
Georgia O'Keefe, mossandfog.com

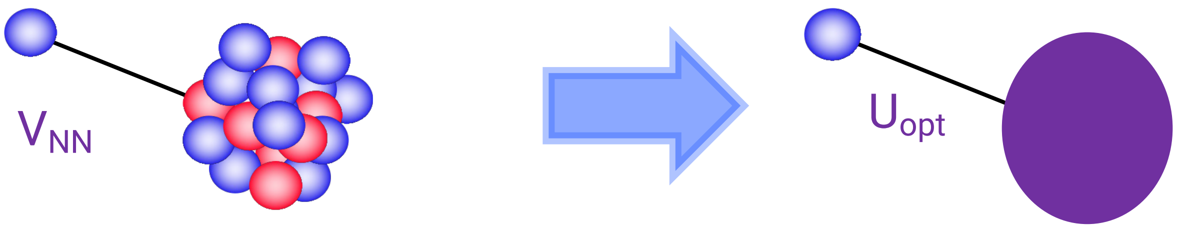
How to constrain optical potentials

Filomena Nunes
Michigan State University

Outline

- What is an optical potential?
- Status of optical potentials
- Bayesian analyses of optical potentials
- Propagation to other observables
  - Transfer
  - Charge-exchange
  - Knockout
- Emulators
  - Application to model for breakup
- Opportunities for the future

What is an optical potential?



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)

FRIB-TA Topical Program on Optical Potentials 2022

The goal of the program was to:

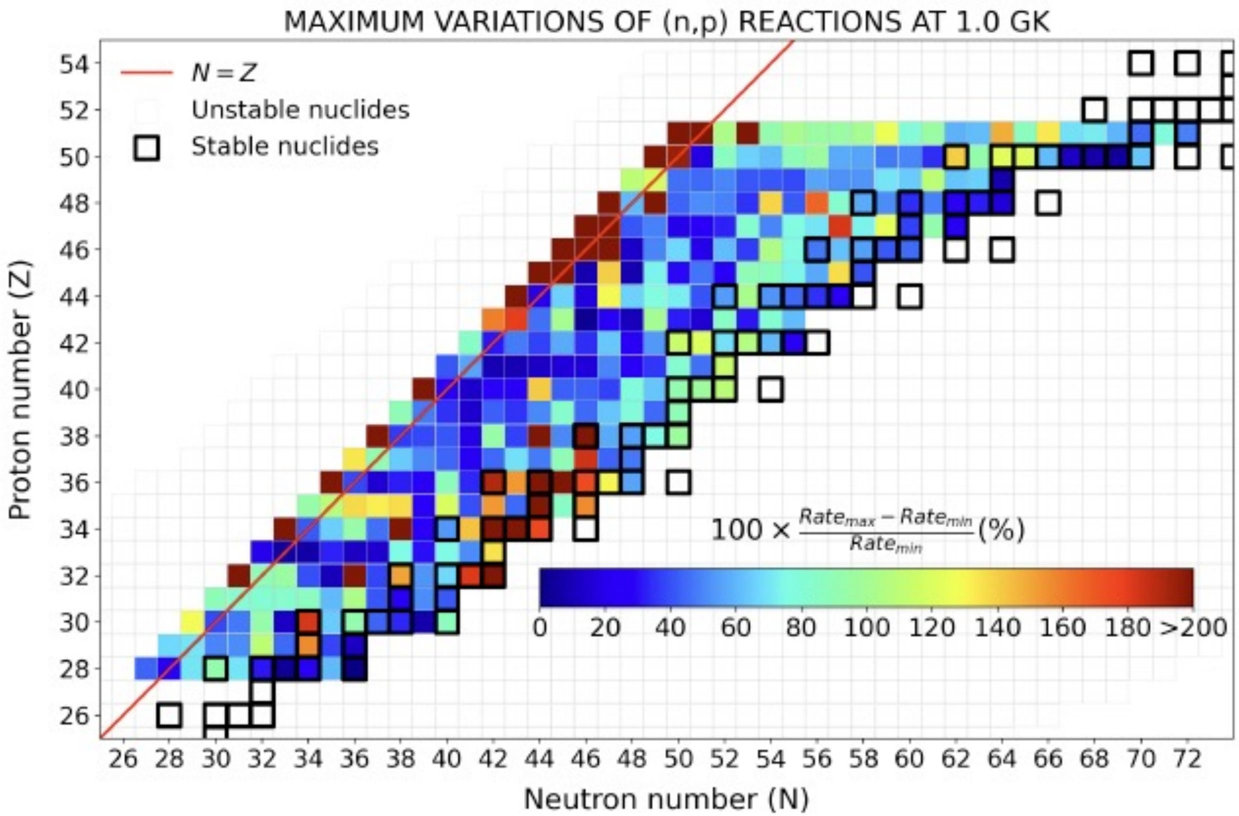
• Review strategies to derive optical potentials, and the underlying associated structure theory approaches.
• Assess the reliability and ranges of validity of the different approaches, as a function of beam energies and mass numbers.
• Make recommendations concerning the future developments, and provide a road map both for the derivation of the new generation of optical potentials and the associated uncertainty quantification.

❑ Over 60 participants
❑ The whitepaper published in JPG covers the many different approaches and the needs for the future.

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

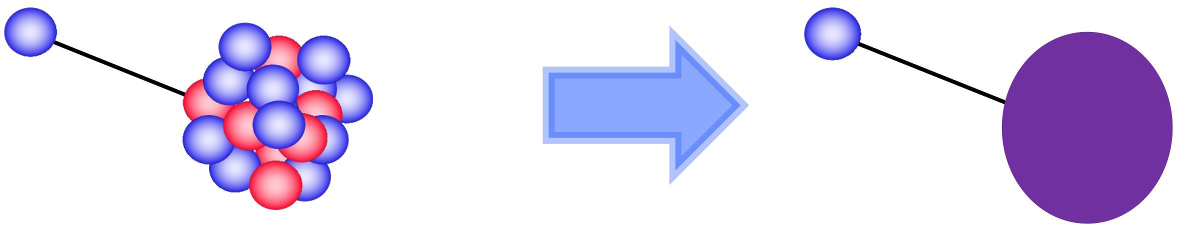
Optical potentials are pervasive in reaction models

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



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

Optical potentials from data

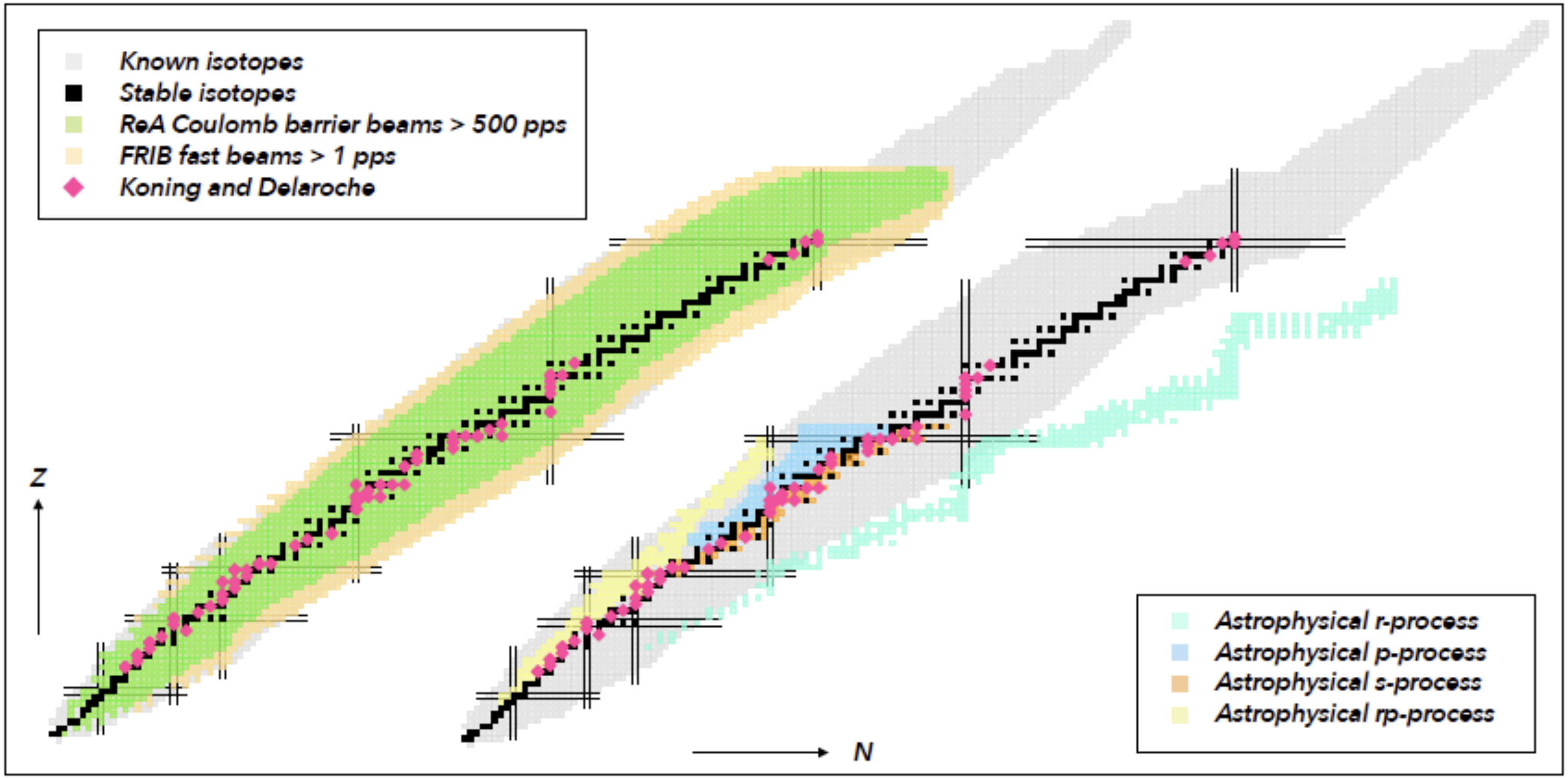


Phenomenological approach:

