Bayesian UQ in transfer reactions for astrophysics

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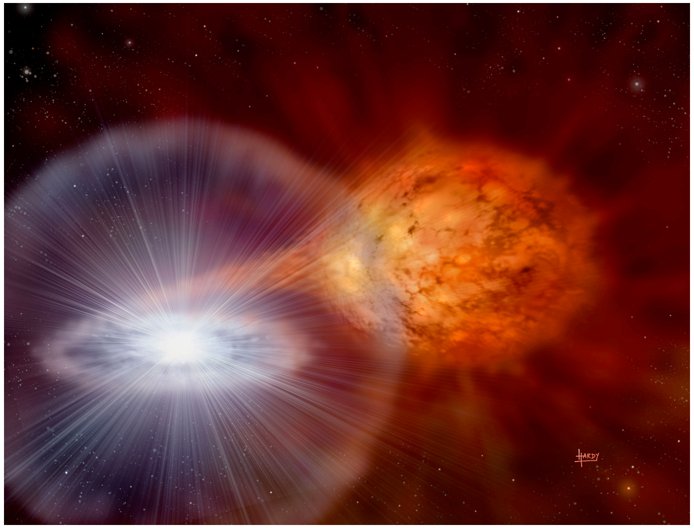
Work supported by NSF

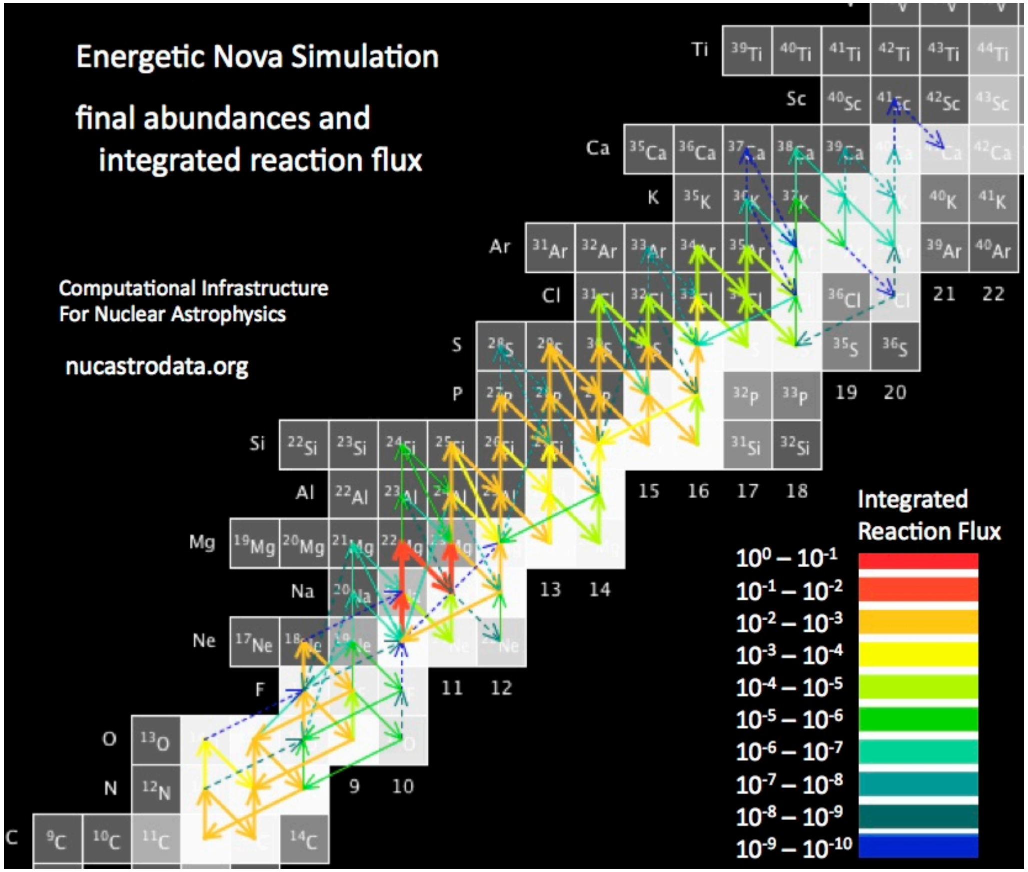
Outline

- Transfer reactions in the astrophysical context
- Source of uncertainties in reaction models
- Uncertainty quantification approaches
- Bayesian analysis to reduce uncertainties
- Challenges and Opportunities

From novae to nuclear reactions



apod.nasa.gov/

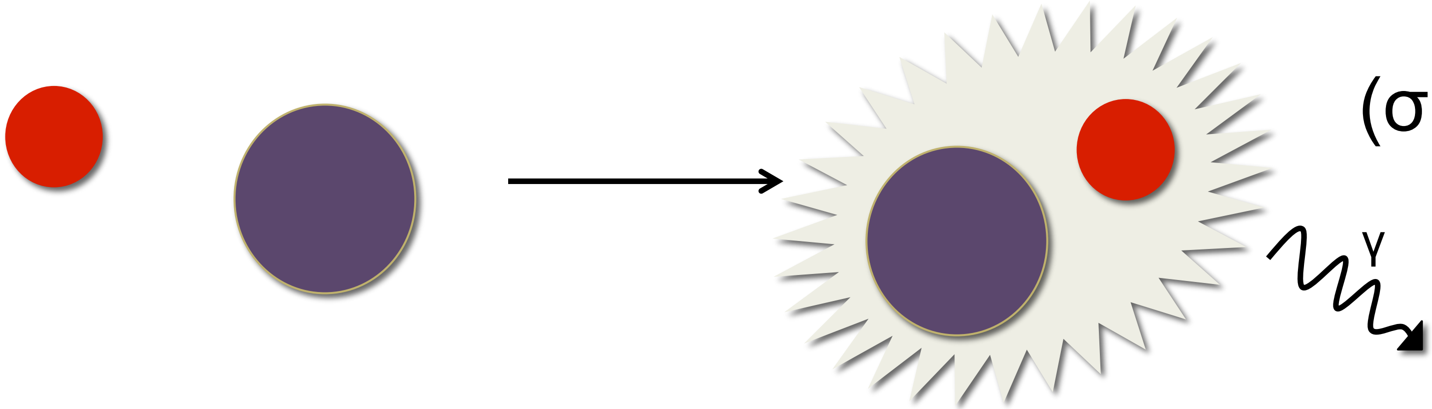


phy.ornl.gov/

need:
proton capture rates on
proton-rich nuclei

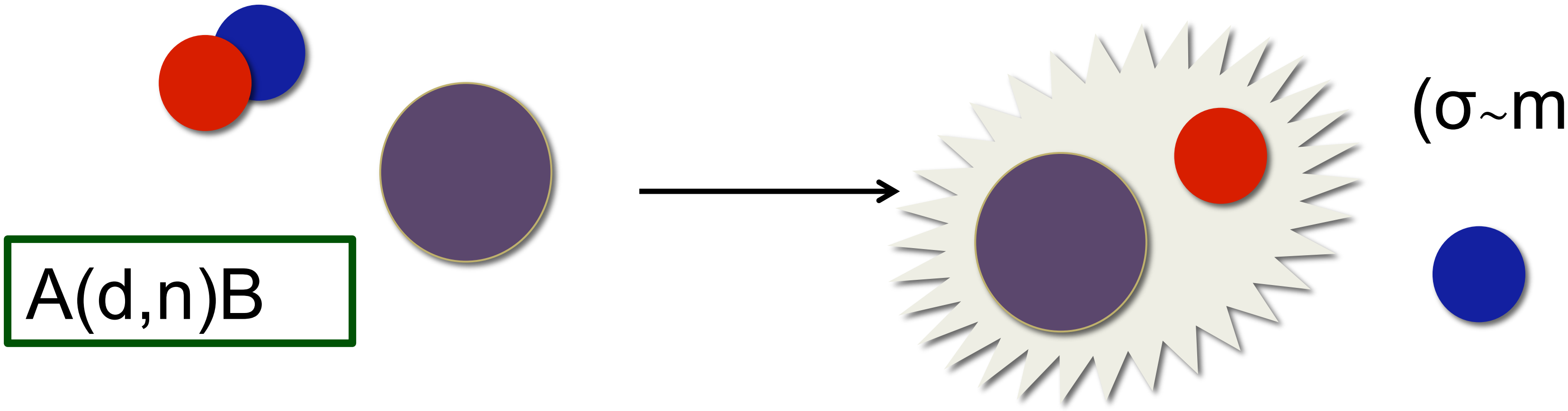
how do we measure charged- particle capture in the Gamow window?

- ✧ (p,γ) cross sections are very low



(σ~pb)

- ✧ (d,n) cross sections are many orders of magnitude higher!



