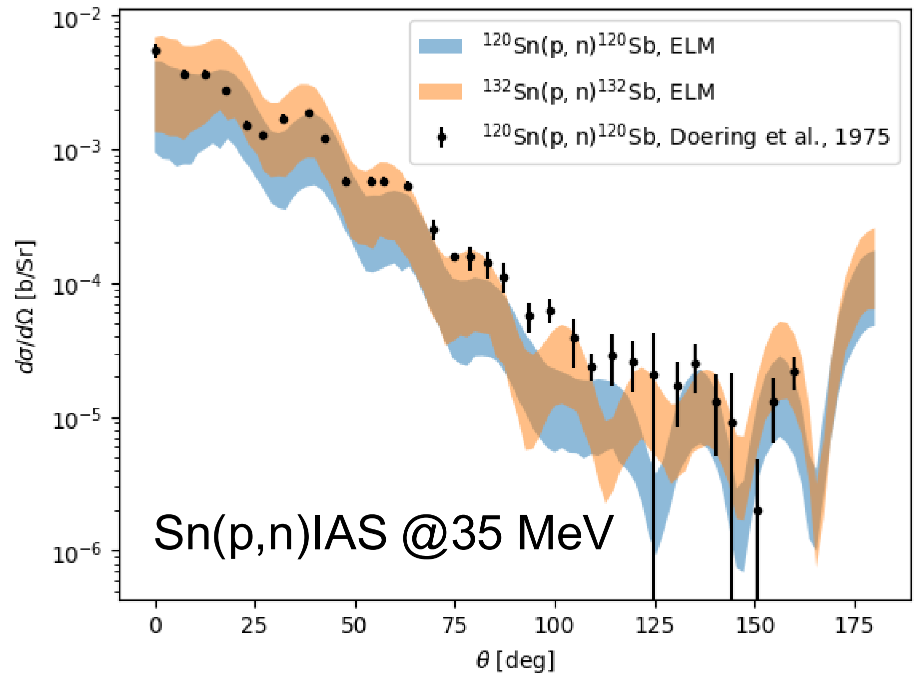
$$\begin{aligned} U_0(r,E,A) &= V_0(E) f((r-R_0(A))/a_0) + iW_0(E) f((r-R_w(A))/a_w) \\ &\quad - 4ia_w W_{s,0}(E) \frac{d}{dr} f((r-R_w(A))/a_w) + 2\,(\boldsymbol{\sigma}\cdot\boldsymbol{\ell})\; V_{so} \frac{1}{r}\frac{d}{dr} f((r-R_{so}(A))/a_{so}) \\ U_1(r,E,A) &= V_1(E) f((r-R_1(A))/a_1) - 4ia_w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

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

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

ELM: extrapolation to neutron-rich isotopes



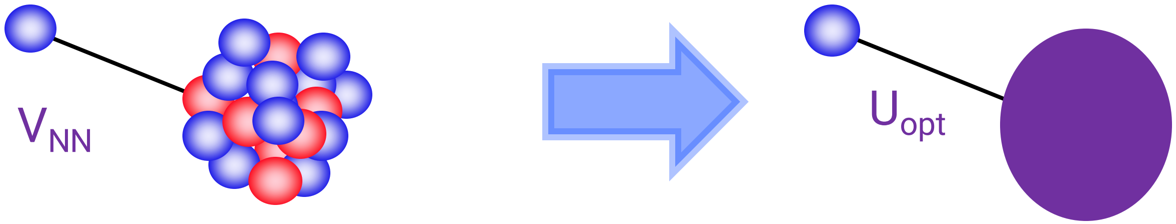


Uncertainties dominated by model uncertainties

defined as percent of cross section: grows as (N-Z)/A

Beyer, Nunes, in preparation

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:

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

$U_{opt} = V(R) + iW(R)$

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

Bayesian statistics

Thomas Bayes (1701–1761)

Bayes' Theorem

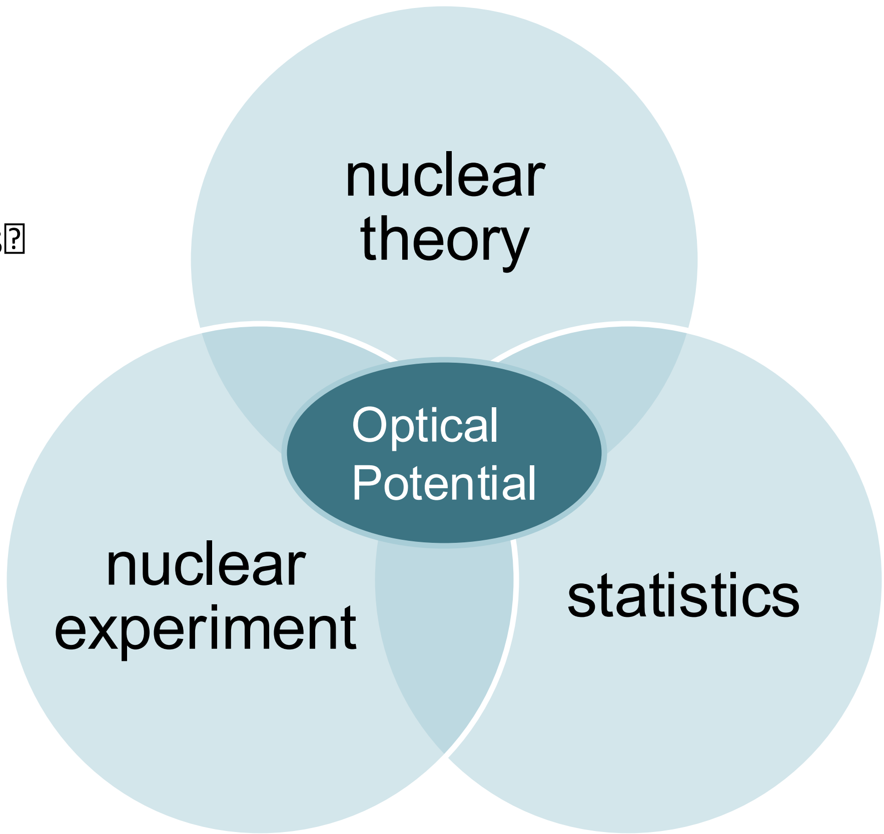
$$\boxed{P(\mathcal{H}|\mathcal{D})} = \frac{\boxed{P(\mathcal{D}|\mathcal{H})}\boxed{P(\mathcal{H})}}{\boxed{P(\mathcal{D})}}$$

Posterior – probability that the model/parameters are correct after seeing the data

Prior – what is known about the model/parameters before seeing the data

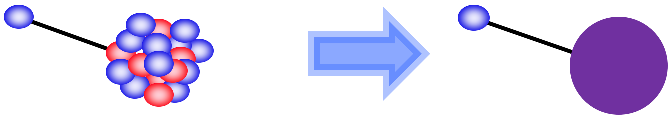
Likelihood – how well the model/parameters describe the data $p(D|H) = e^{-\chi^2/2}$

Evidence – marginal distribution of the data given the likelihood and the prior



Amy Lovell (LANL)

How to quantify uncertainties in reaction theory?