fit a large set of elastic data – extract *global* optical potential

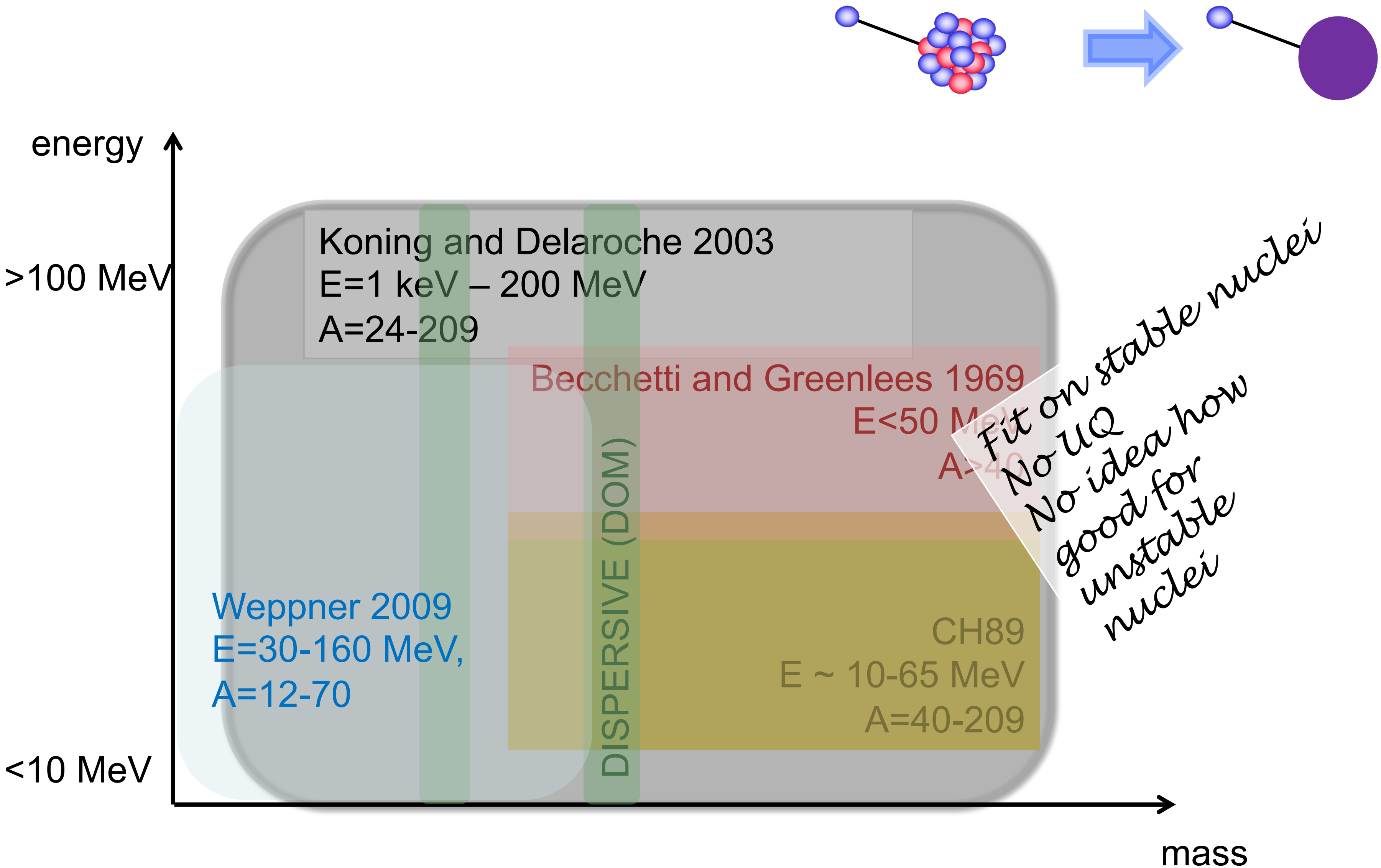
typically local, L-independent but strongly E-dependent

Phenomenological potentials fitted to stable nuclei



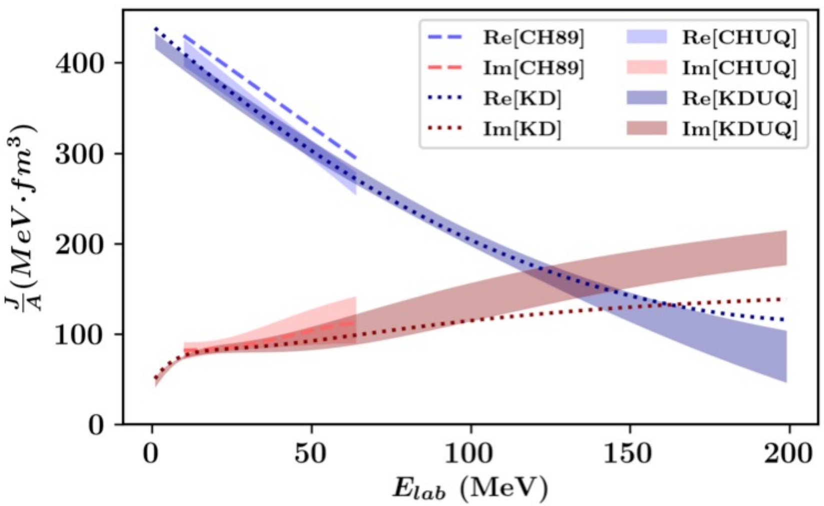
Hebborn, Nunes, et al., JPG 50, 060501 (2023)

Landscape of global optical potentials



Uncertainty quantified phenomenological optical potential (CHUQ and KDUQ)

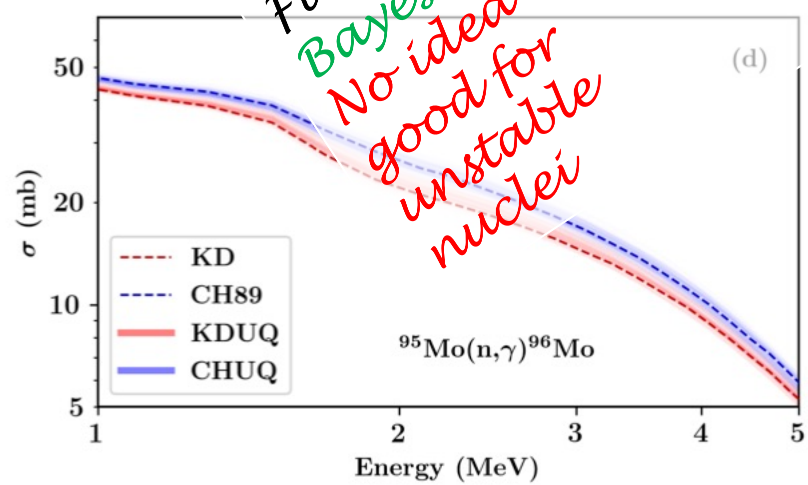
Bayesian analysis using the same experimental protocol as in the original CH89 and KD2003 parameterizations