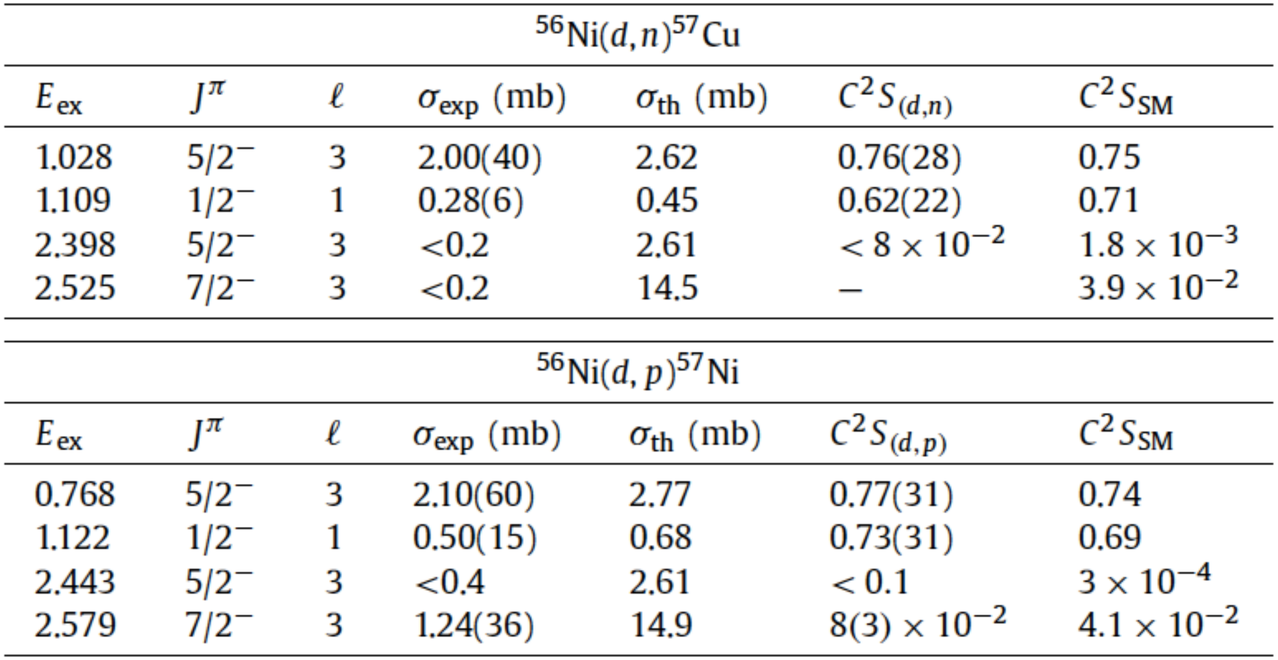
(σ~mb)

A(d,n)B

Applications to recent (p,g) measurements

^{56}Ni(d,nγ)^{57}Cu to extract ^{56}Ni(p,γ)^{57}Cu

NSCL: S800 for PID (^{57}Cu) + GRETINA for γ



^{56}Ni$(d,n)^{57}$Cu

E_{ex}	J^{π}	ℓ	σ_{exp} (mb)	σ_{th} (mb)	$C^2S_{(d,n)}$	C^2S_{SM}
1.028	$5/2^-$	3	2.00(40)	2.62	0.76(28)	0.75
1.109	$1/2^-$	1	0.28(6)	0.45	0.62(22)	0.71
2.398	$5/2^-$	3	<0.2	2.61	$< 8 \times 10^{-2}$	1.8×10^{-3}
2.525	$7/2^-$	3	<0.2	14.5	–	3.9×10^{-2}

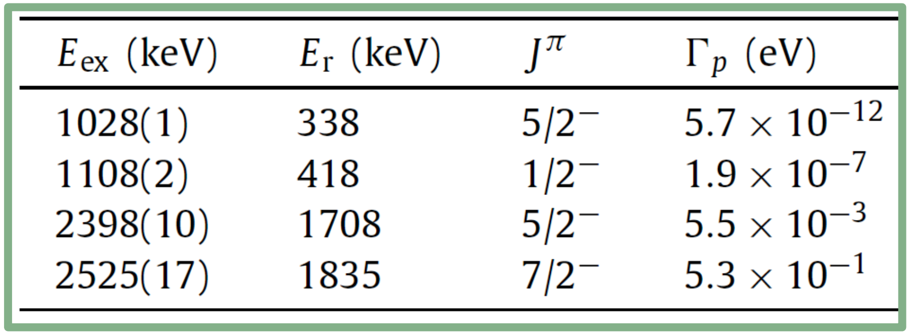
^{56}Ni$(d,p)^{57}$Ni

E_{ex}	J^{π}	ℓ	σ_{exp} (mb)	σ_{th} (mb)	$C^2S_{(d,p)}$	C^2S_{SM}
0.768	$5/2^-$	3	2.10(60)	2.77	0.77(31)	0.74
1.122	$1/2^-$	1	0.50(15)	0.68	0.73(31)	0.69
2.443	$5/2^-$	3	<0.4	2.61	< 0.1	3×10^{-4}
2.579	$7/2^-$	3	1.24(36)	14.9	$8(3) \times 10^{-2}$	4.1×10^{-2}

Angle integrated cross section only

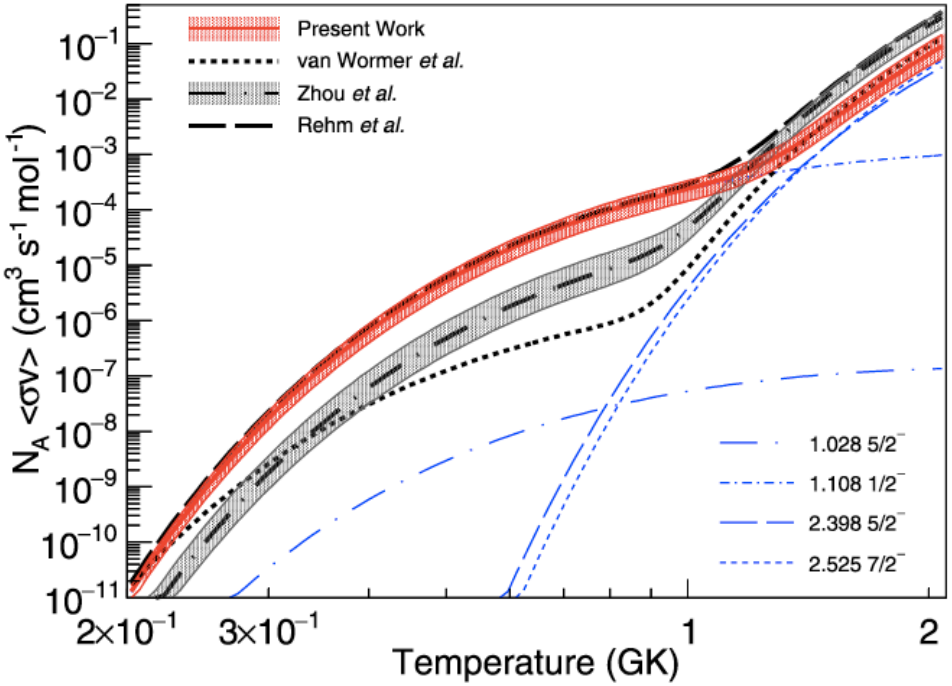
Dahl, Woods, Poxon-Pearson, et al, PLB 797 (2019) 134803

Applications to recent (d,n) measurements



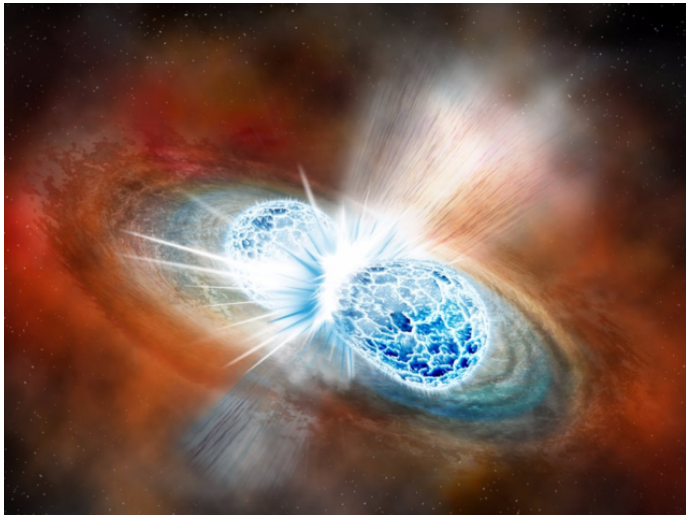
E_{ex} (keV)	E_r (keV)	J^π	Γ_p (eV)
1028(1)	338	$5/2^-$	5.7×10^{-12}
1108(2)	418	$1/2^-$	1.9×10^{-7}
2398(10)	1708	$5/2^-$	5.5×10^{-3}
2525(17)	1835	$7/2^-$	5.3×10^{-1}