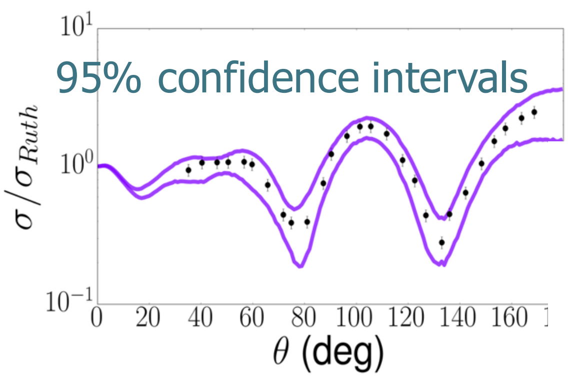


We develop a hypothesis (model) with a set of parameters (priors)

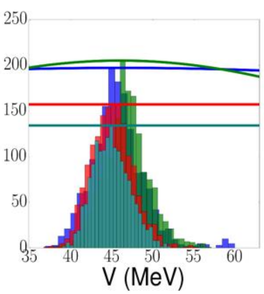
optical model
$[T+U(R)-E]\psi=0$

We confront it with reality (data) typically elastic scattering angular distributions (likelihood)

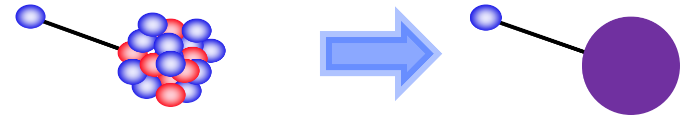
Use Bayes' Theorem + Markov Chain Monte Carlo with Metropolis to sample parameter space



Constraints on the model



Setting up the UQ part



Priors p(H): Gaussians with mean at the BG global parameters and wide width

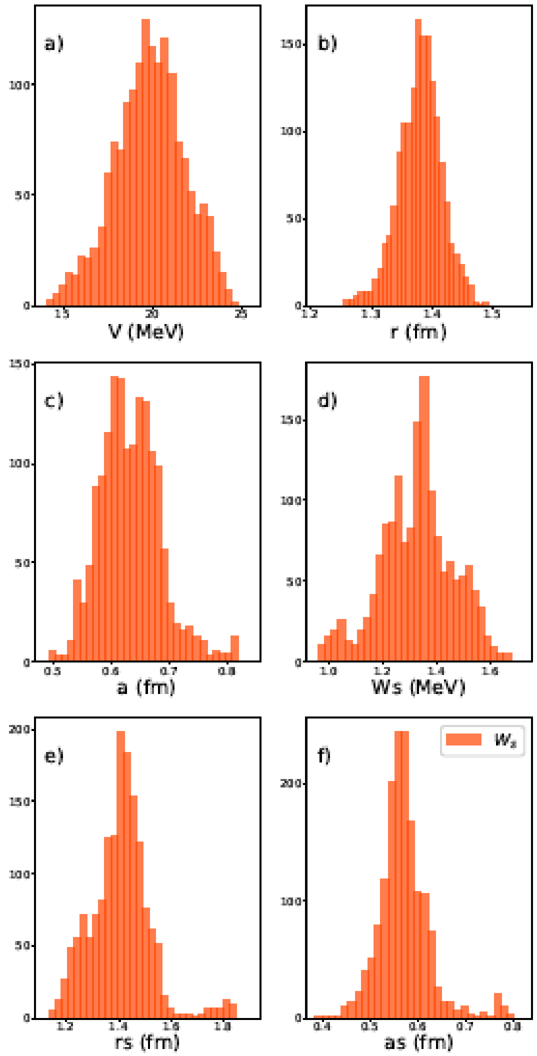
Data (D): real data or mock data generated from KD global parameters with 10% error

Likelihood p(D,H): assumption that data points are independent and errors are normally distributed

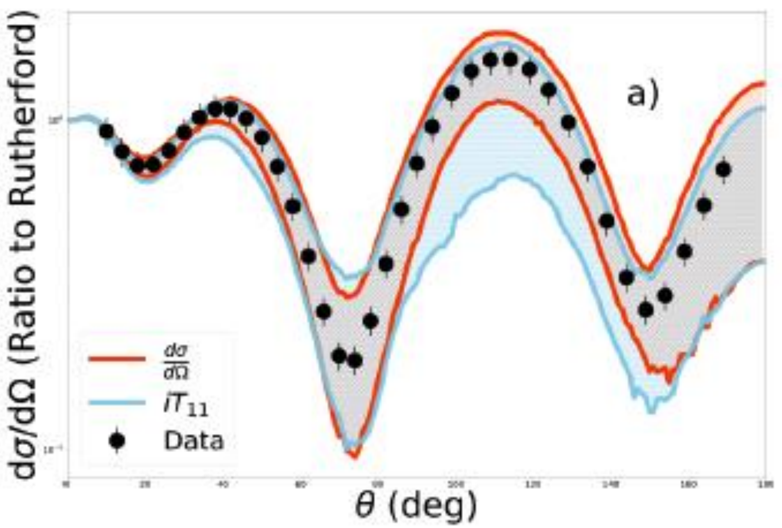
$$p(\mathbf{D}|\theta, f, \{\sigma_i^2\}) \propto \exp\left(\frac{-1}{2n} \sum_{i=1}^{n} \frac{\left(y_i - f(x_i, \theta)\right)^2}{\sigma_i^2} \right)$$

θ: parameters
σ: independent errors
x: angles
y: experimental cross section
f: model prediction for cross section

Bayesian: parameter posterior distributions

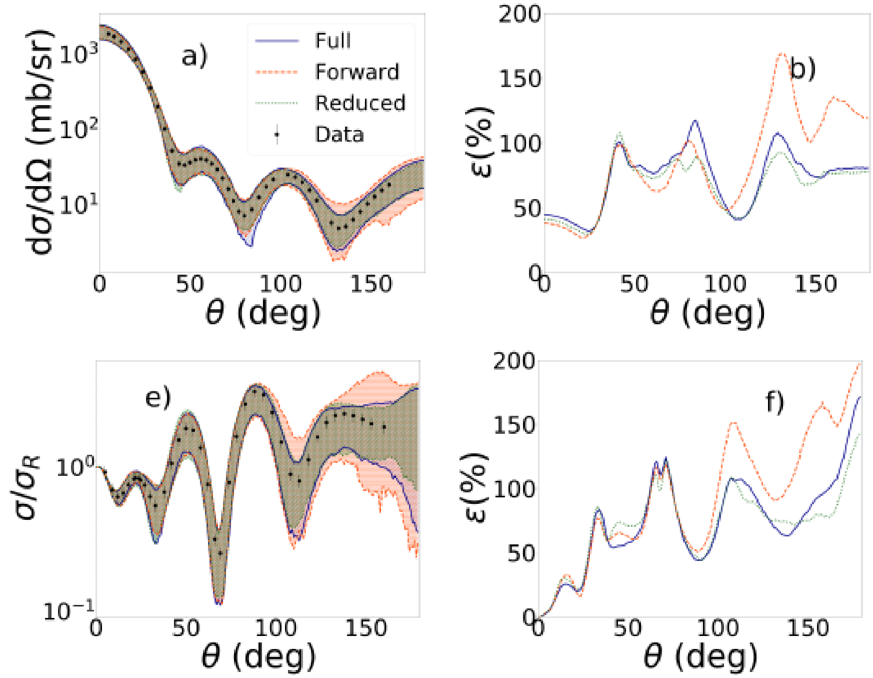


Create 95% confidence intervals for observable



Manuel Catacora-Rios

What angular information needed?