Fit on stable nuclei

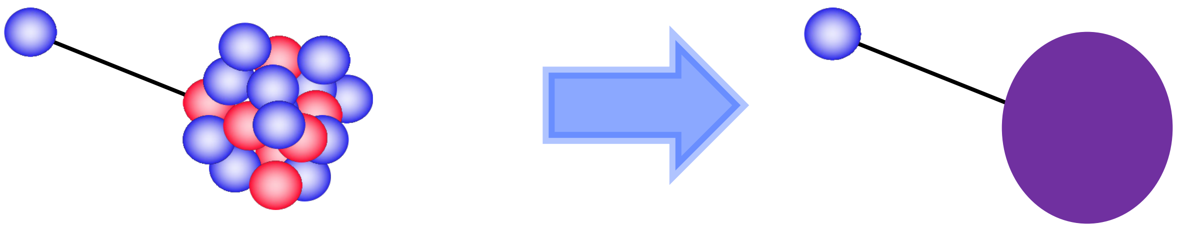
Bayesian UQ

No idea how good for unstable nuclei



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

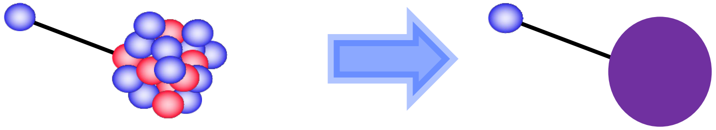
Optical potentials from theory

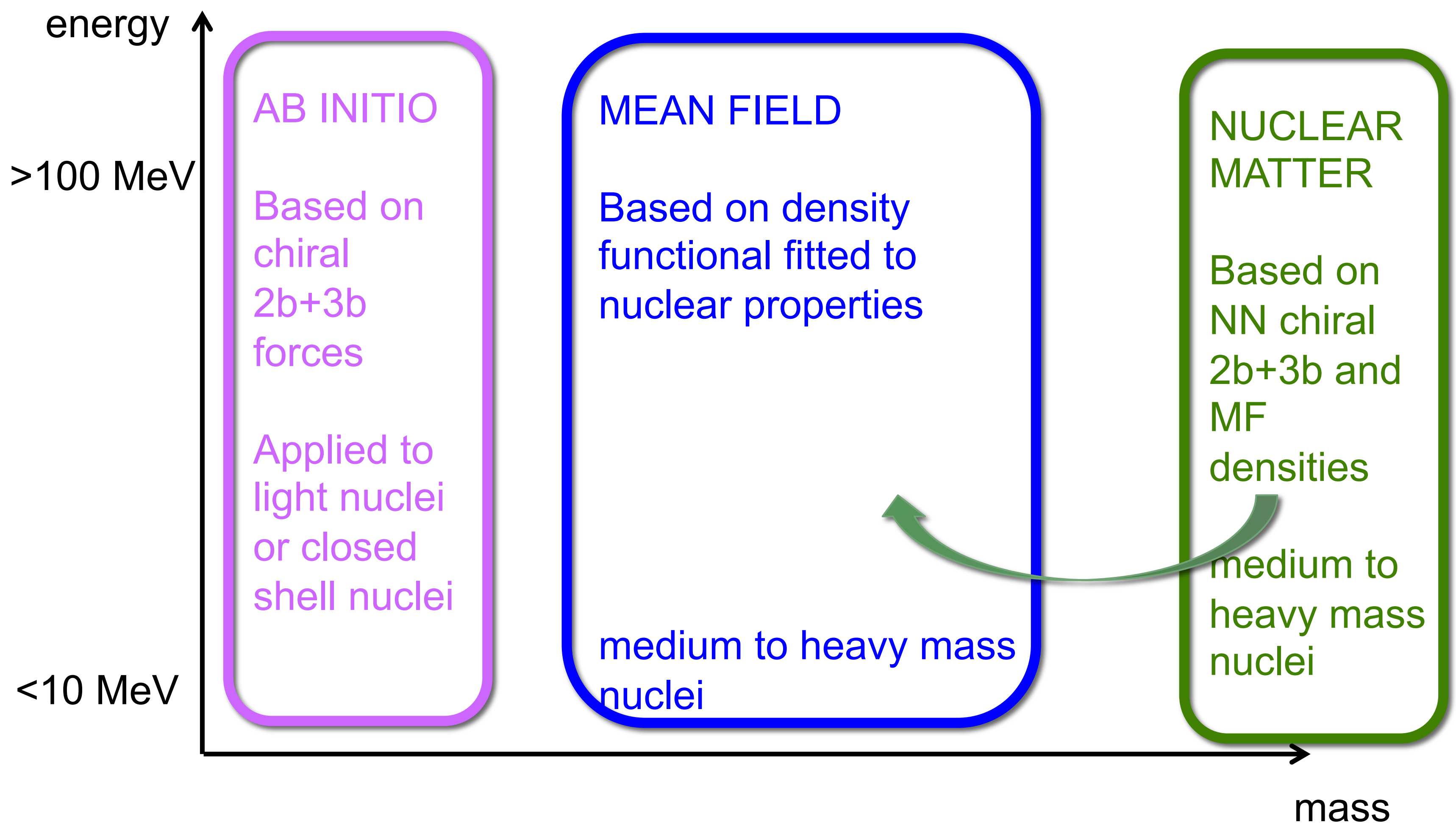


Microscopic optical potential:

- 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





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	$E < 40\ \text{MeV}$	✓	✓	✗
SCGF	O, Ca, Ni isotopes	$E < 100\ \text{MeV}$	✓	✓	✗
MST-B	$A \leq 20$	$E \gtrsim 70\ \text{MeV}$	✗	✓	✗
MST-V	$4 \leq A \leq 16$	$E \gtrsim 60\ \text{MeV}$	✗	✓	✗
WLH	$12 \leq A \leq 242$	$0 \leq E \leq 150\ \text{MeV}$	✗	✓	✓
JLMB	$A > 30$	$1\ \text{keV} < E < 340\ \text{MeV}$	✗	✓	✗

Mean field

Ab-initio

Nuclear Matter

phenomenological

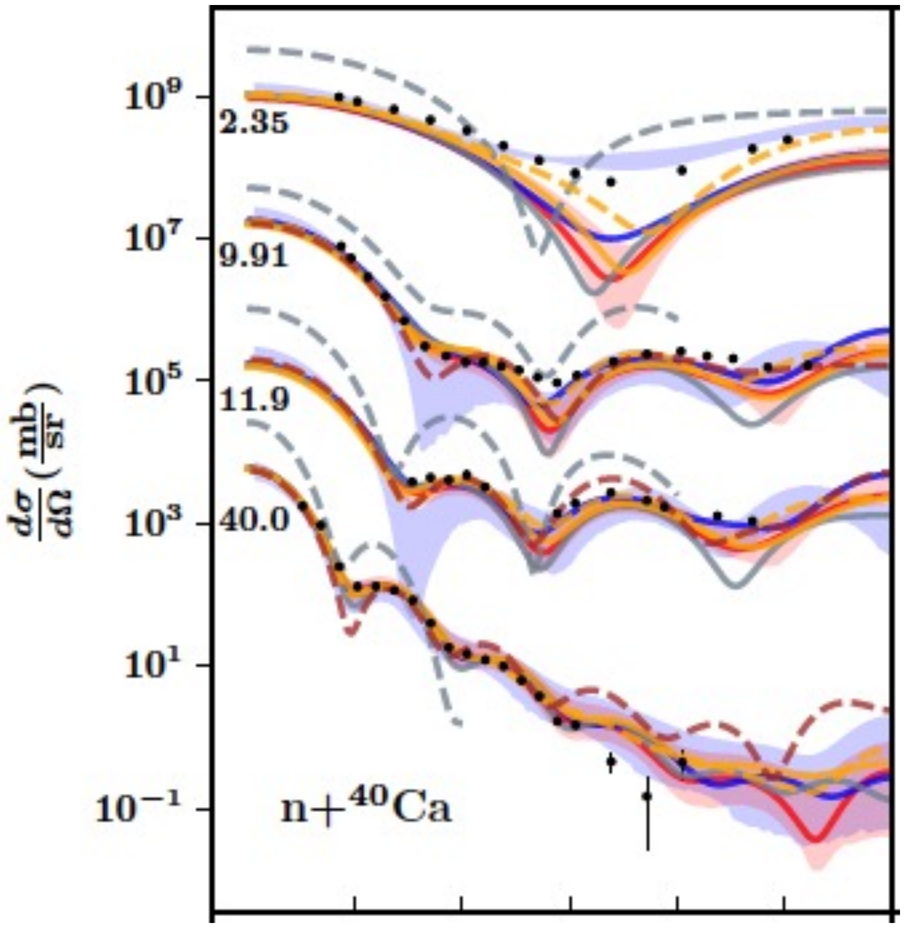
microscopic

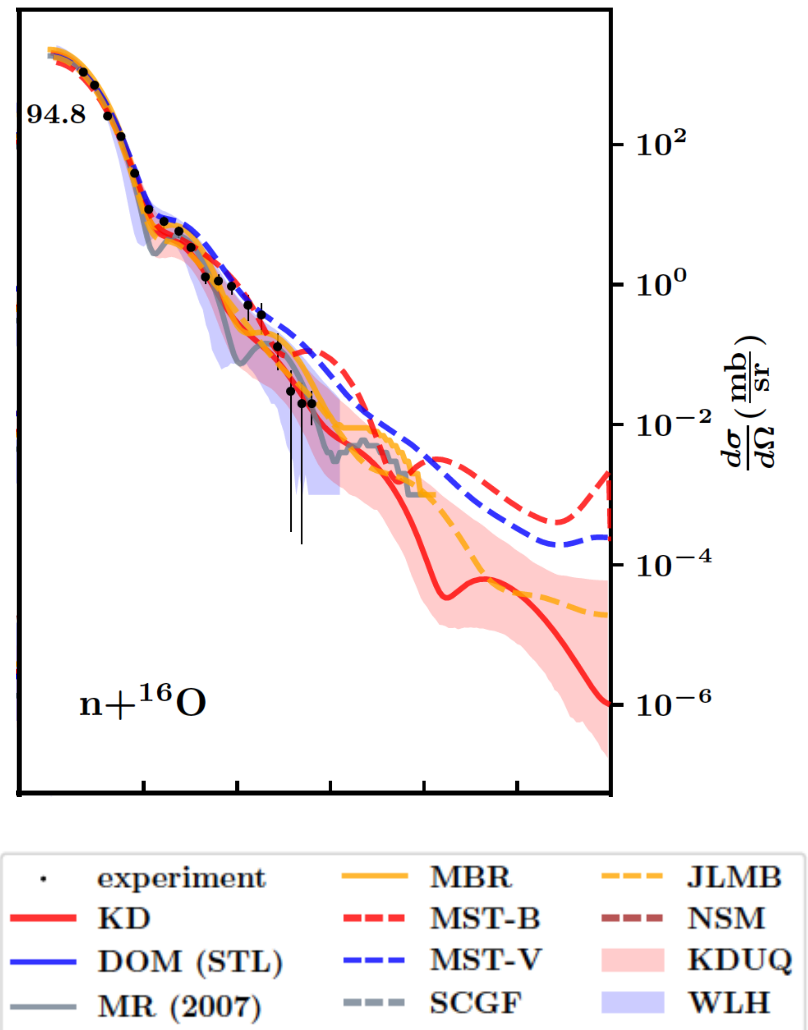
Semi-phenomenological

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

How do optical models compare?