^{56}Ni(p,γ)^{57}Cu rate

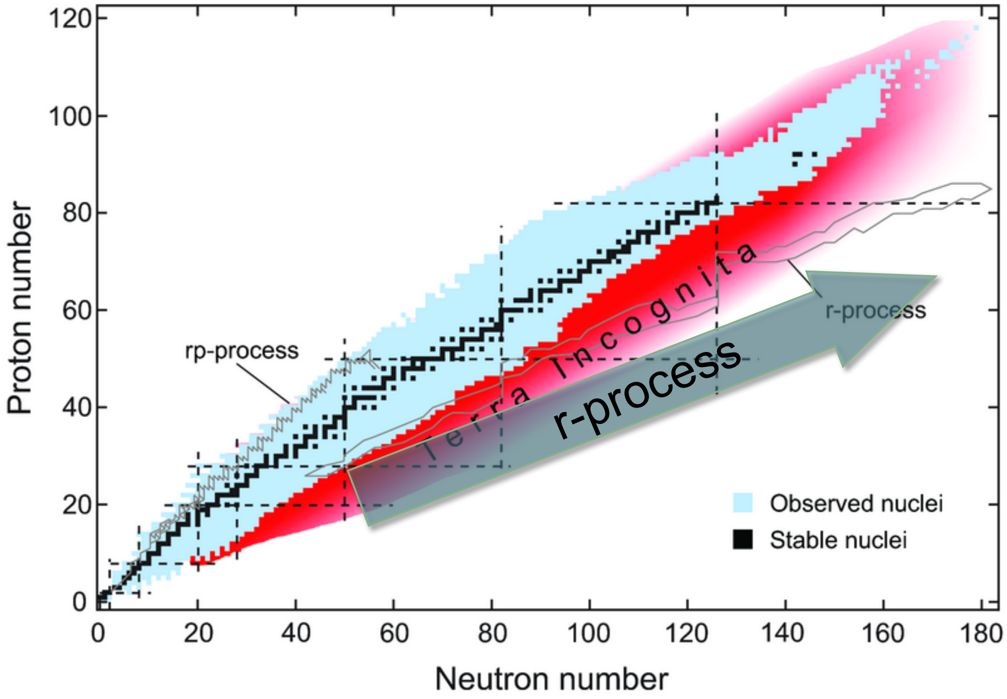


Dahl, Woods, Poxon-Pearson, et al, PLB 797 (2019) 134803

From neutron star mergers to reactions



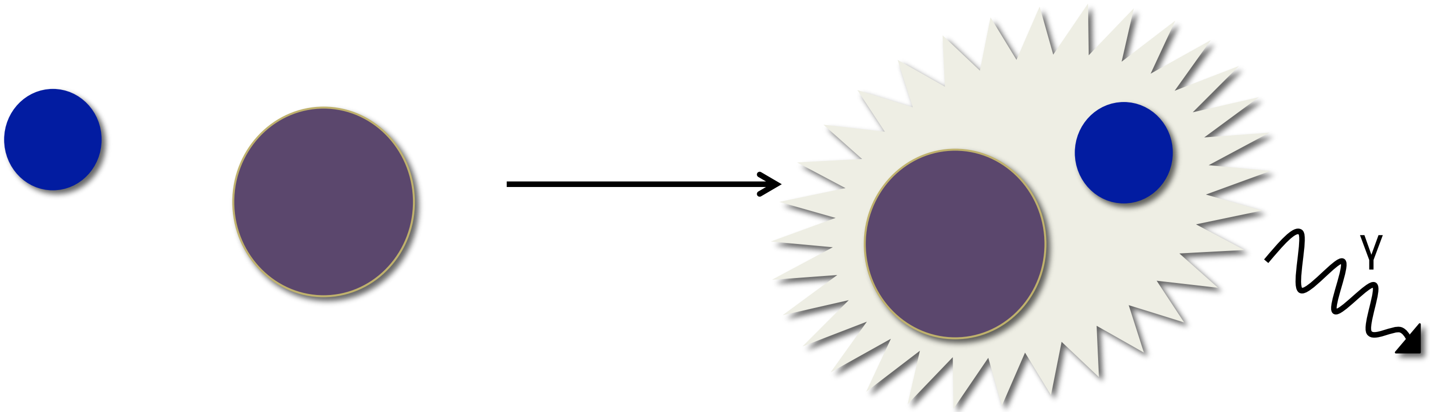
carnegiescience.edu/



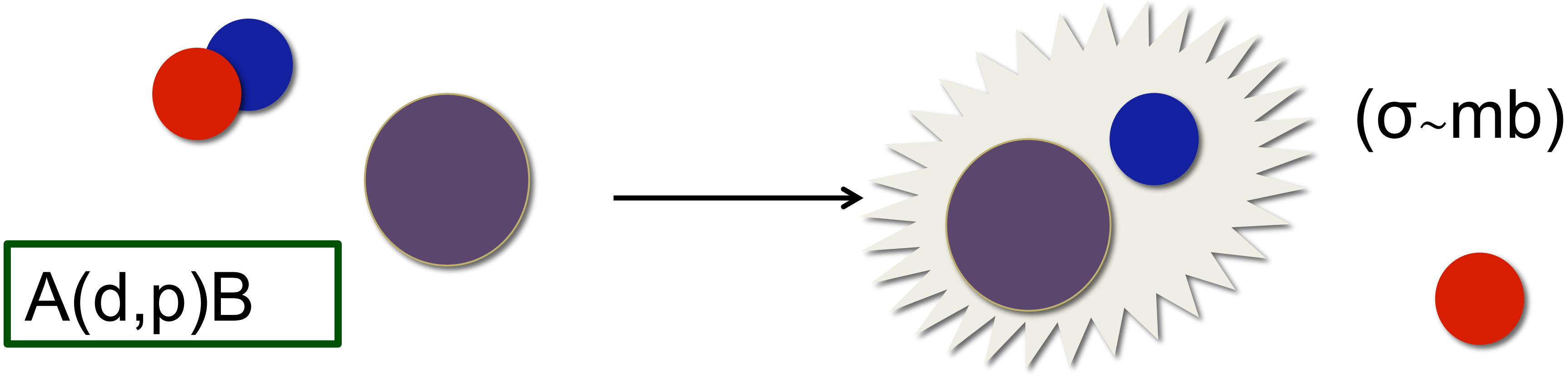
need:
neutron capture rates

how do we measure neutron capture on unstable nuclei?

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



- transfer offers an indirect measurement!



Applications to recent (n,γ) measurements

^{95}Mo(d,pγ)^{96}Mo to extract ^{95}Mo(n,γ)^{96}Mo

Compound nucleus (n,γ) is determined through:

$$\sigma_{\alpha\chi}(E_n) = \sum_{J,\pi} \sigma_{\alpha}^{\mathrm{CN}}(E_{ex}, J, \pi) G_{\chi}^{\mathrm{CN}}(E_{ex}, J, \pi)$$

xs for formation of CN
(depends on OP)

branching ratios
from surrogate
experiment

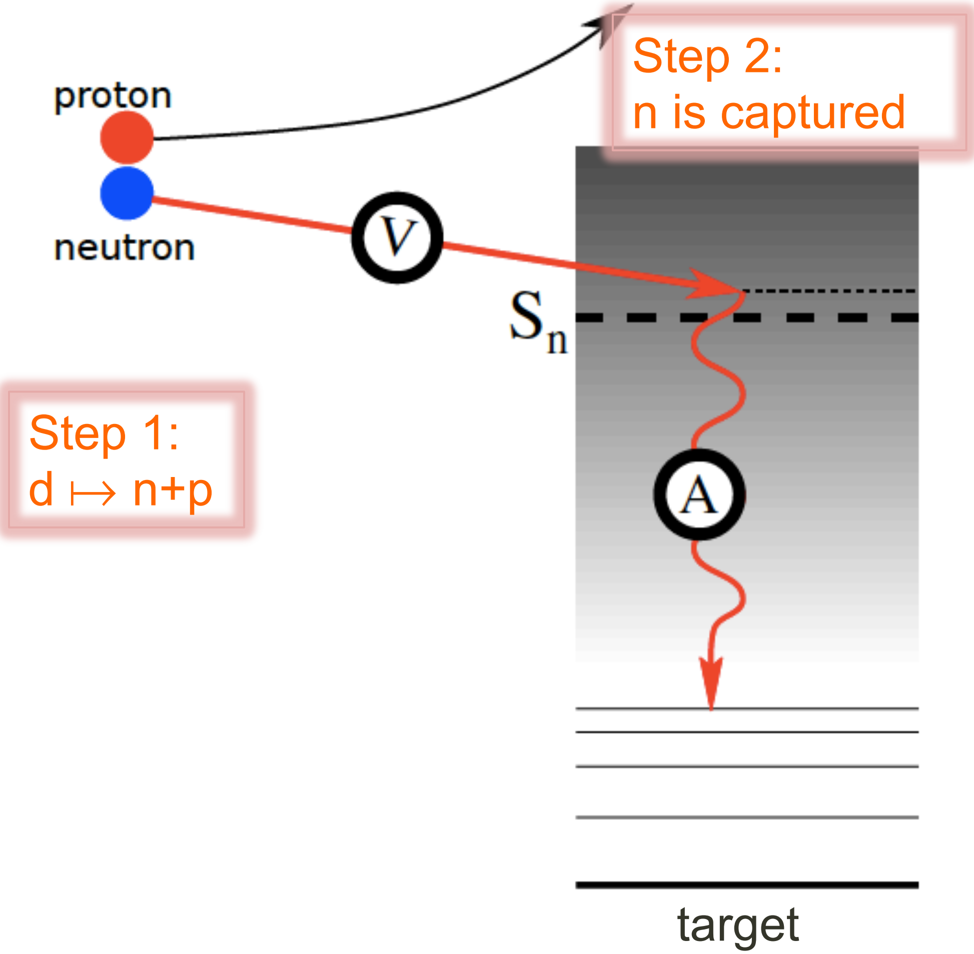
Compound nucleus (d,pγ) is determined through:

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

Ratkiewicz, Cizewski, Escher, Potel, et al. PRL 122, 052502

Theory for deuteron induced transfer: populating compound states in continuum

- ✧Two-step process



Step 2:
n is captured

Step 1:
d ↦ n+p

Source term generates flux from breakup

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

Neutron propogates in the field of the target after breakup

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

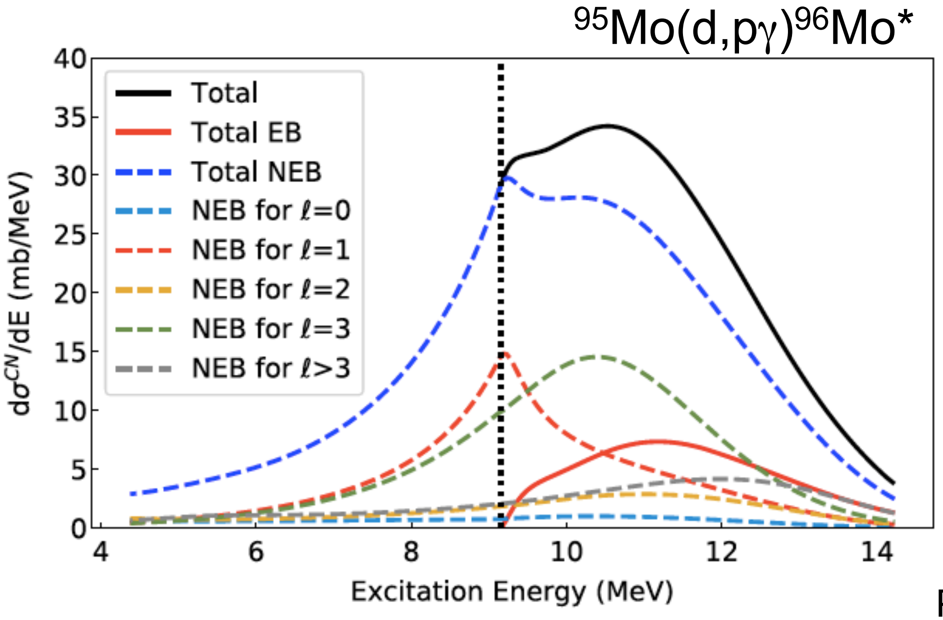
Potel, Nunes, Thompson, PRC92 (2015) 034611