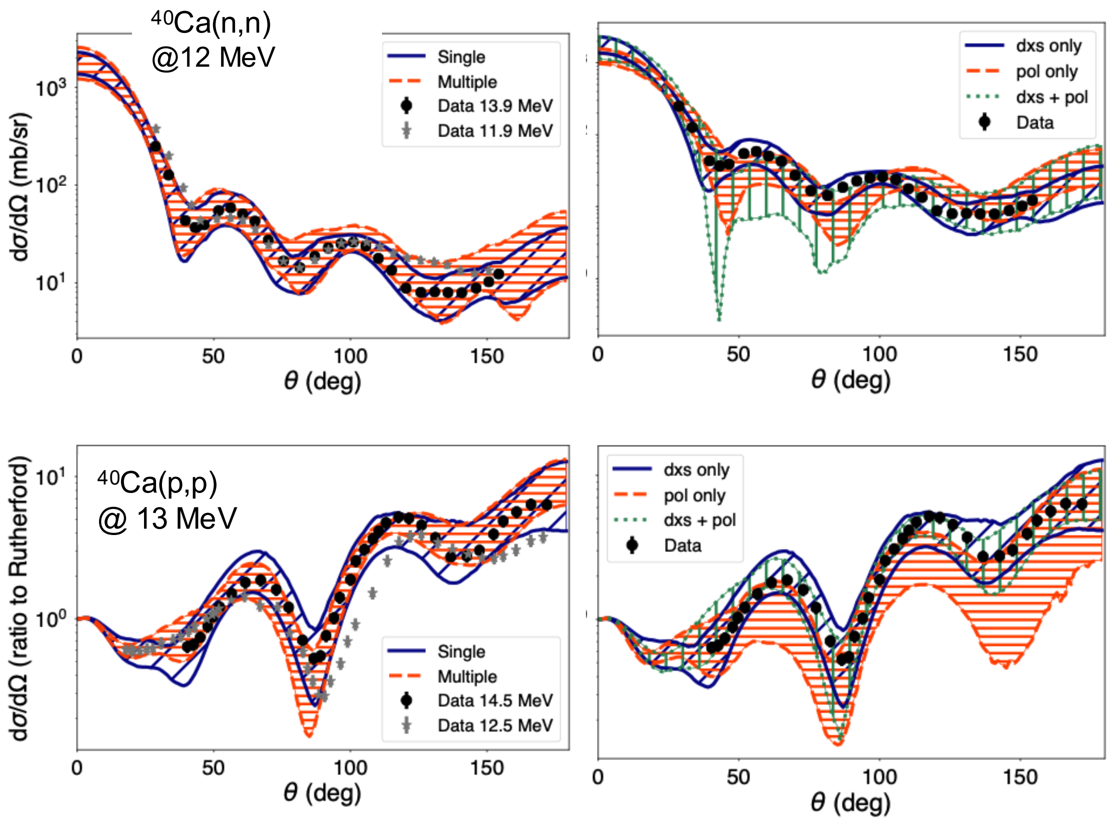
^{48}Ca(n,n)^{48}Ca at 12 MeV

^{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% confidence intervals

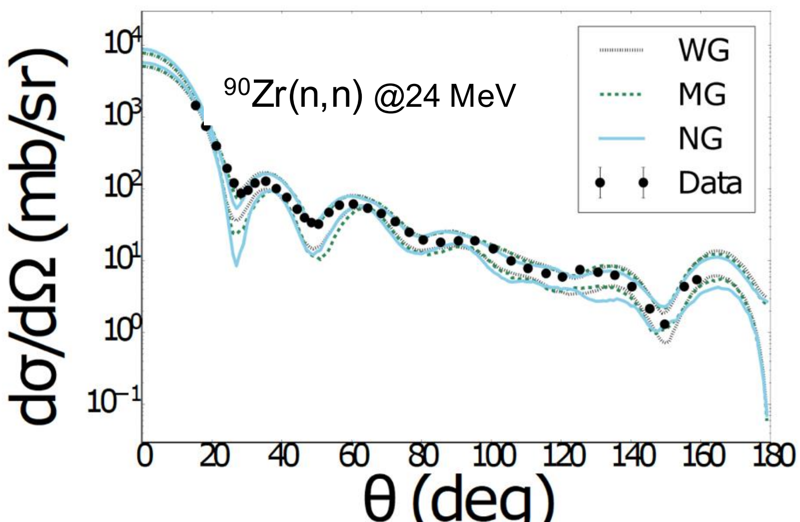


King, Lovell, Neufcourt, Nunes PRL (2019)
Catacora-Rios et al. PRC 100, 064615 (2019)
Lovell, Nunes, Catacora-Rios, King, JPG (2020)
Catacora-Rios et al. PRC 104, 064611 (2021)

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?



Lovell and Nunes PRC (2018)

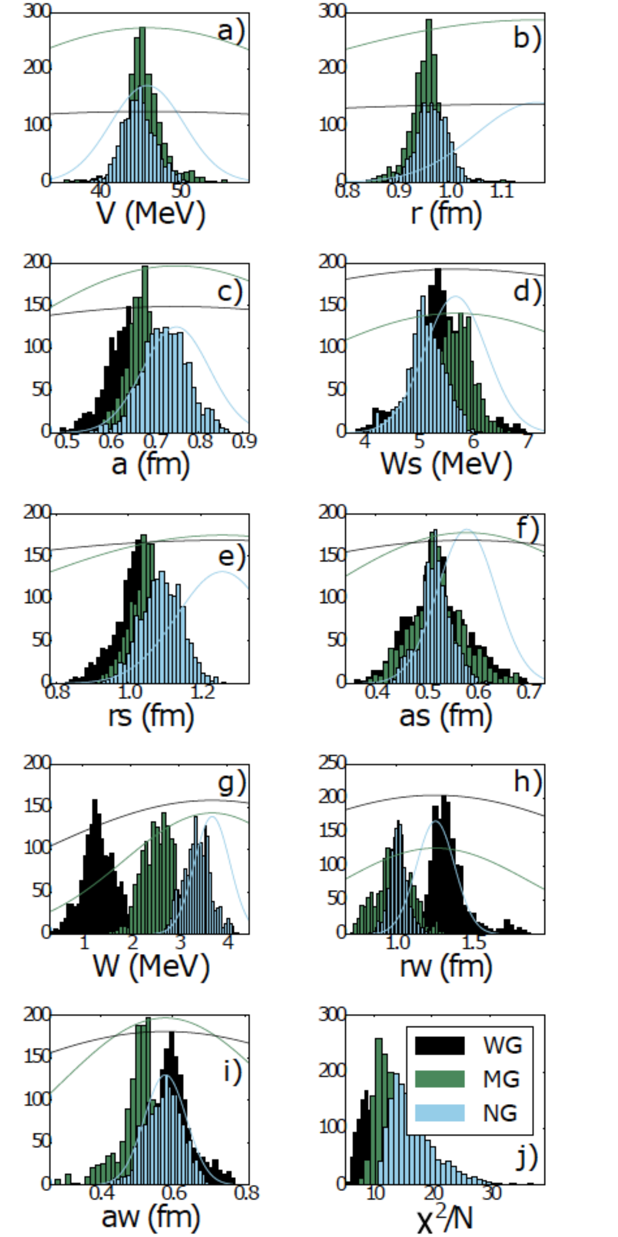


FIG. 2: (Color online) Comparison of the posterior distributions (histograms) resulting from various prior distributions (corresponding solid lines) for a wide Gaussian (WG), medium Gaussian (MG), and narrow Gaussian (NG) as defined in Table II for ^{90}Zr(n,n)^{90}Zr at 24.0 MeV.

Which likelihood?