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



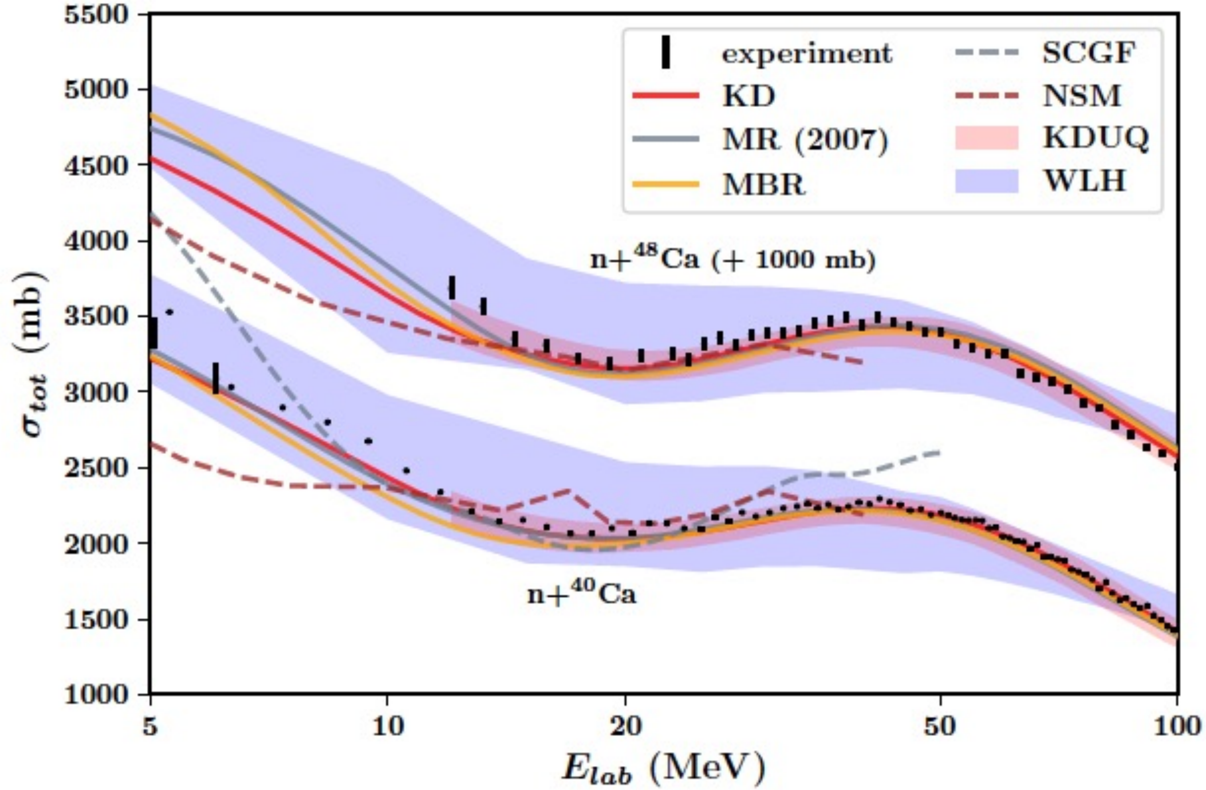


Hebborn, Nunes, et al., JPG 50, 060501 (2023)

How do optical models compare?

95% credible intervals

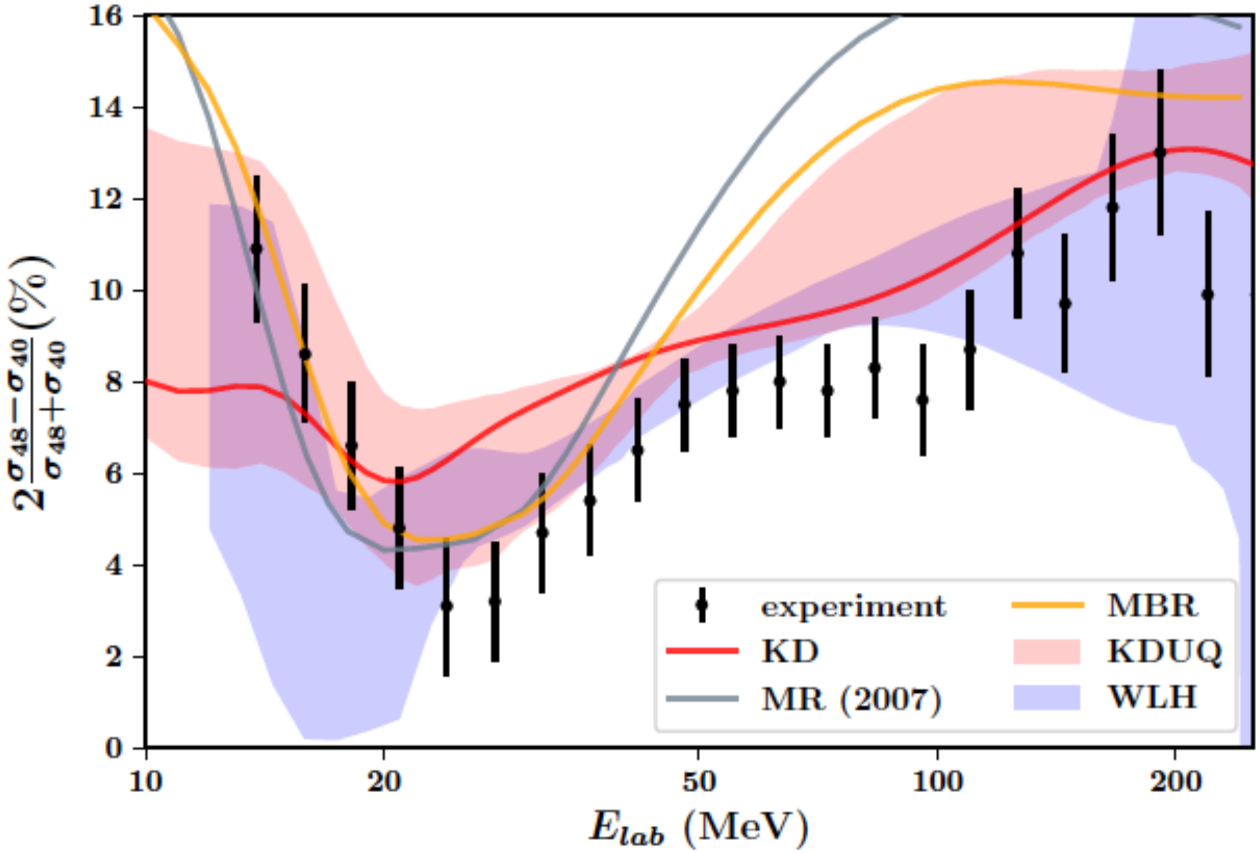
Total cross section as a function of energy



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)

FRIB-TA Topical Program on Optical Potentials Recommendations

While at stability various methods agree, the situation for rare isotopes is dire. We need:

- Experiments specifically targeting optical potential extractions
- Inclusion of UQ by theorists
- Inclusion of systematic errors in experimental analyses
- Collaborations amongst the various theory methods
- Ab-initio methods need to expand beyond current truncations
- Microscopic theories need to be tested on a variety of reaction observables (not just spectra and radii)
- Other considerations:
    - dispersion relation, non-locality, isospin dependence
- Heavy ion optical potentials?