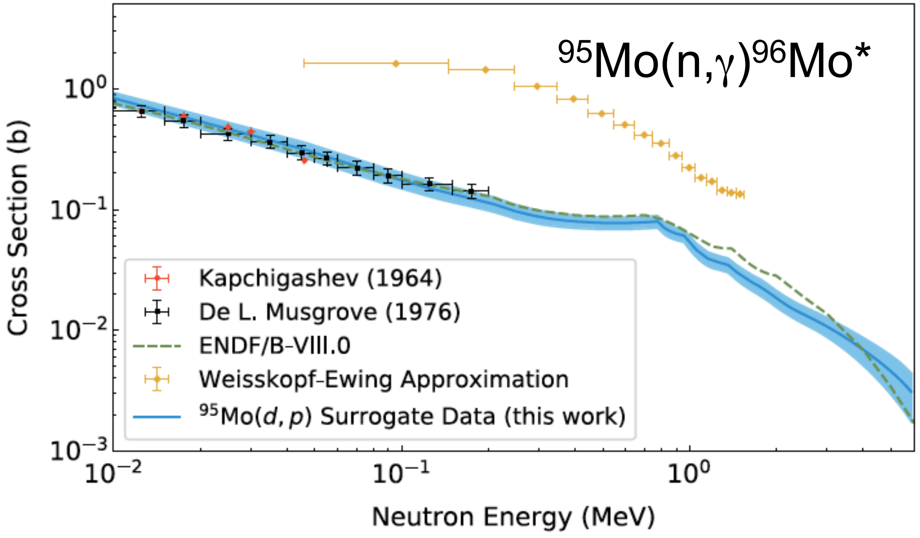
Applications to recent (n,γ) measurements

Compound nucleus (d,pγ) is determined through:

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

L-distributions in (d,p) are different from those in (n,g)
reaction theory provides essential input


^{95}Mo(d,pγ)^{96}Mo*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Ratkiewicz, Cizewski, Escher, Potel, et al. PRL 122, 052502

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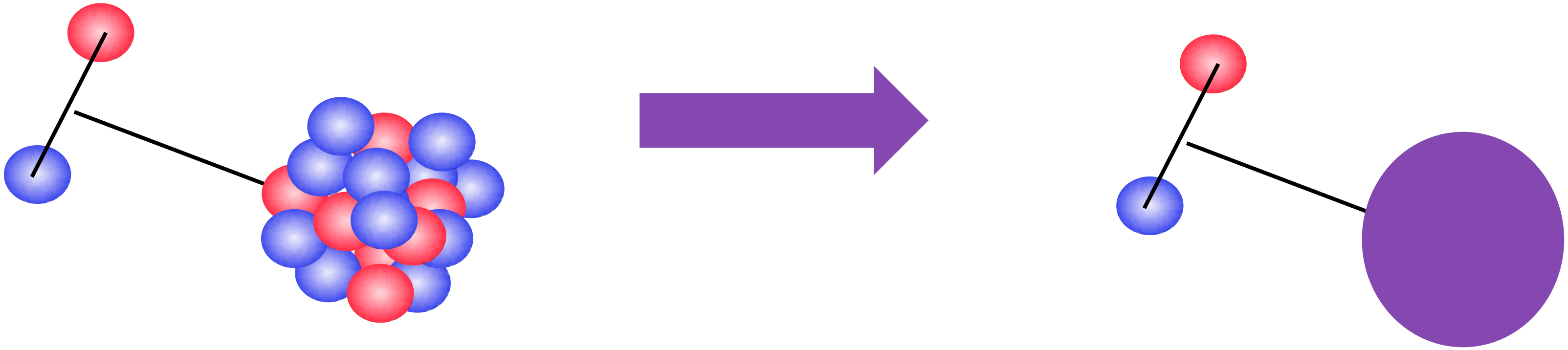
Mapping the many-body onto the few-body



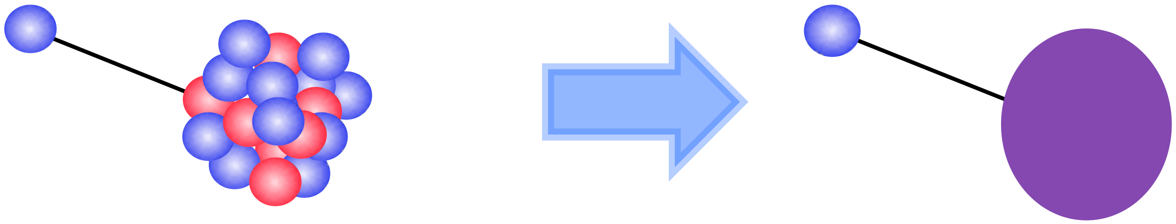
✓ solving the few-body scattering problem?

? the effective interactions (parametric uncertainties)

? target excitations/3-body force/other channels

(model uncertainties)

Effective interactions? Optical potentials



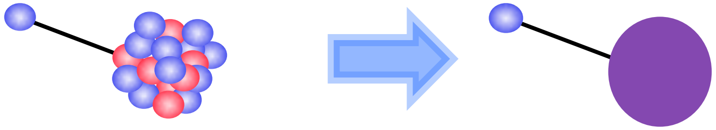
U_{opt} is intrinsically non-local, L-dependent, E-dependent

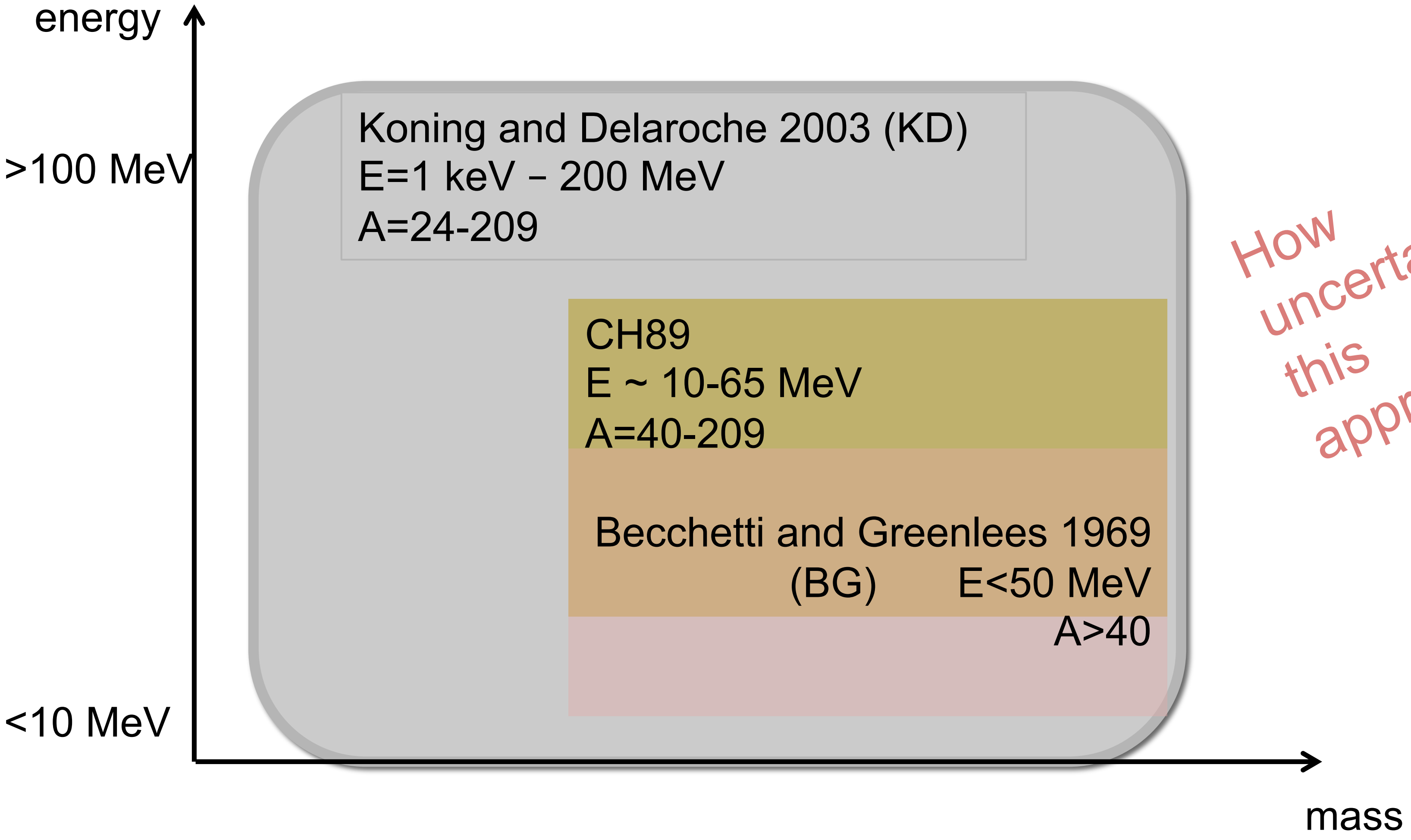
Phenomenological approach:

fit a set of data (typically elastic scattering)
extract model parameters of an assumed shape
typically local, L-independent, strongly E-dependent

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

A map of global optical potentials





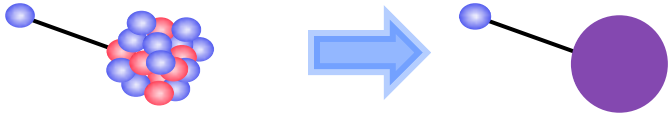
Koning and Delaroche 2003 (KD)
E=1 keV – 200 MeV
A=24-209

CH89
E ~ 10-65 MeV
A=40-209

Becchetti and Greenlees 1969
(BG) E<50 MeV
A>40

How uncertain is this approach?