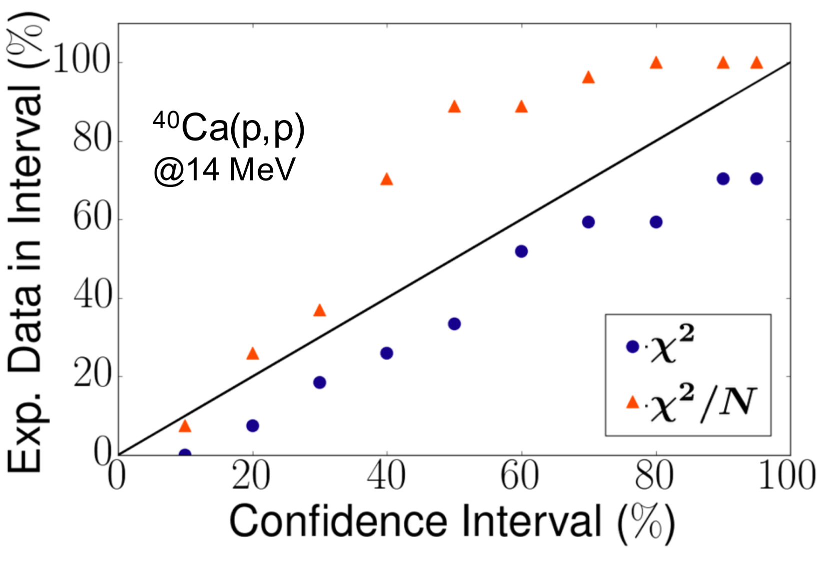
Complications:
- data correlations
- systematic errors on data underestimated
- model correlations
- model uncertainties

How to combine sets of angular distributions?

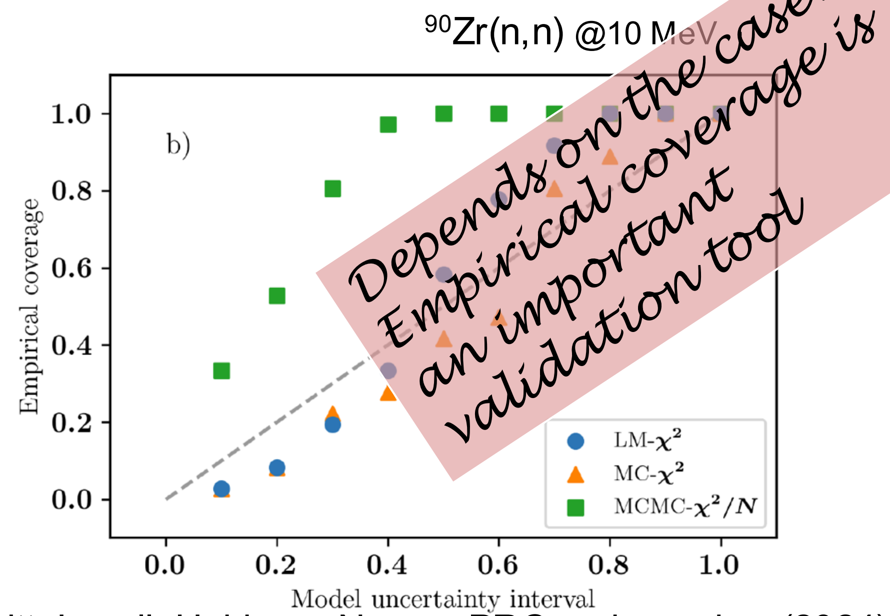
$$\chi^2 = \sum_{i=1}^{N} \frac{[\sigma_{\exp}(\theta_i) - \sigma_{\rm th}(\theta_i, x)]^2}{[\Delta\sigma_{\exp}(\theta_i)]^2}$$

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

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



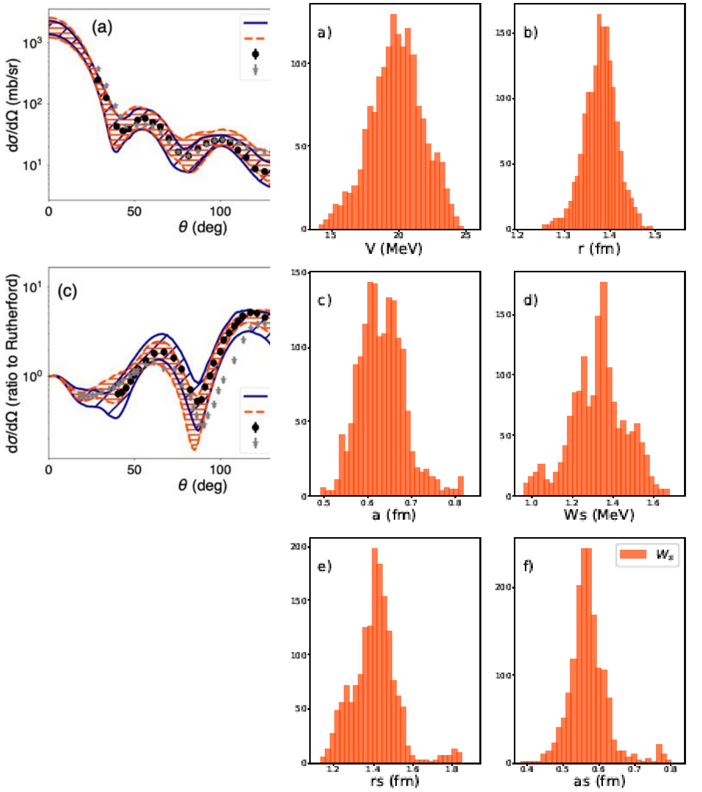
King et al., PRL 2019

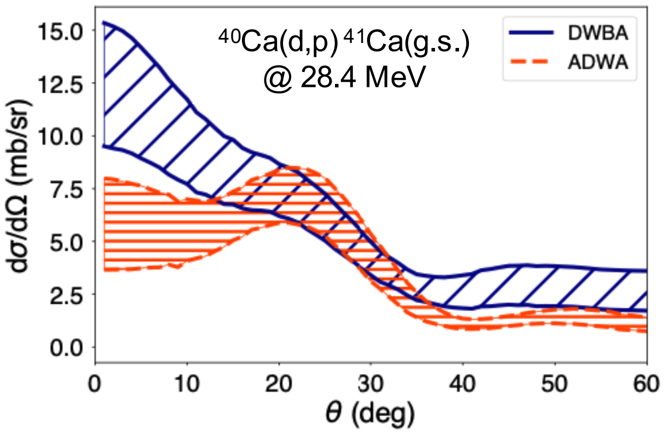


Pruitt, Lovell, Hebborn, Nunes, PRC under review (2024)

Propagating uncertainties to transfer

OP constrained with elastic scattering to obtain posterior distributions for parameters