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

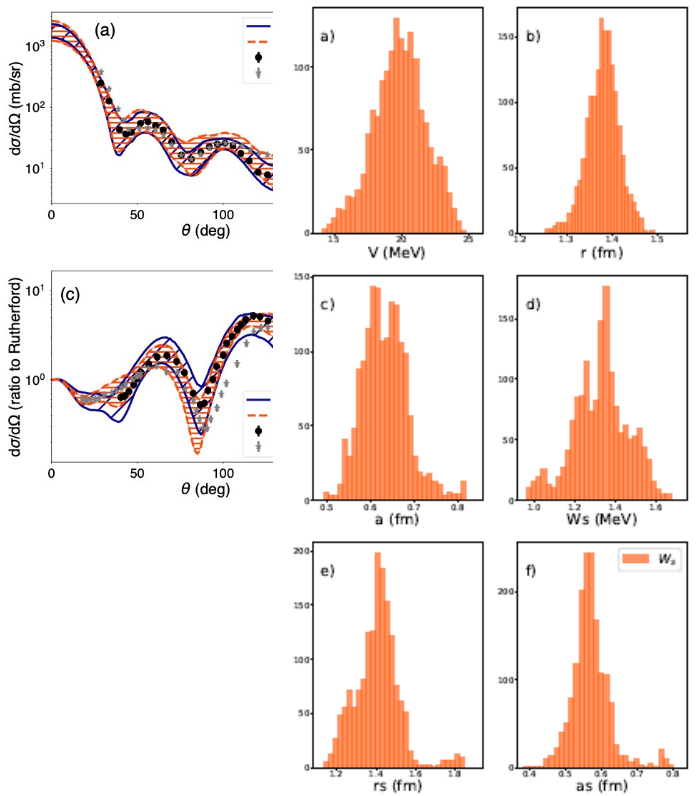
And here we are today!

Outline

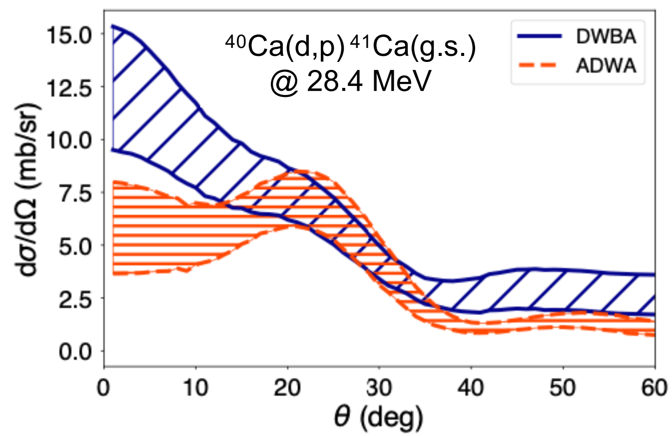
- What is an optical potential?
- Status of optical potentials
- Bayesian analyses of optical potentials
- Propagation to other observables
  - Transfer
  - Charge-exchange
  - Knockout
- Emulators
  - Application to model for breakup
- Opportunities for the future

Propagating uncertainties to transfer

OP constrained with elastic scattering to obtain posterior distributions for parameters



95% credible intervals



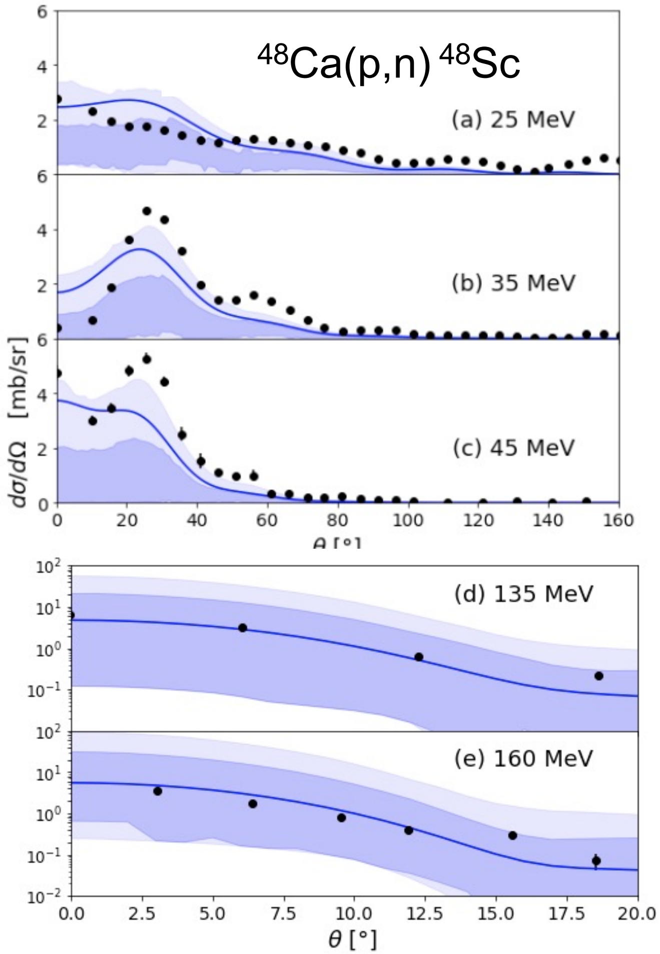
Propagate to other reaction observables

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

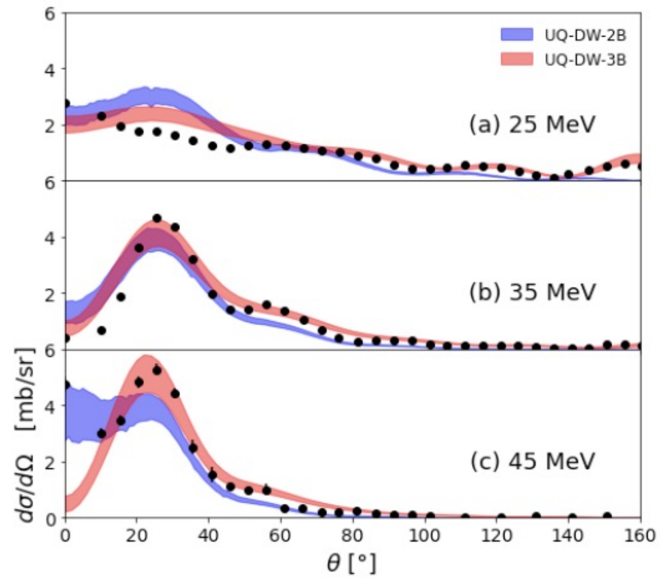
OP uncertainties to charge exchange to IAS

- 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



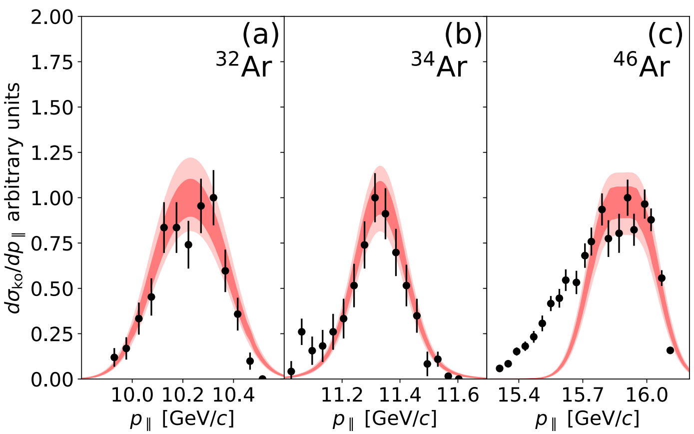
Smith, Hebborn, Nunes, Zegers, PRC under review (2024)

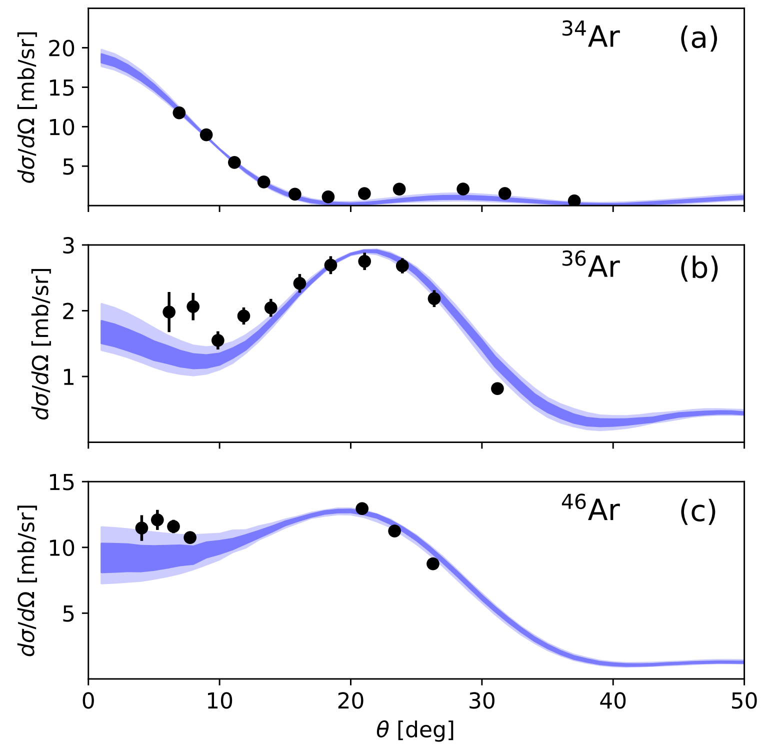
Propagating uncertainties to neutron knockout