How to quantify uncertainties



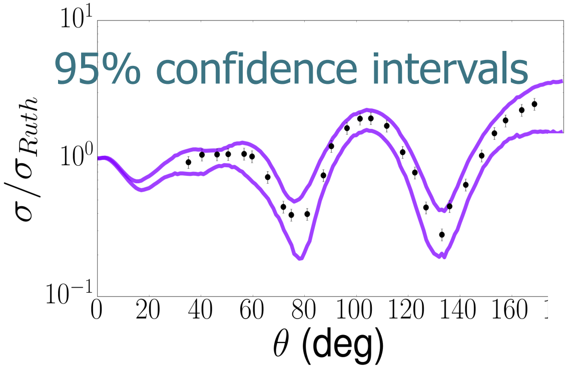
We develop a hypothesis (model) with a set of parameters (priors)

optical model

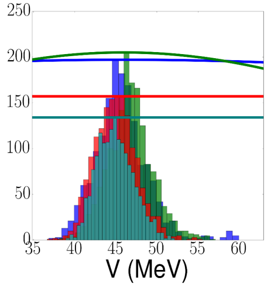
$[T+U(R)-E]\psi=0$

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

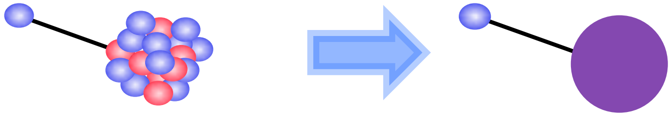
Use Bayes' Theorem + Markov Chain Monte Carlo to sample parameter space


95% confidence intervals

Constraints on the model



Setting up the UQ part



Priors: Gaussians with mean at the BG global parameters and width 100% of the mean

Data: real data versus mock generated from KD global parameters with 10% error

Likelihood: assumption that data points are independent and errors are normally distributed

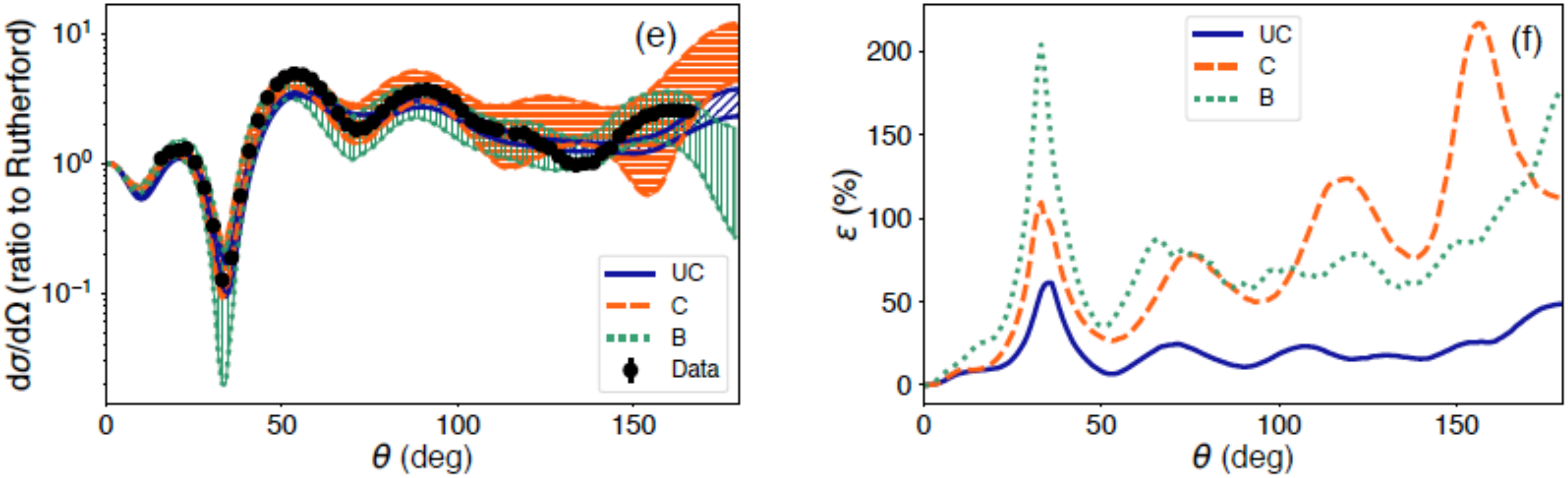
θ: parameters
σ: independent errors
x: angles
y: experimental cross section
f: model prediction for cross section

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

The formulation of the likelihood matters

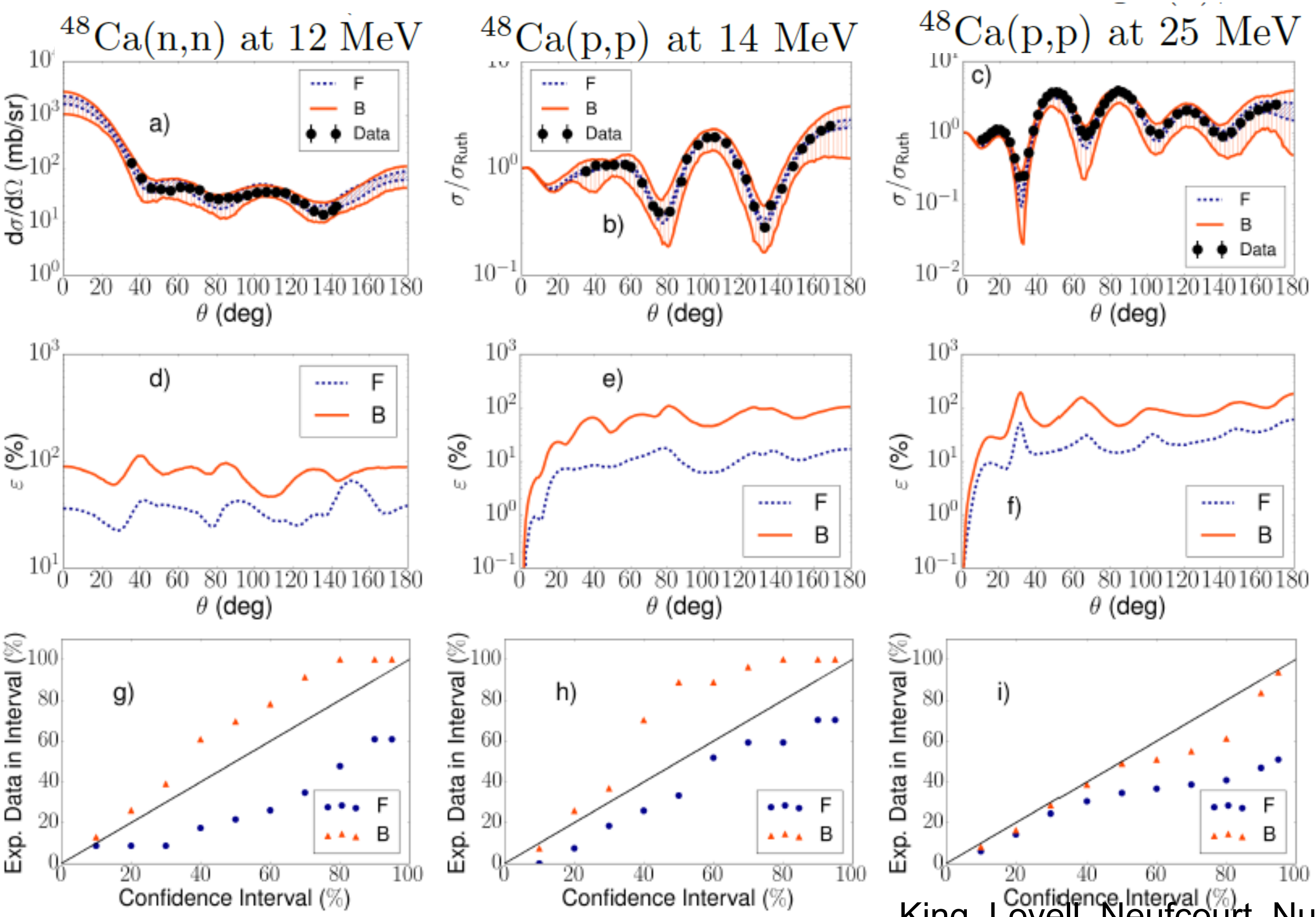
UC – uncorrelated chi2 frequentist
C – correlated chi2 frequentist
B - Bayesian

^{40}Ca(p,p)^{40}Ca at 26.3 MeV



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

Optical model uncertainties: comparing frequentist and Bayesian



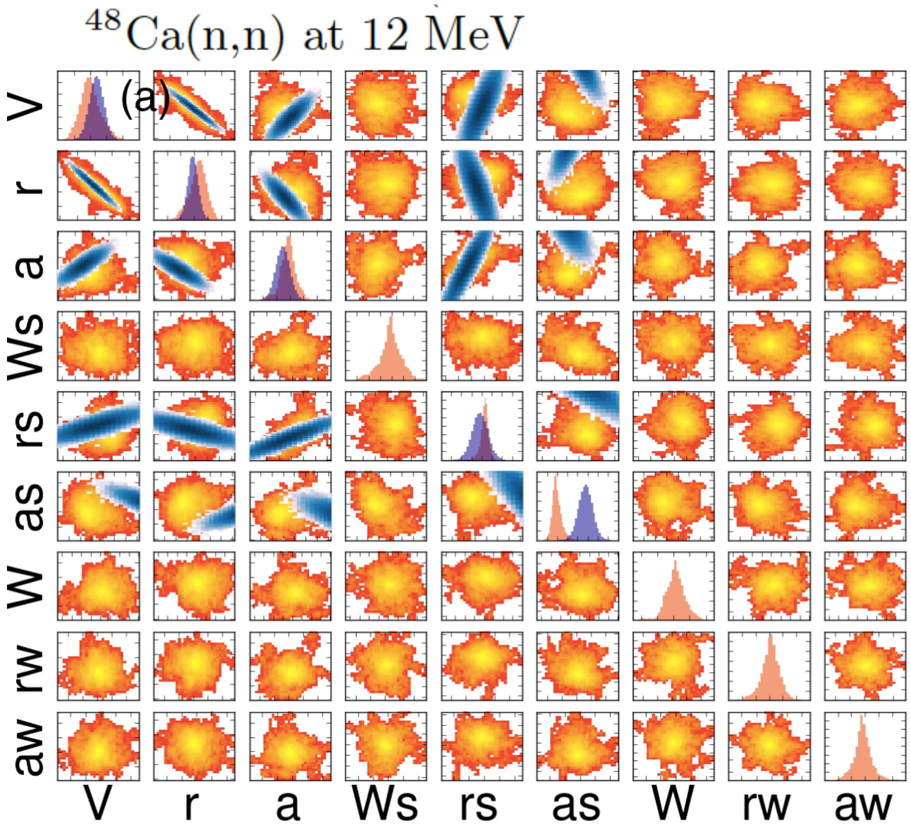
Cross section angular distributions

Percentage uncertainty width

Empirical coverage

King, Lovell, Neufcourt, Nunes PRL (2019)