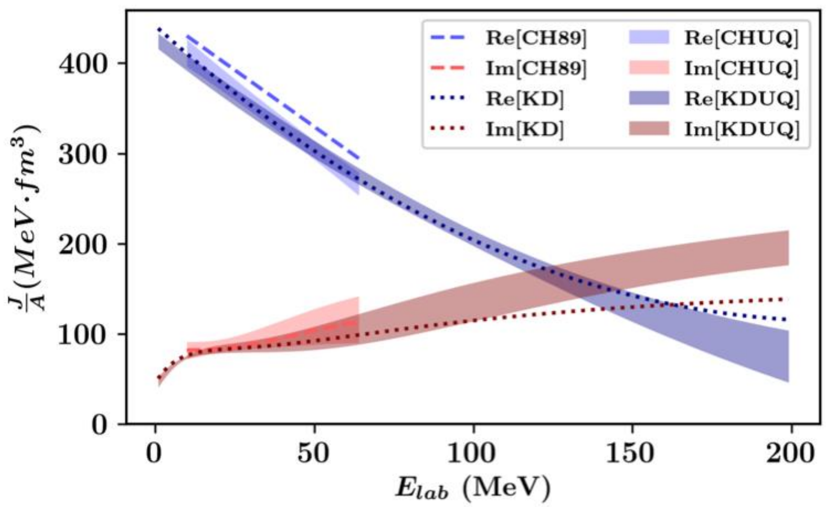


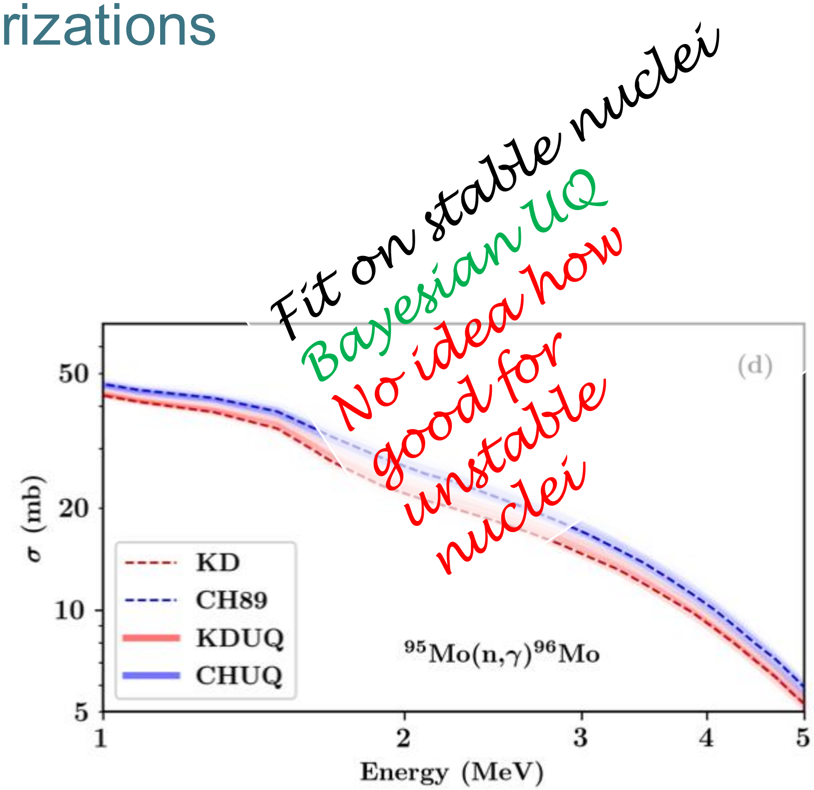
Propagate to other reaction observables

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





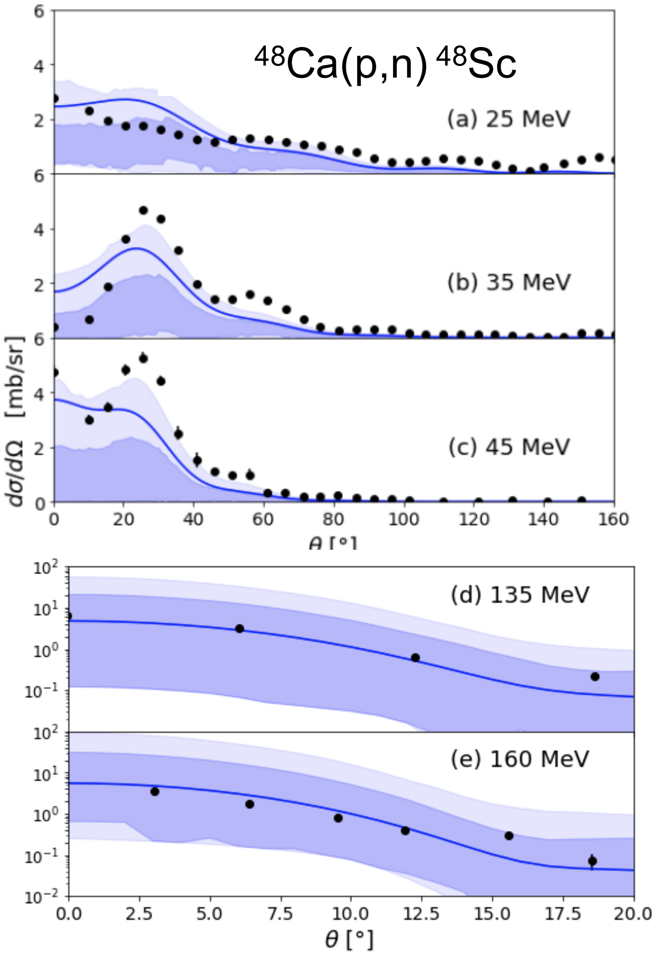
Pruitt et al., Phys. Rev. C 107, 014602 (2023)

Andy Smith

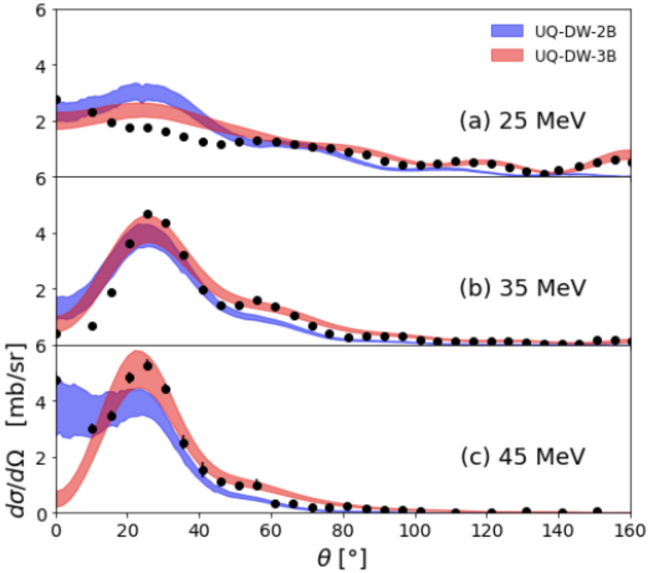
OP uncertainties in charge exchange to IAS

- 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

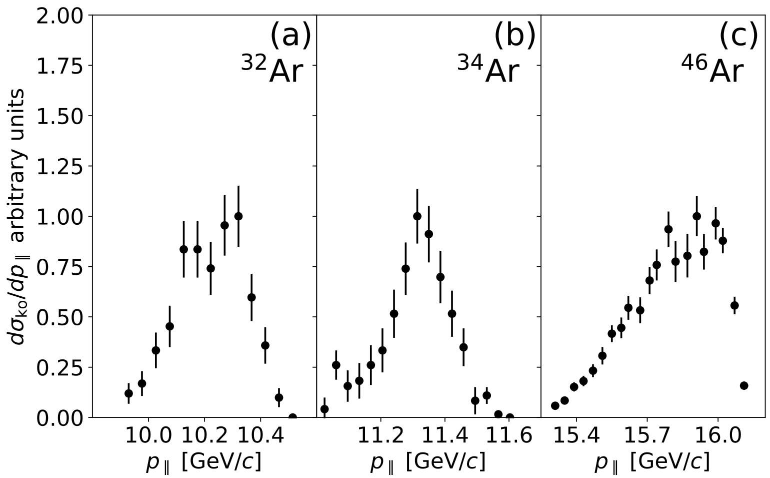


Smith, Hebborn, Nunes, Zegers, PRC accepted (2024)