Using parameter posterior from KDUQ

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

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





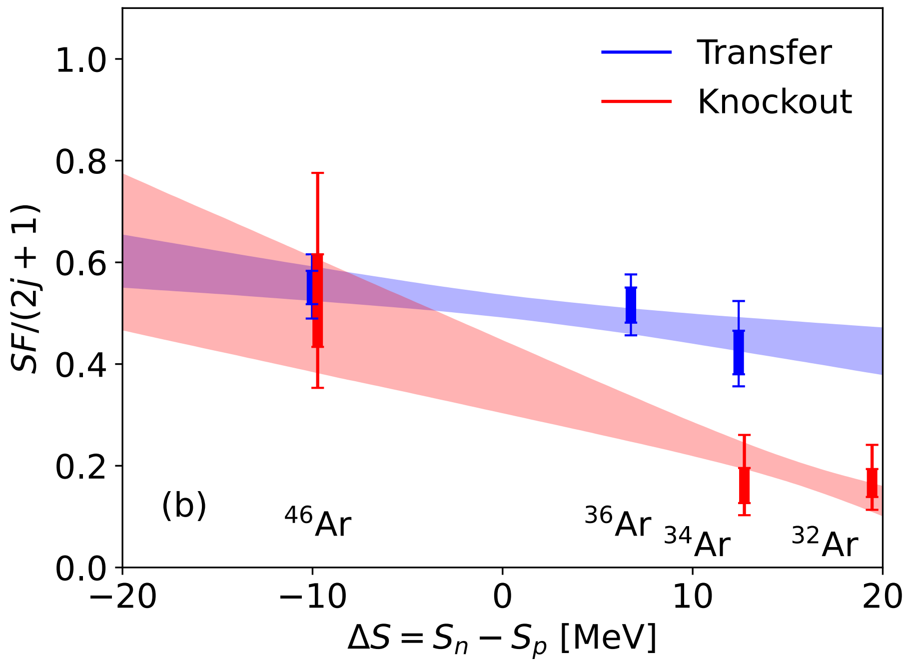
constrained n-^{9}Be elastic scattering to obtain knockout xs within the Eikonal model

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% credible intervals

^{32,34,46}Ar on ^{9}Be @ ~70 MeV A
a=-0.0122 (0.0043)
b=0.51(0.02)

^{34,26,46}Ar(p,d)@ 70 MeV A
a=-0.0044(0.0022)
b=0.37(0.07)

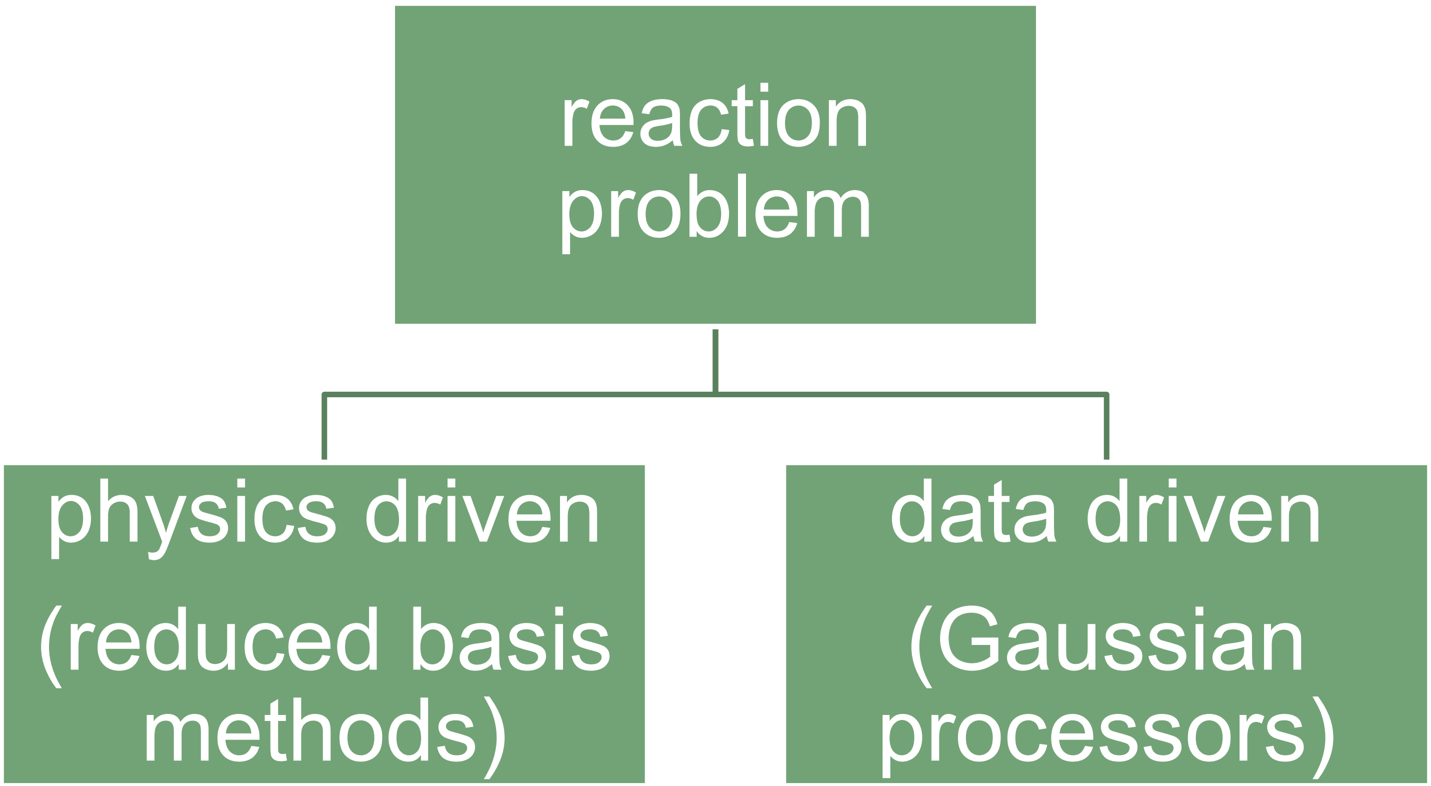
Hebborn, Nunes, Lovell, PRL 131, 212503(2023)

Outline

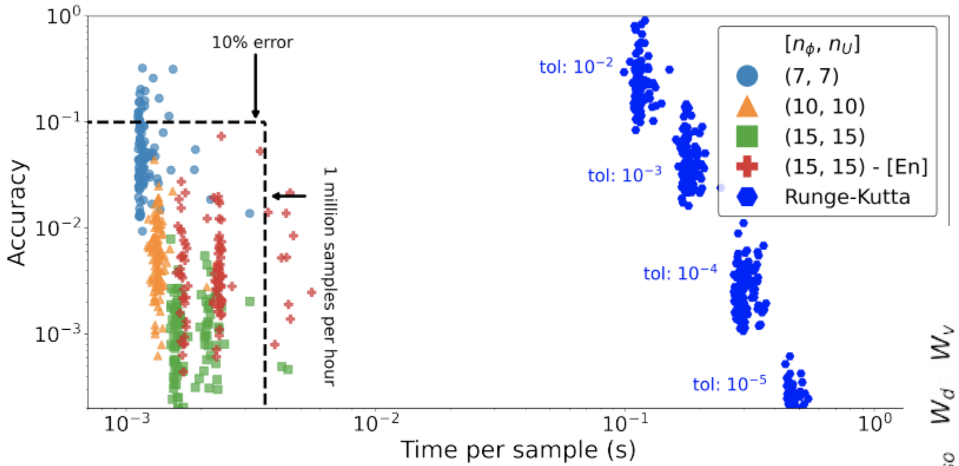
- What is an optical potential?
- Status of optical potentials
- Bayesian analyses of optical potentials
- Propagation to other observables
  - Transfer
  - Charge-exchange
  - Knockout
- Emulators
  - Application to model for breakup
- Opportunities for the future

Emulators for nuclear reactions

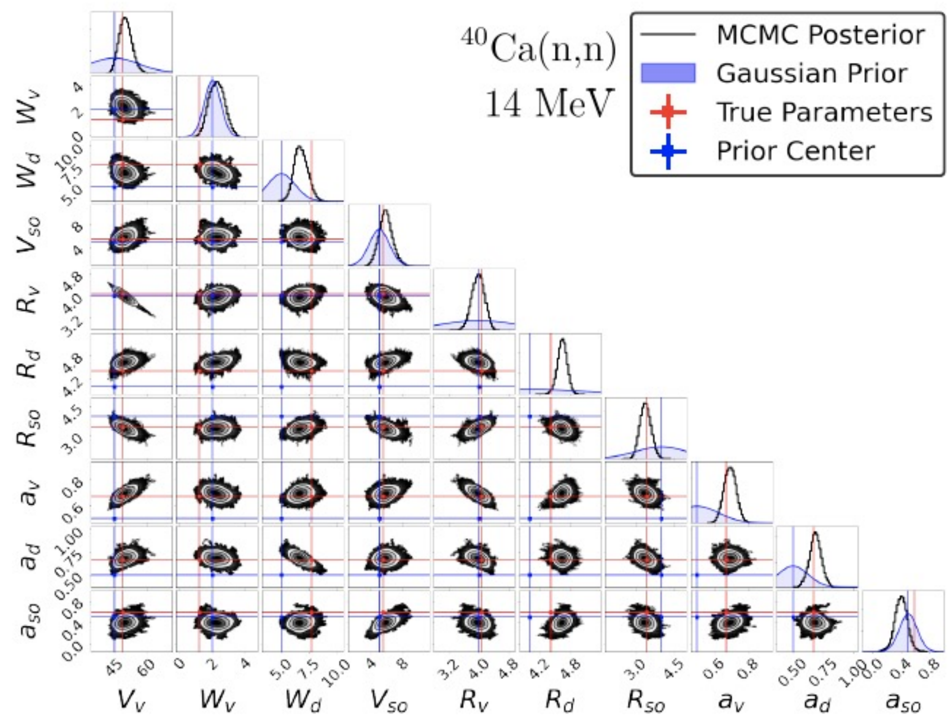
An emulator is a fast and efficient replacement for a complex physics model