Optical model uncertainties: comparing frequentist and Bayesian

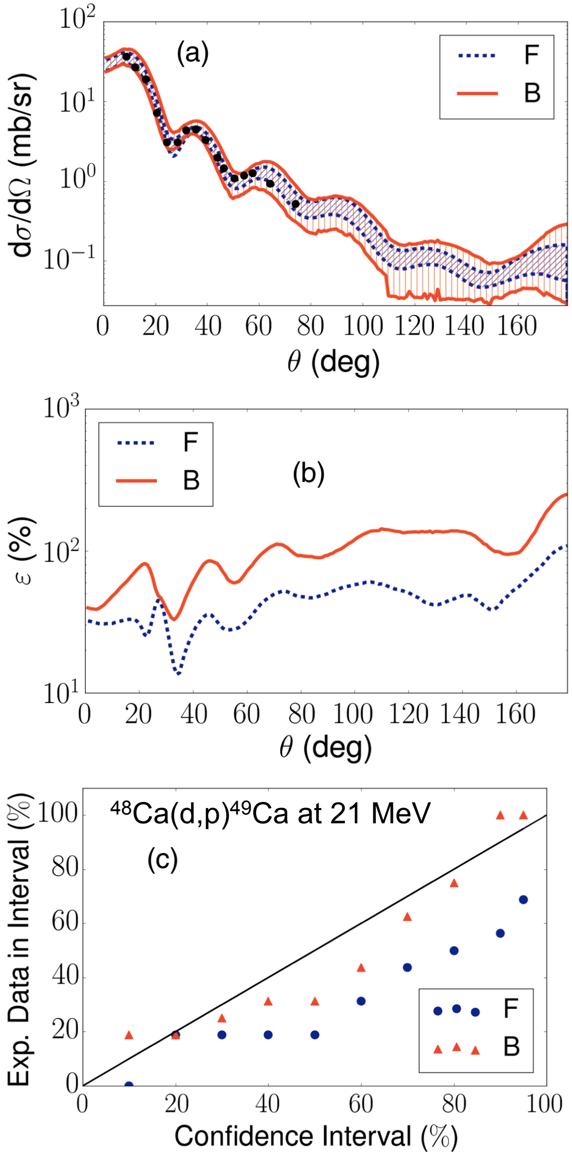


parameter correlations in Bayesian look very different to the frequentist approach

blue (frequentist)
orange (Bayesian)

King, Lovell, Neufcourt, Nunes PRL (2019)

Propagating optical model uncertainties to (d,p) comparing frequentist and Bayesian



Uncertainties are larger than previously thought

Must explore other ways to reduce optical potential uncertainties

King, Lovell, Neufcourt, Nunes PRL (2019)

Outline

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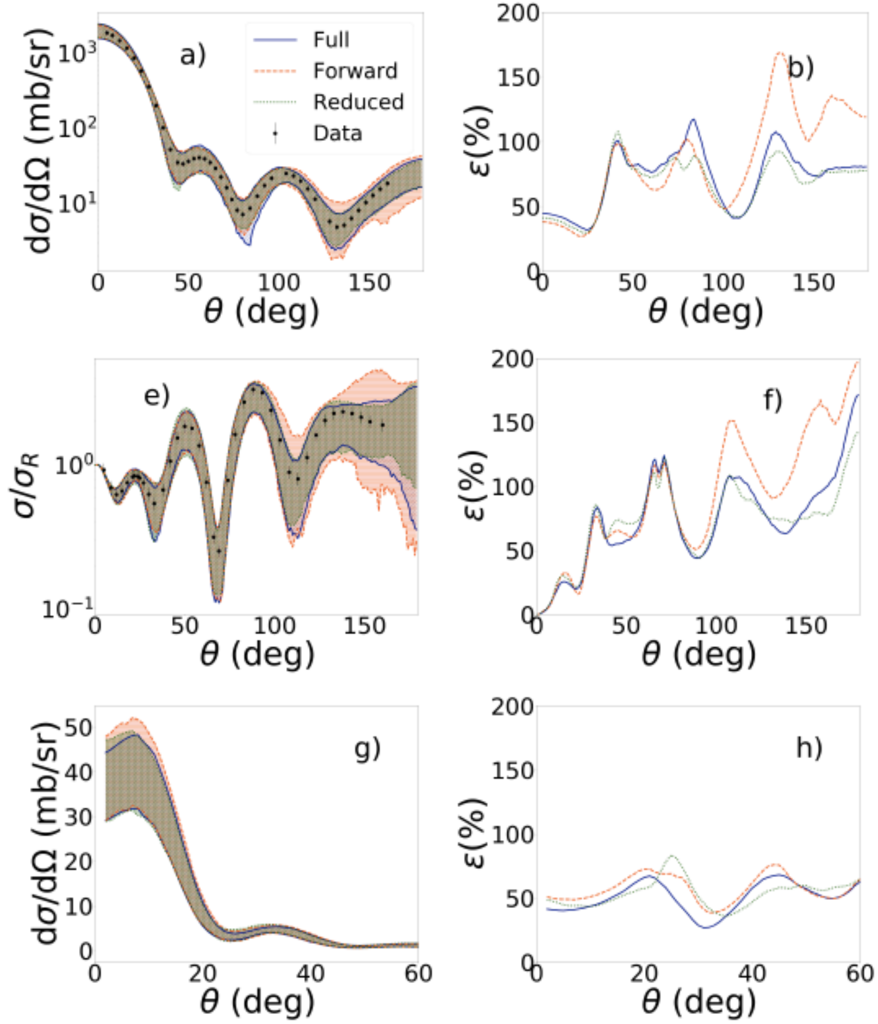
Angular information needed?



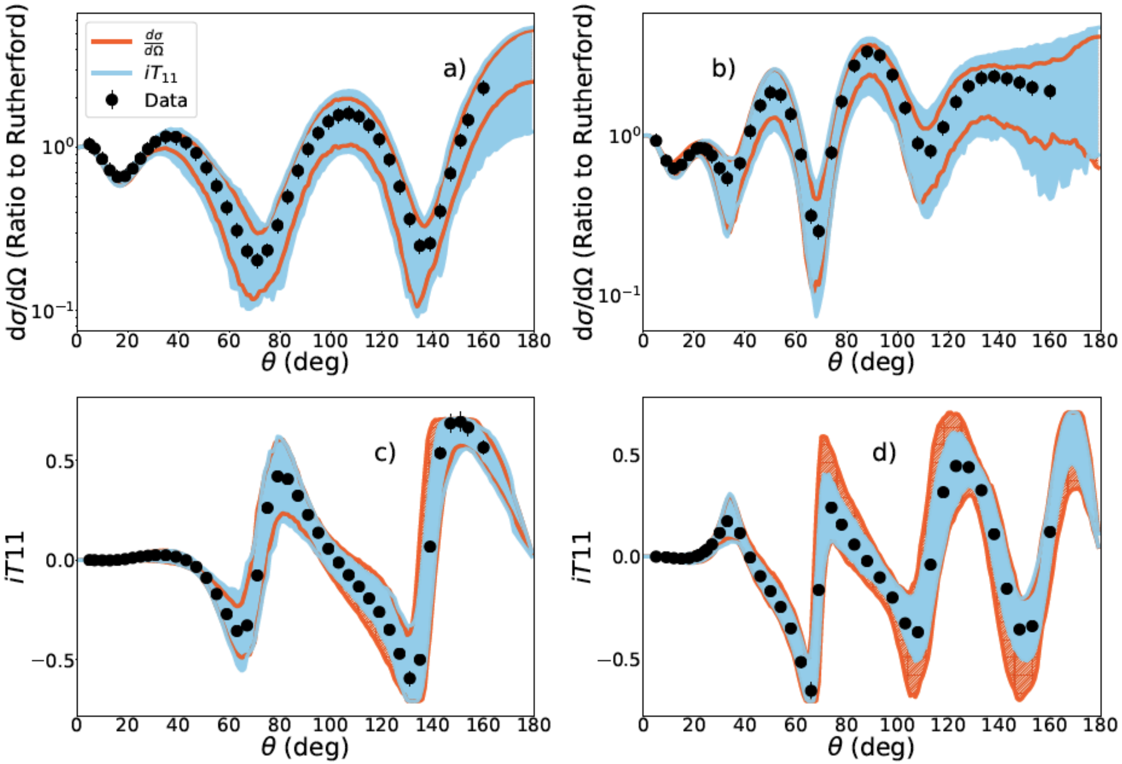
^{48}Ca(n,n)^{48}Ca at 12 MeV

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

^{48}Ca(d,p)^{49}Ca at 21 MeV

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

Which observable offers best constraint?