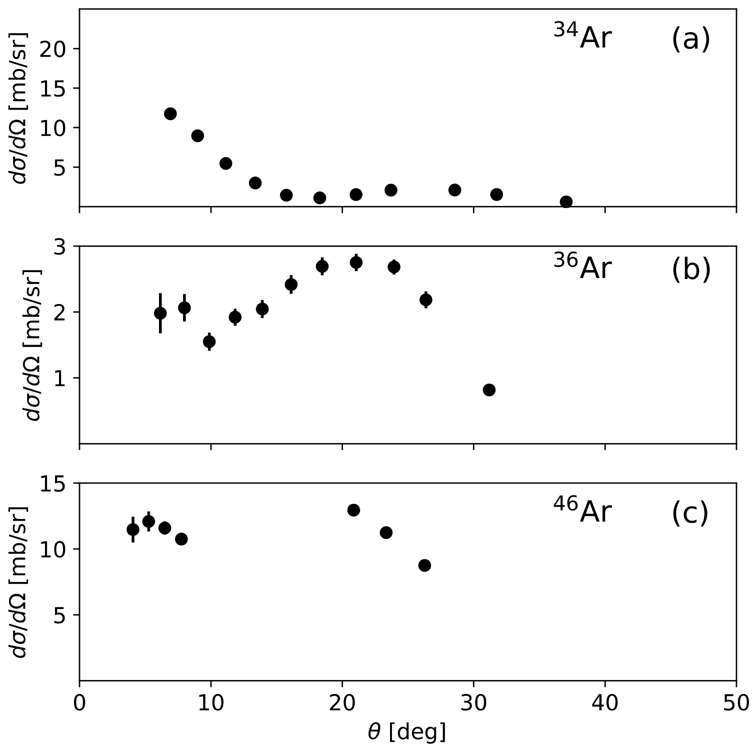
Propagating uncertainties to knockout

- 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)

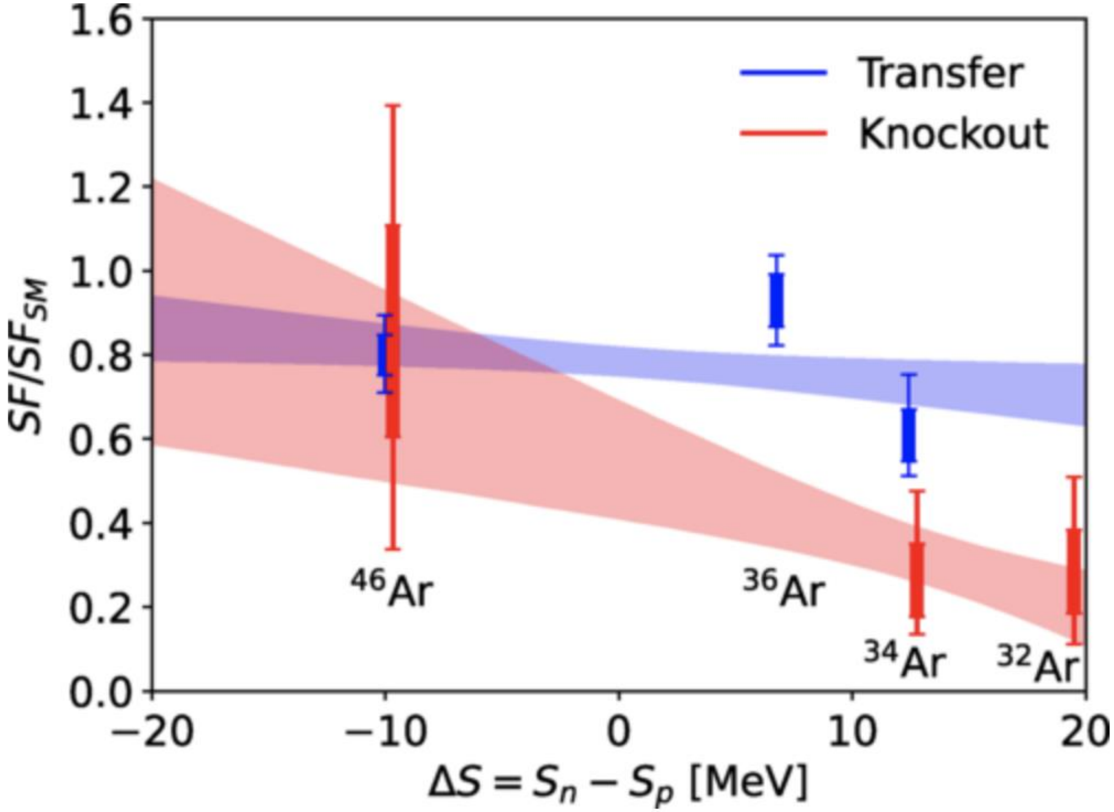


dark (light) shade:
68% (95%) credible intervals

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)

Emulators for nuclear reactions

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

reaction problem

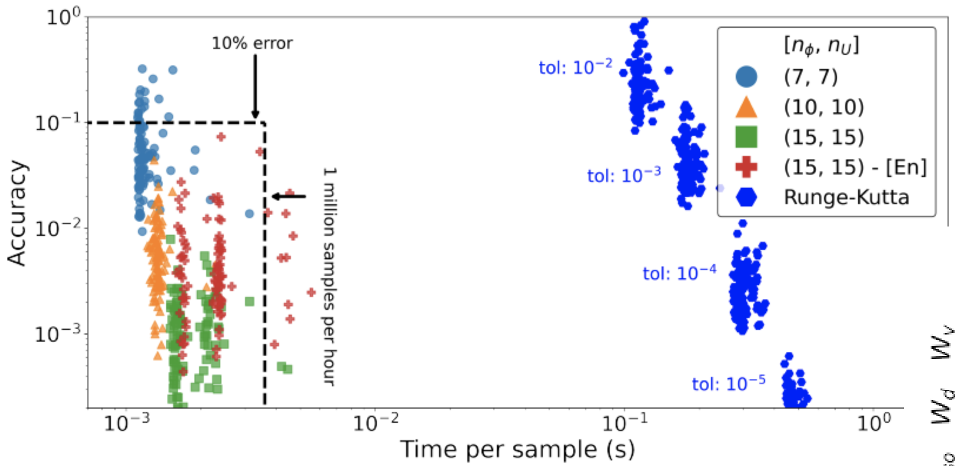
physics driven

(reduced basis methods)

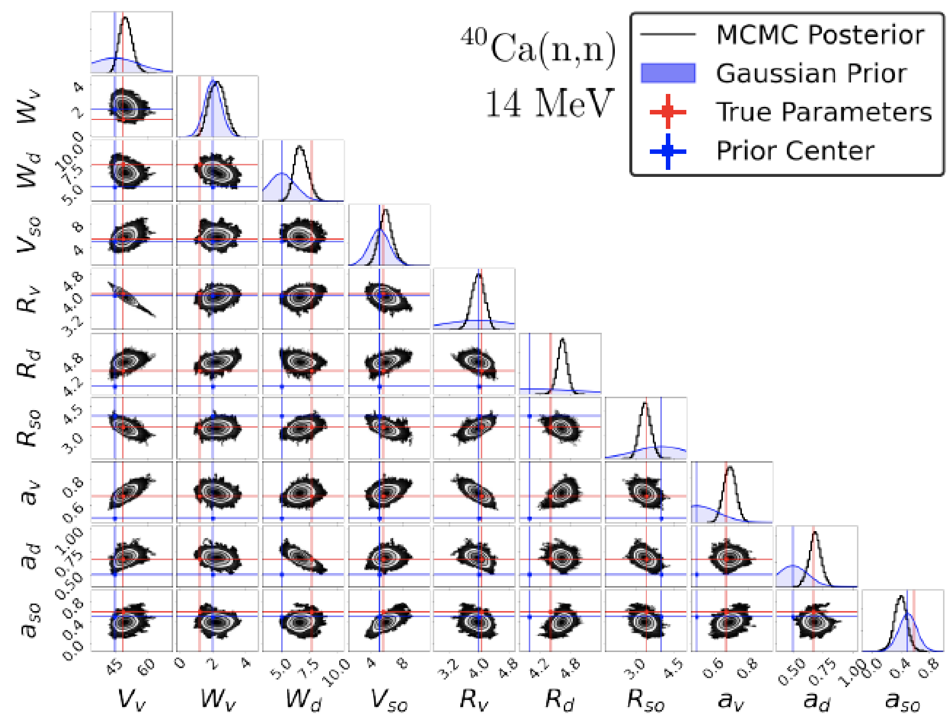
data driven

(Gaussian processors)