Physics Driven Emulator
ROSE: Reduced Order Scattering Emulator



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

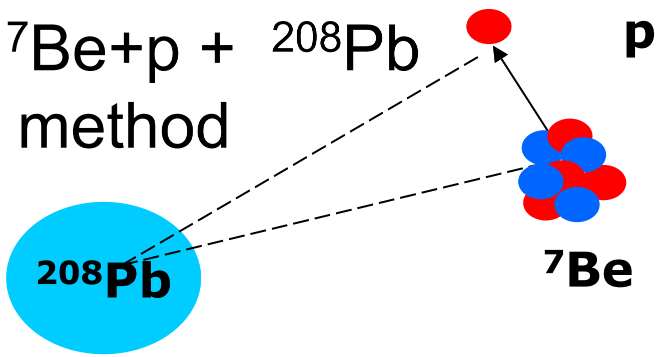


Odel et al., Phys. Rev. C (2024)

Data driven emulator
Breakup cross sections needed for astrophysics

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

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

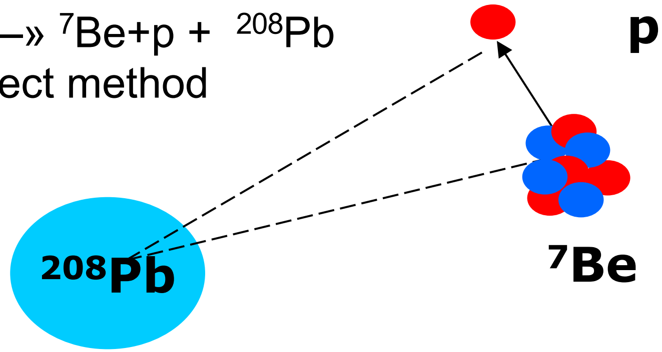
Predictions: Angular distributions and energy distributions of fragments

Bayesian Analysis of Nuclear Dynamics

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



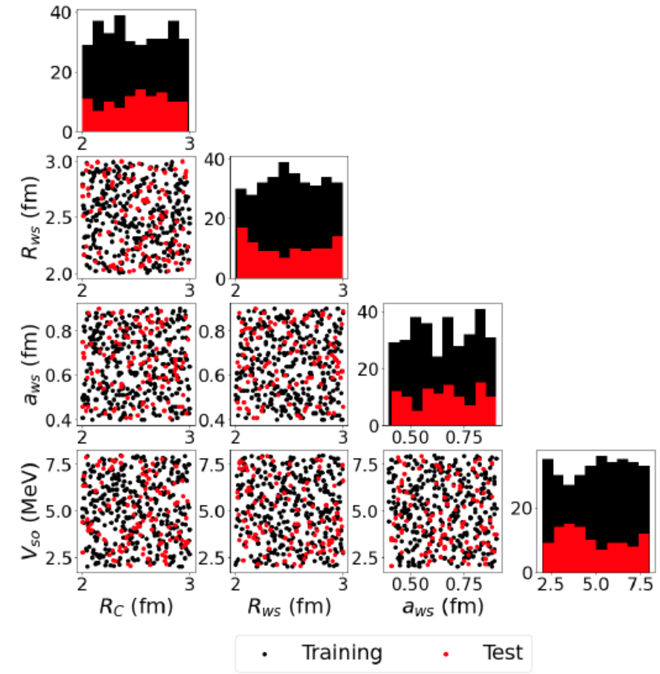
Continuum Discretized Coupled Channel
Gaussian-processors emulator for breakup:
Angular distribution and energy distribution

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.

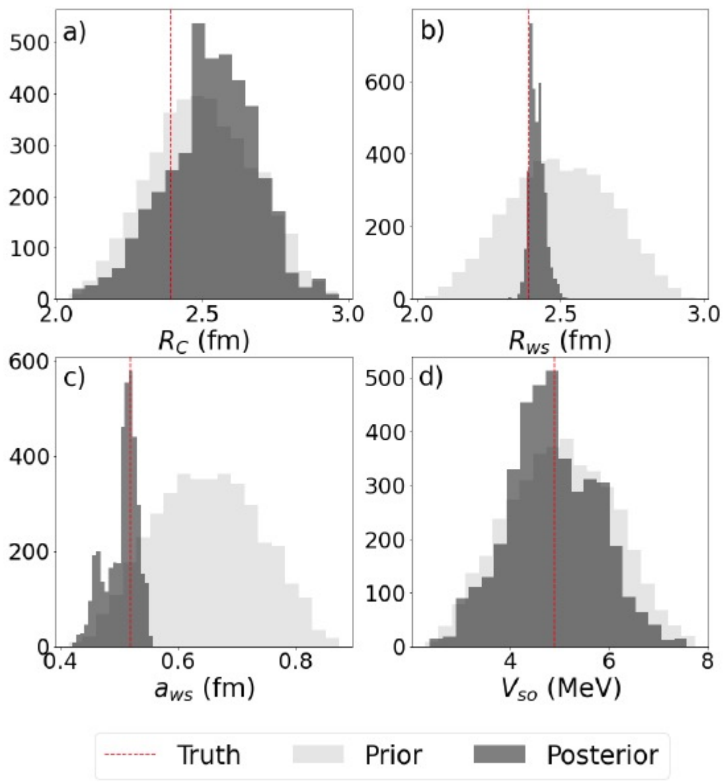
Parameter	Label	Range $[\underline{\rho_i}, \overline{\rho_i}]$
R_C	ρ_1	[2, 3] (fm)
R_{ws}	ρ_2	[2, 3] (fm)
a_{ws}	ρ_3	[0.4, 0.9] (fm)
V_{so}	ρ_4	[2, 8] (MeV)

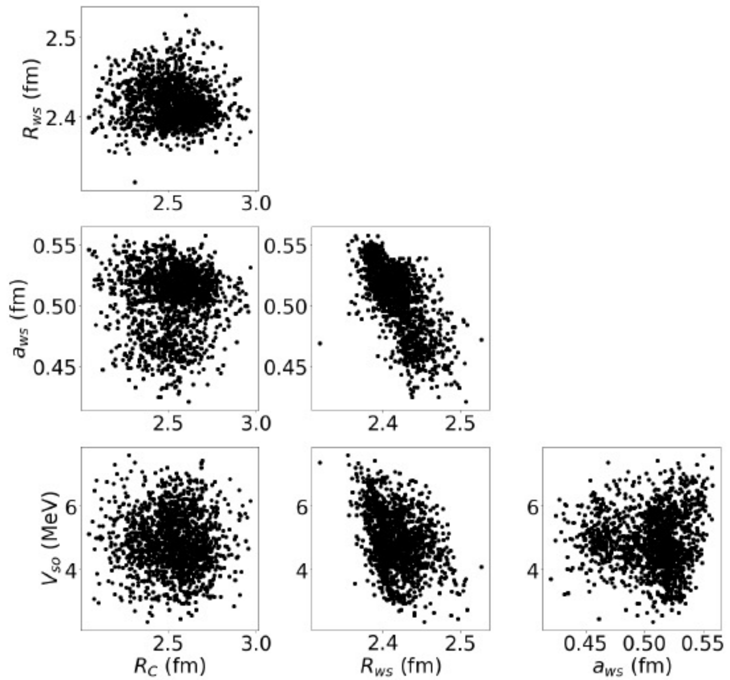


Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Emulators for breakup cross sections

Posterior distributions and correlation plots

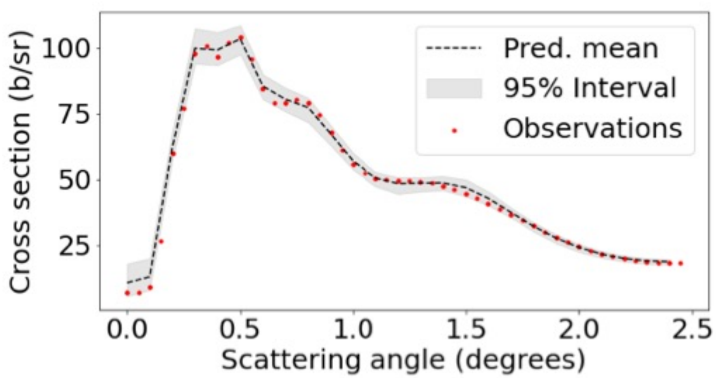




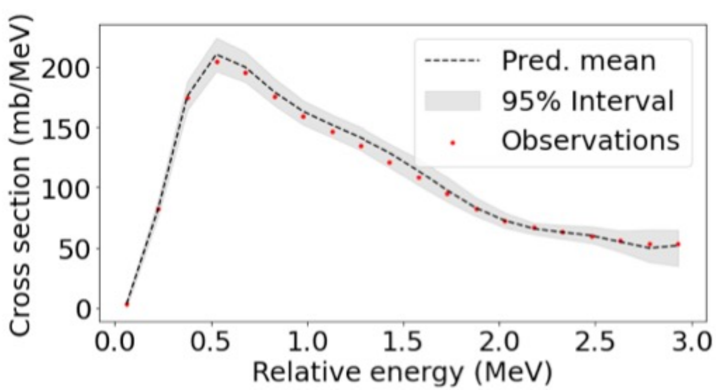
Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

Emulators for breakup cross sections

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



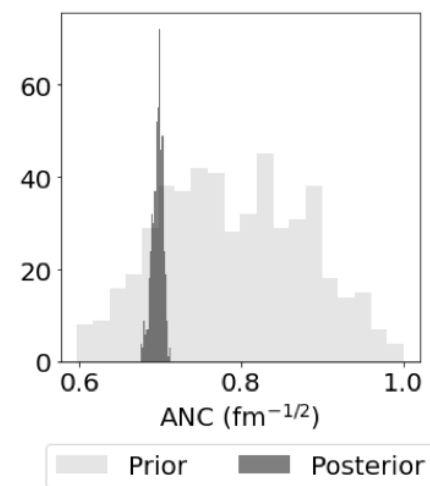
(a) Angular distribution.