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

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

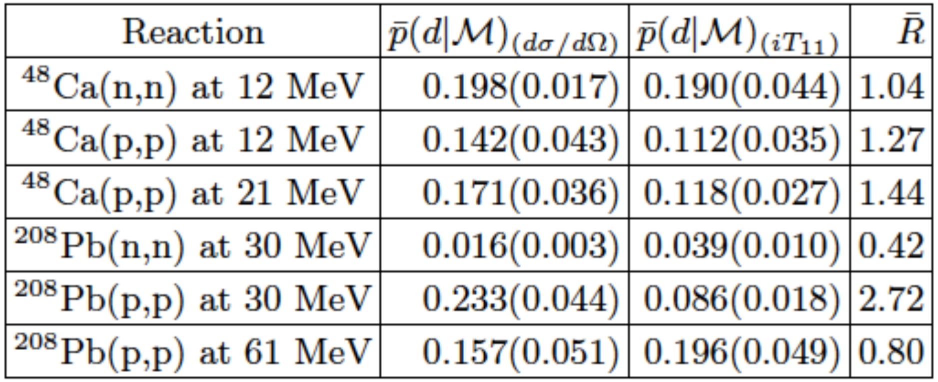
Observable	E (MeV)	V (MeV)	r (fm)	a (fm)	W_s (MeV)	r_s (fm)	a_s (fm)
$\frac{d\sigma}{d\Omega}$	12.0	59.48 (4.12)	1.173 (0.052)	0.699 (0.051)	9.476 (0.960)	1.294 (0.084)	0.571 (0.049)
iT_{11}	12.0	60.65 (5.22)	1.159 (0.057)	0.699 (0.067)	9.704 (0.954)	1.273 (0.079)	0.595 (0.080)
$\frac{d\sigma}{d\Omega}$	21.0	55.57 (4.11)	1.178 (0.052)	0.661 (0.057)	7.857 (0.767)	1.297 (0.083)	0.572 (0.051)
iT_{11}	21.0	57.16 (4.44)	1.165 (0.047)	0.691 (0.046)	8.011 (1.007)	1.260 (0.073)	0.579 (0.076)

Catacora-Rios, King, Lovell and Nunes, PRC (2020) under review

What is the information content of the data?

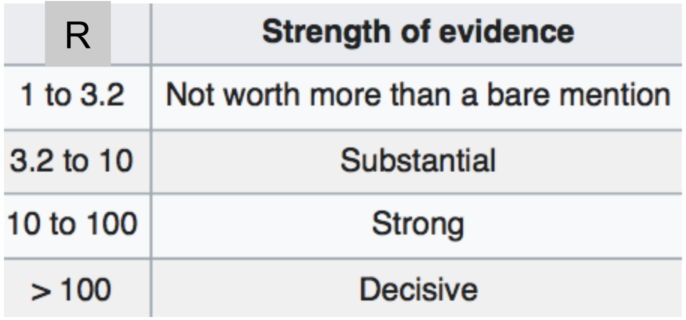
Bayesian evidence: provides information contained in a data set.
Integral of the likelihood times the prior over full parameters space

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



Reaction	$\bar{p}(d\vert\mathcal{M})_{(d\sigma/d\Omega)}$	$\bar{p}(d\vert\mathcal{M})_{(iT_{11})}$	$\bar{R}$
^{48}Ca(n,n) at 12 MeV	0.198(0.017)	0.190(0.044)	1.04
^{48}Ca(p,p) at 12 MeV	0.142(0.043)	0.112(0.035)	1.27
^{48}Ca(p,p) at 21 MeV	0.171(0.036)	0.118(0.027)	1.44
^{208}Pb(n,n) at 30 MeV	0.016(0.003)	0.039(0.010)	0.42
^{208}Pb(p,p) at 30 MeV	0.233(0.044)	0.086(0.018)	2.72
^{208}Pb(p,p) at 61 MeV	0.157(0.051)	0.196(0.049)	0.80

TABLE II: Bayesian evidence (multiplied by 10^{-3}) for the different reactions considered: using only cross section data (2nd column), using only polarization data (3rd column), and the ratio between the Bayesian evidence with cross section data over that with polarization data (the Bayes' factor).



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

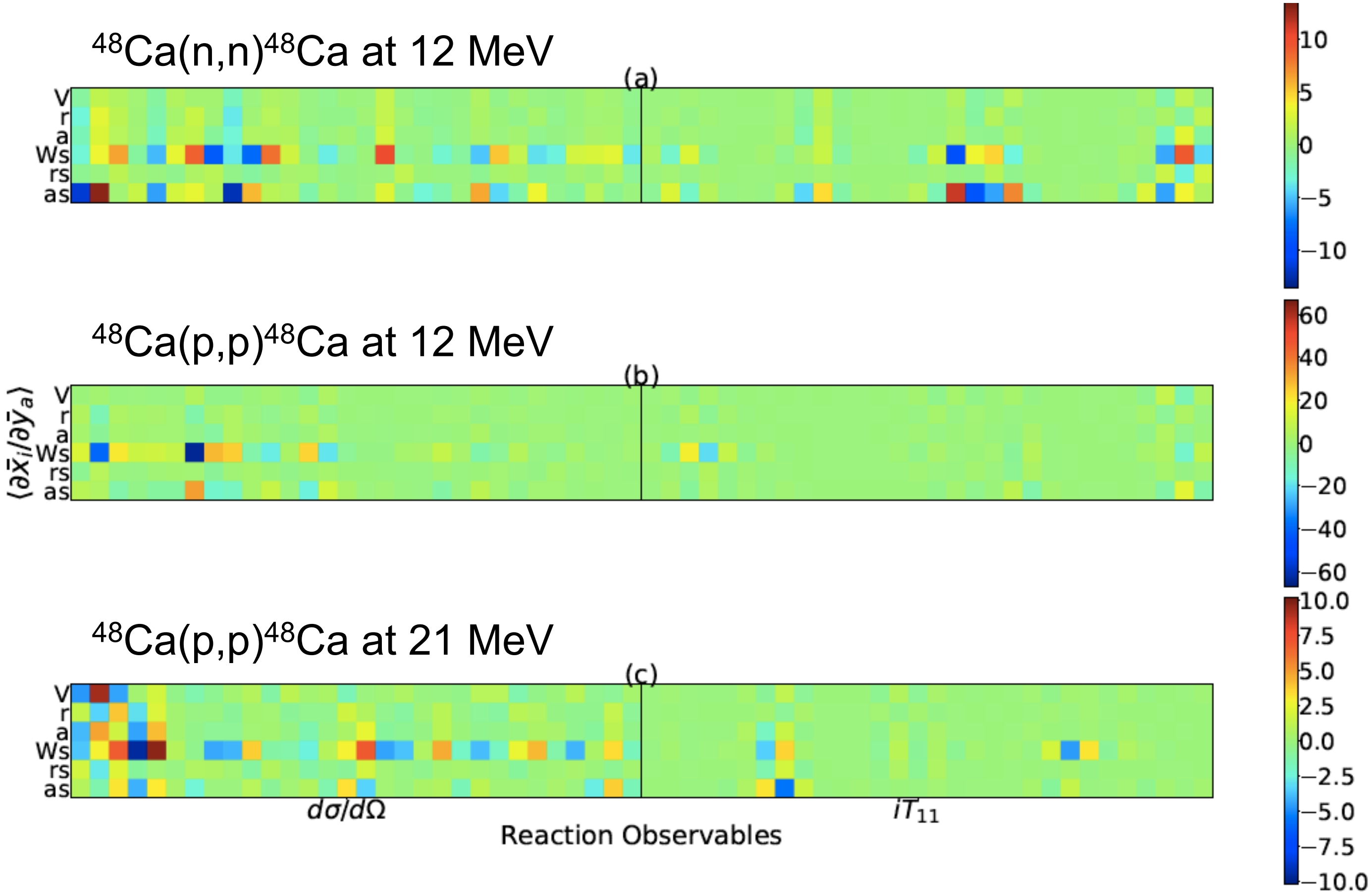
Kass and Raftery,
J. Amer. Stat. Assoc 9 (430) 791

Catacora-Rios, King, Lovell and Nunes, PRC (2020) under review

What do we learn from sensitivities?

how much variation in parameter x_i is produced by a variation on observable y_a?

$$\left\langle \frac{\partial \bar{x}_i}{\partial \bar{y}_a} \right\rangle = \widetilde{\mathbb{C}}_{ib} \mathbb{C}^{-1}_{ba}$$



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

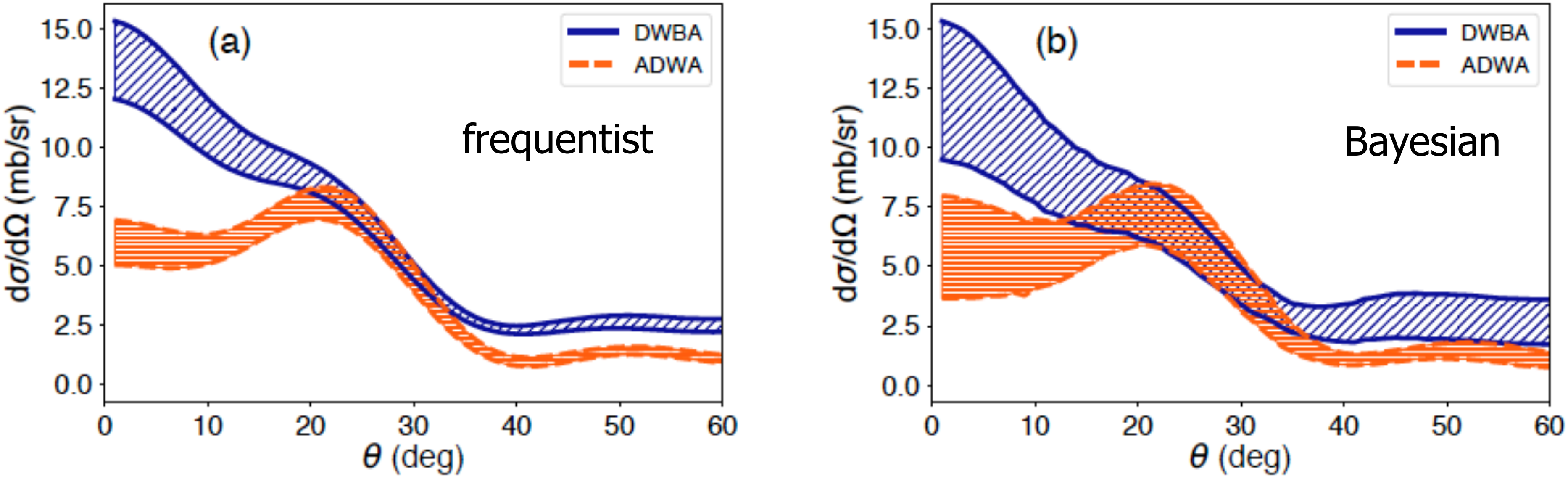
^{48}Ca(p,p)^{48}Ca at 12 MeV

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

Catacora-Rios, King, Lovell and Nunes, PRC (2020) under review

Comparing models

^{40}Ca(d,p)^{41}Ca at 28.4 MeV



Can we discriminate between models?