Physics Driven Emulator
ROSE: Reduced Order Scattering Emulator



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

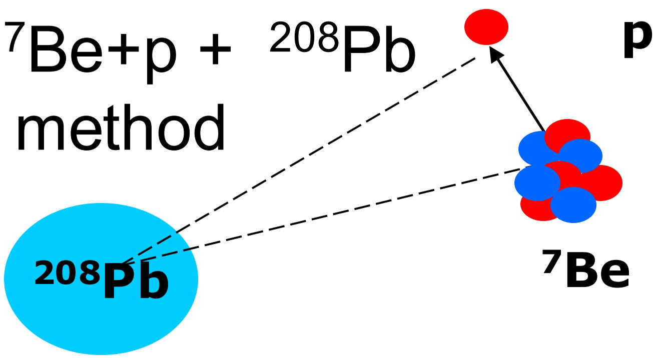


Odel et al., Phys. Rev. C (2024)

Data driven emulator
Breakup cross sections needed for astrophysics

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

$^{8}B + {}^{208}Pb \longrightarrow {}^{7}Be + p + {}^{208}Pb$
Indirect method



Working horse for modeling these reactions:
Continuum Discretized Coupled Channel (CDCC)
Large scale (large memory requirements)
Long runs (many hours to days)

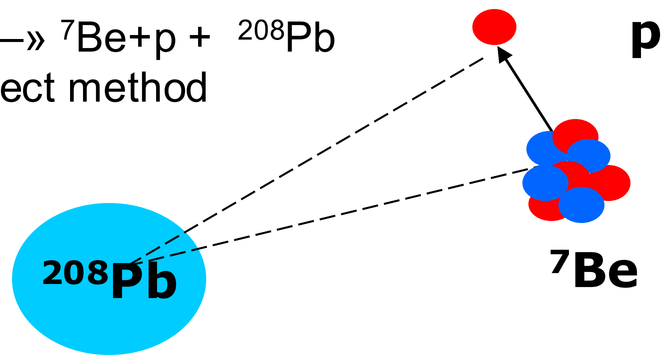
Impossible to do Bayesian analysis directly with CDCC!

Predictions: Angular distributions and energy distributions of fragments

Emulators for breakup cross sections

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

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



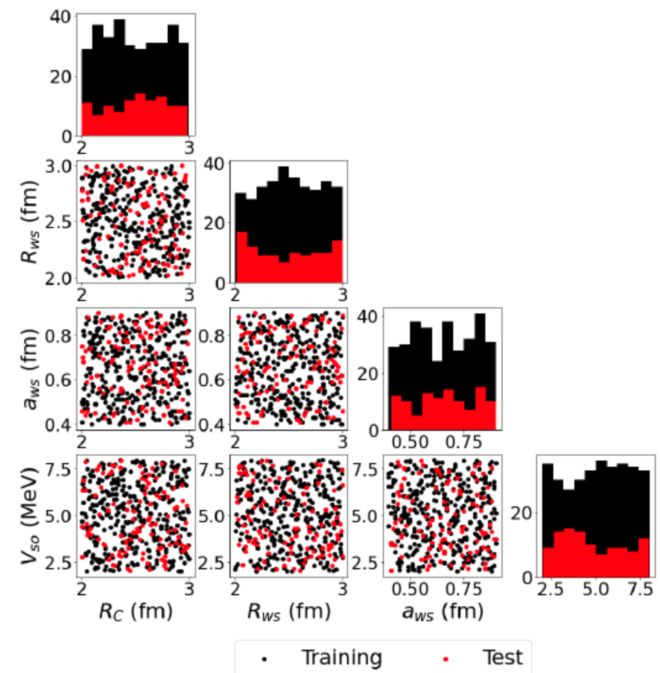
Continuum Discretized Coupled Channel
Gaussian-processors emulator for breakup:
Angular distribution and energy distribution

uncertainty from ^7Be+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.

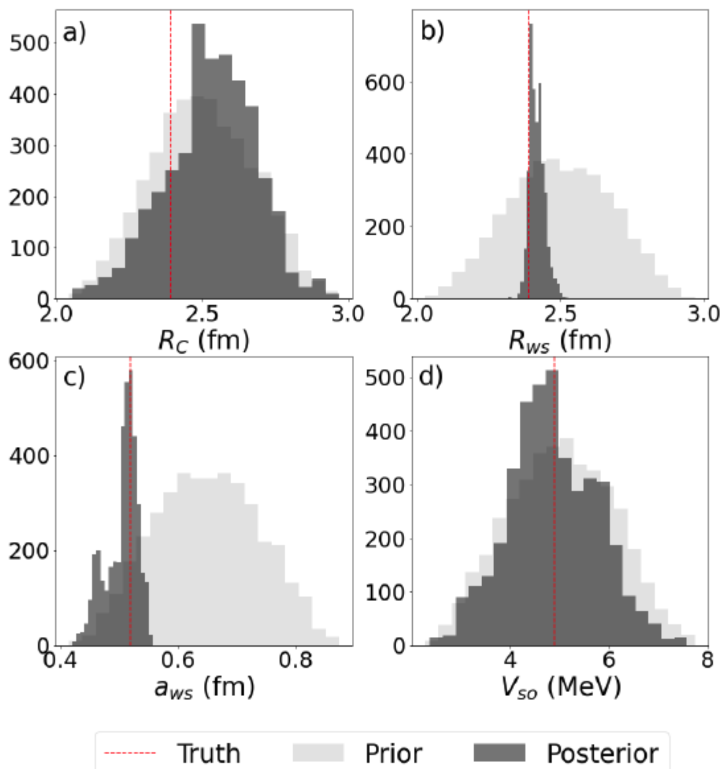
Parameter	Label	Range $[\underline{\rho_i}, \overline{\rho_i}]$
R_C	ρ_1	[2, 3] (fm)
R_{ws}	ρ_2	[2, 3] (fm)
a_{ws}	ρ_3	[0.4, 0.9] (fm)
V_{so}	ρ_4	[2, 8] (MeV)

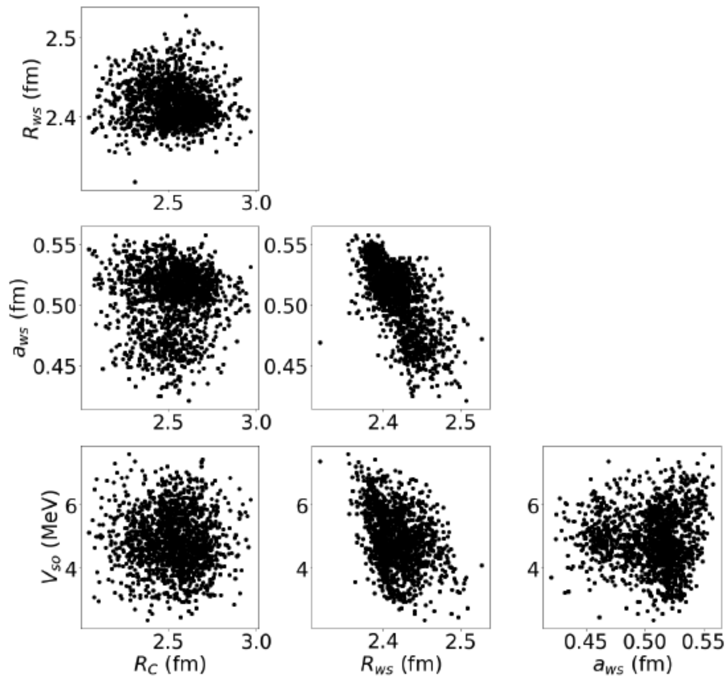


Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Emulators for breakup cross sections