(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}

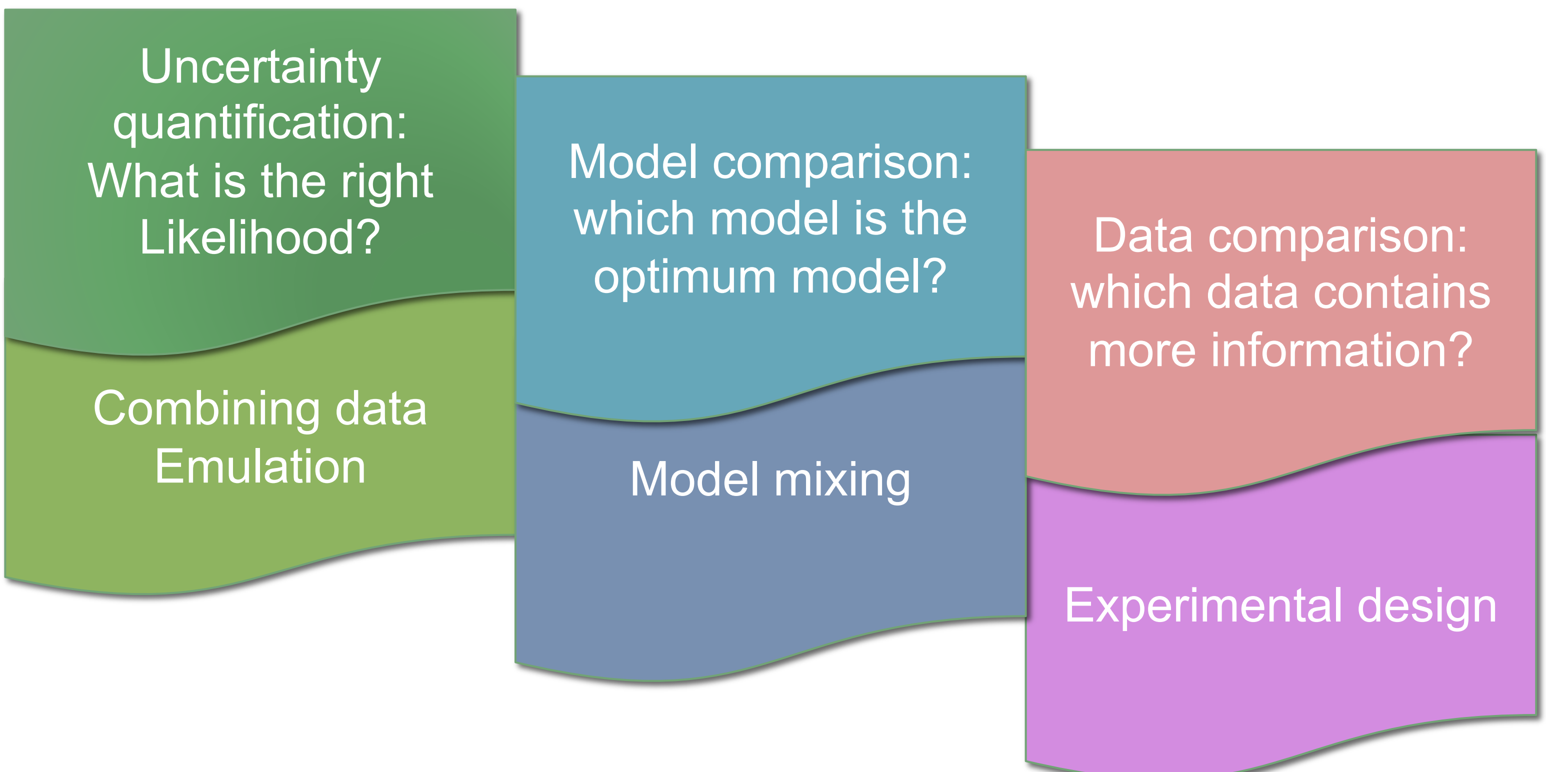
Surer, Nunes, Plumlee, Wild, PRC106, 024607(2022)

And now what?

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



Which is the correct likelihood?

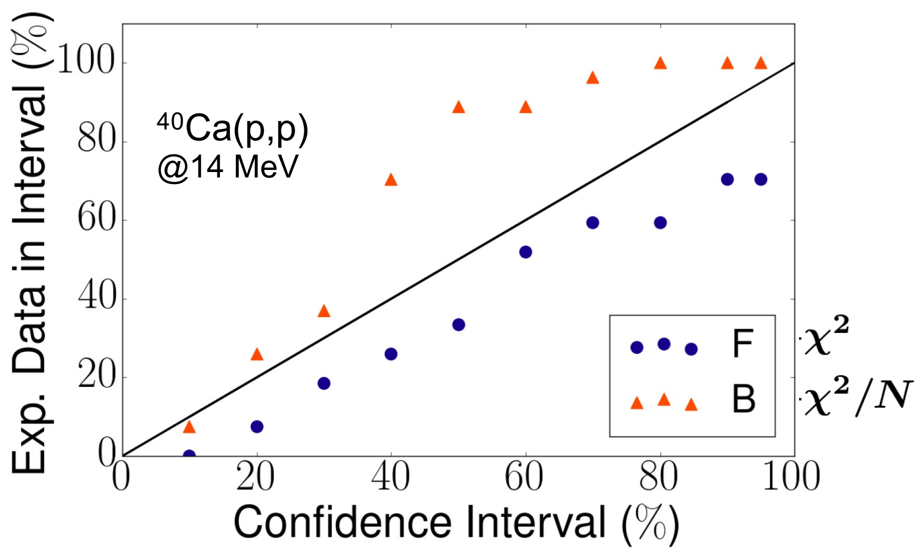
Complications:
- data correlations
- systematic errors on data underestimated
- model correlations
- model uncertainties

How to combine sets of angular distributions?

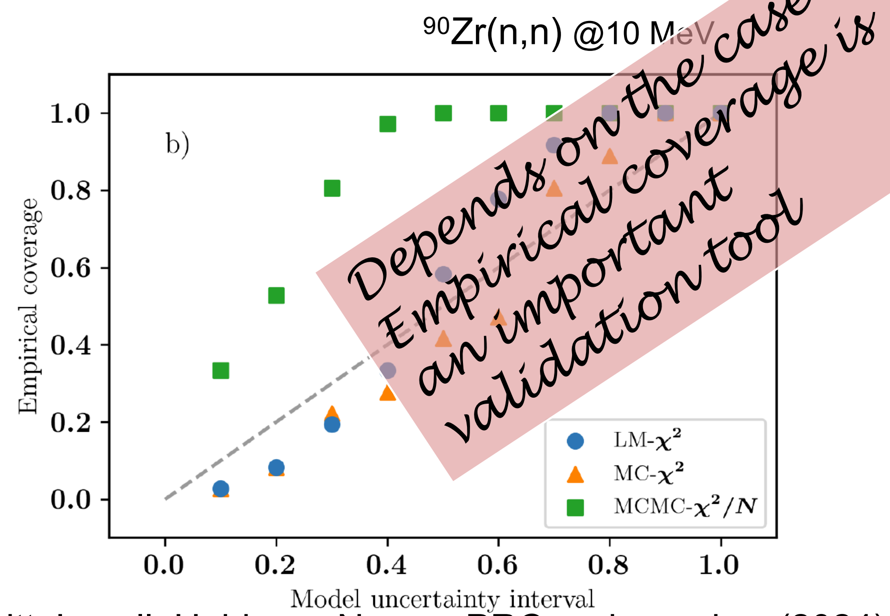
$$\chi^2 = \sum_{i=1}^{N} \frac{[\sigma_{\mathrm{exp}}(\theta_i) - \sigma_{\mathrm{th}}(\theta_i, x)]^2}{[\Delta\sigma_{\mathrm{exp}}(\theta_i)]^2}$$

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

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



King et al., PRL 2019



Depends on the case!!
Empirical coverage is an important validation tool

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

Georgia O'Keefe, mossandfog.com

thanks to all of you!

Work supported by NSF and DOE