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

Opportunities for the next 5yrs

- ❑ go beyond the simplest reaction models
- ❑ quantify model uncertainties
- ❑ perform model mixing

Computational challenge: need Emulators

Eigenvector continuation method for scattering
to reduce the dimensionality of the problem
Furnstahl et al. PLB 809 (2020) 135719

$$|\psi_{\text{trial}}\rangle = \sum_{i=1}^{N_b} c_i |\psi_E(\boldsymbol{\theta}_i)\rangle$$

QUILTR

Quantifying Uncertainties in Low energy Theory for Reactions

It's a suite of codes including Bayesian MCMC for optical model calibration and propagation of uncertainties to transfer reactions


LRDesignsQuilting.com

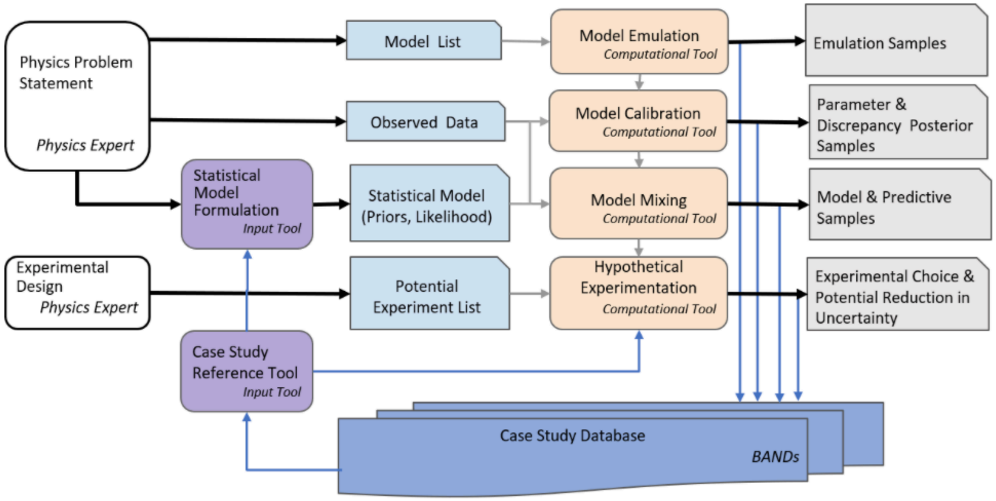
(by Amy Lovell)

Wrappers built on:
FRESCO (by Ian Thompson)

BAND

Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io



Physics Problem Statement
Physics Expert

Experimental Design
Physics Expert

Statistical Model Formulation
Input Tool

Case Study Reference Tool
Input Tool

Model List

Observed Data

Statistical Model (Priors, Likelihood)

Potential Experiment List

Model Emulation
Computational Tool

Model Calibration
Computational Tool

Model Mixing
Computational Tool

Hypothetical Experimentation
Computational Tool

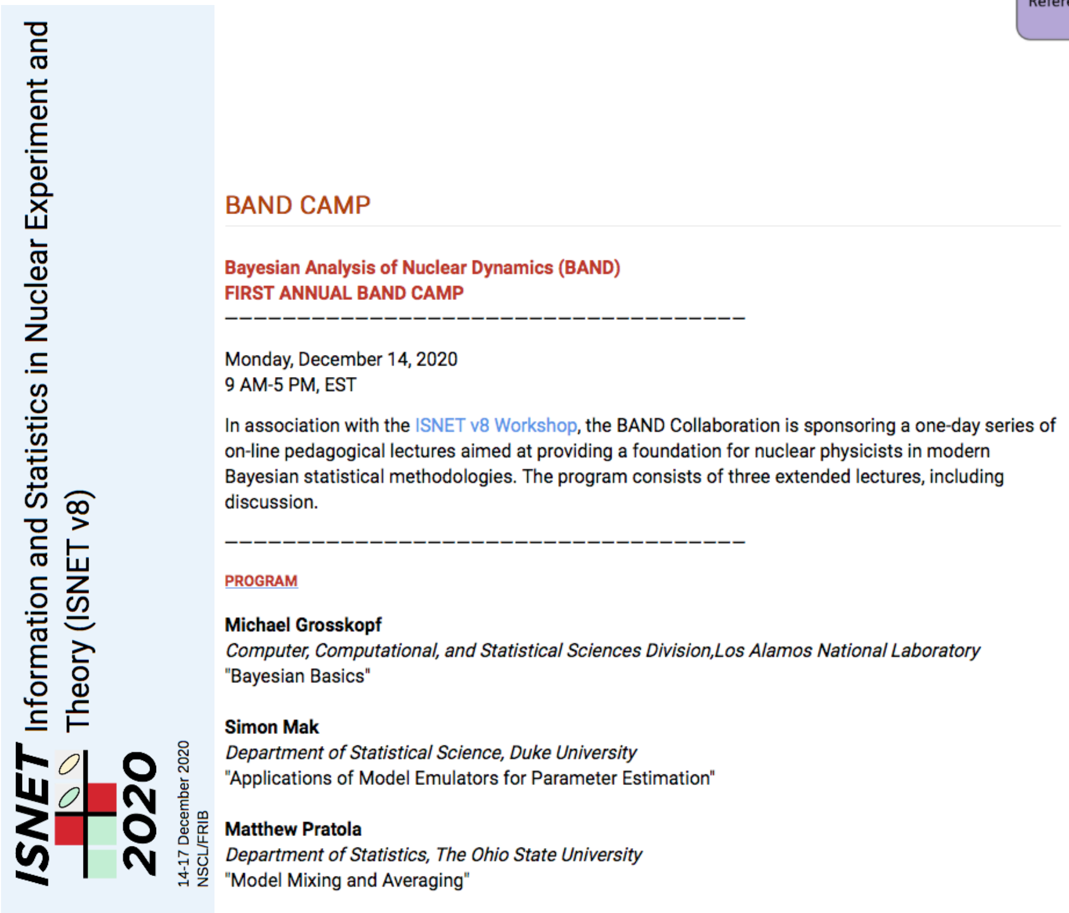
Emulation Samples

Parameter & Discrepancy Posterior Samples

Model & Predictive Samples

Experimental Choice & Potential Reduction in Uncertainty

Case Study Database
BANDs



ISNET 2020 Information and Statistics in Nuclear Experiment and Theory (ISNET v8)

14-17 December 2020
NSCL/FRIB

BAND CAMP

Bayesian Analysis of Nuclear Dynamics (BAND)
FIRST ANNUAL BAND CAMP

————————————————————————————

Monday, December 14, 2020
9 AM-5 PM, EST

In association with the ISNET v8 Workshop, the BAND Collaboration is sponsoring a one-day series of on-line pedagogical lectures aimed at providing a foundation for nuclear physicists in modern Bayesian statistical methodologies. The program consists of three extended lectures, including discussion.

————————————————————————————

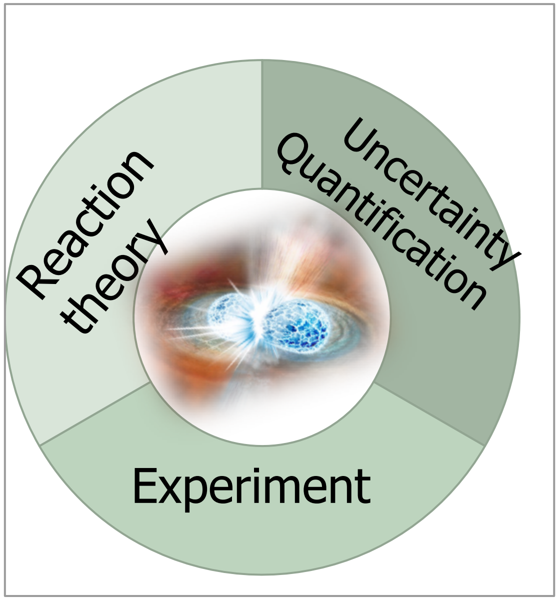
PROGRAM

Michael Grosskopf
Computer, Computational, and Statistical Sciences Division,Los Alamos National Laboratory
"Bayesian Basics"

Simon Mak
Department of Statistical Science, Duke University
"Applications of Model Emulators for Parameter Estimation"

Matthew Pratola
Department of Statistics, The Ohio State University
"Model Mixing and Averaging"

In conclusion:



- Transfer reactions offer a versatile tool for extracting capture rates for astrophysics (many recent applications with impact on astrophysics)
- Reactions theories is needed to interpret the indirect measurements and obtain reliable capture rates
- Uncertainty quantification is an essential ingredient and Bayesian analysis offers many new avenues and a promising future of collaboration with experiment.

Thanks to my collaborators

Amy Lovell
(now staff at LANL)

Garrett King
(now GS WashU)

Manuel Catacora Rios
(now GS UChicago)

Michael
Quinonez

UQ reactions group

Transfer applications

Gregory Potel
(now at LLNL)

Terri Poxon-Pearson
(now at NNSA)

Many thanks to all for zooming in!