Posterior distributions and correlation plots

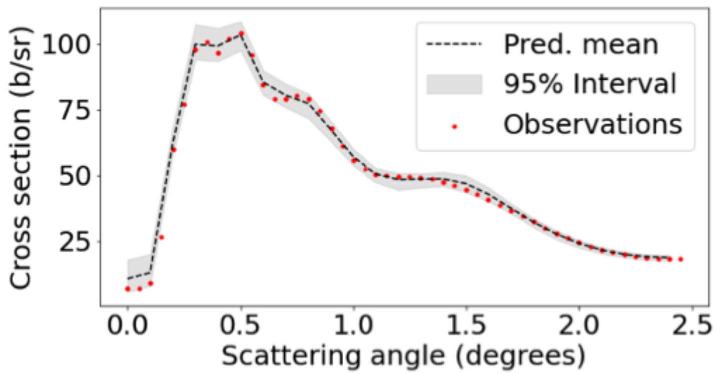




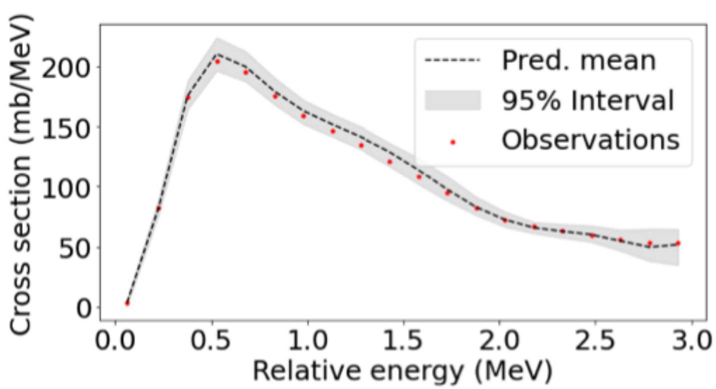
Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Emulators for breakup cross sections

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



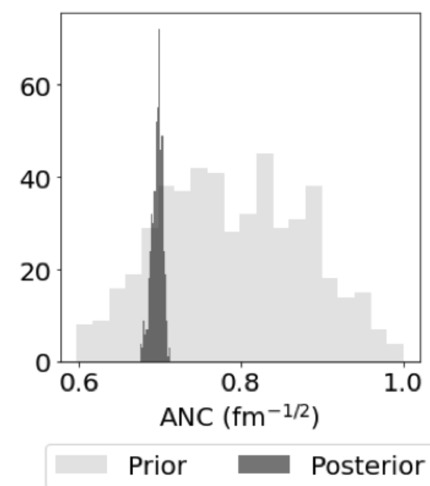
(a) Angular distribution.



(b) Energy distribution.

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

uncertainty from ^7Be+p interaction



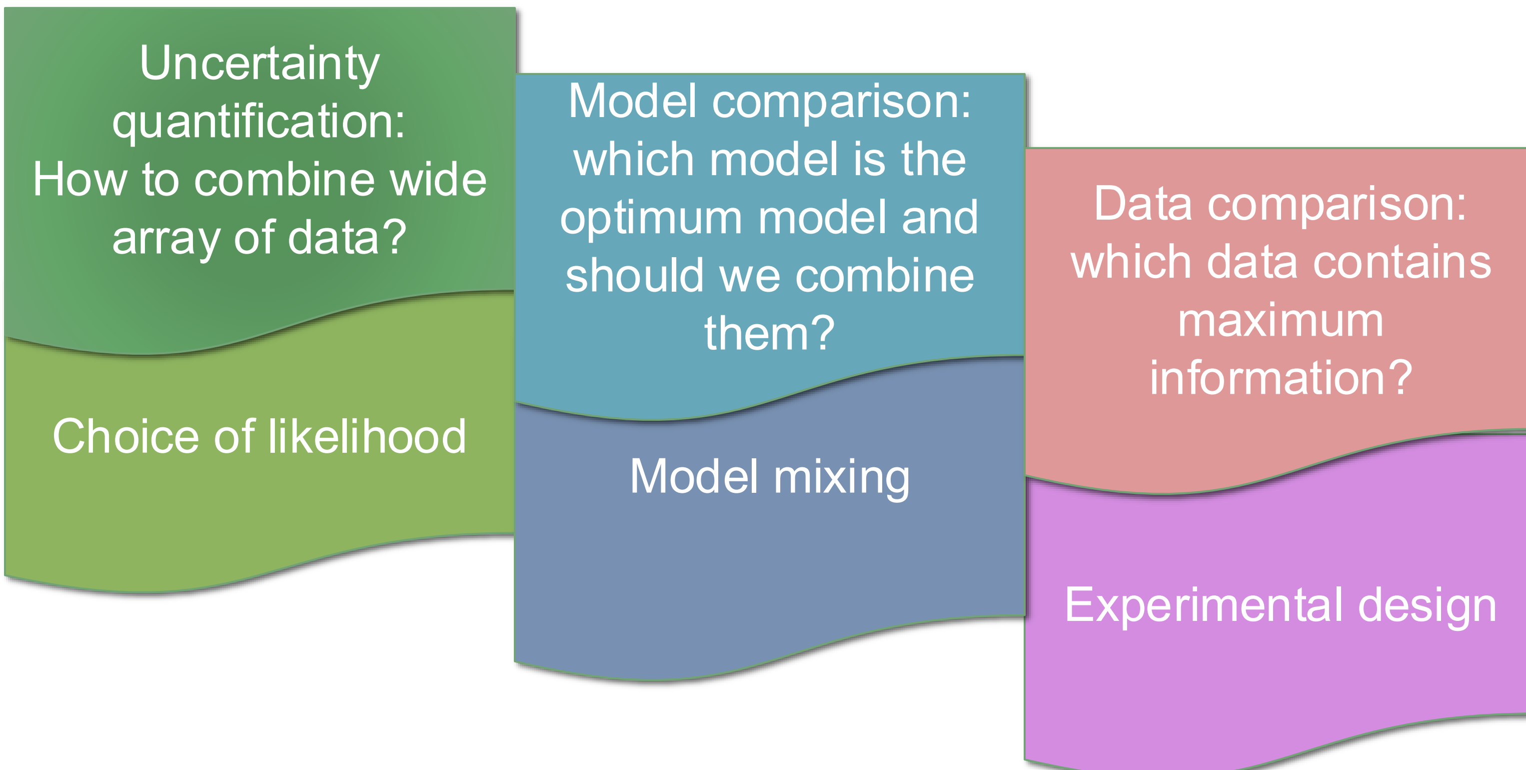
Excellent constraint on S_{17}

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

Opportunities for the future

- Optical potential validated for rare isotopes:
  - full UQ, global; ab-initio priors; extension to heavy-ions
- Bayesian analysis for complex reactions models:

  fast and accurate emulators



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Gregory Potel (LLNL)
Andy Smith (MSU)
Chloe Hebborn
Remco Zegers

Knockout:
Chloe Hebborn
Amy Lovell

Emulators:
BAND collaboration

Work supported by NSF and DOE

Landscape of global optical potentials