Nuclear reaction theory for astrophysics and other applications

Russbach School on Nuclear Astrophysics Russbach, Austria

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Abstract:

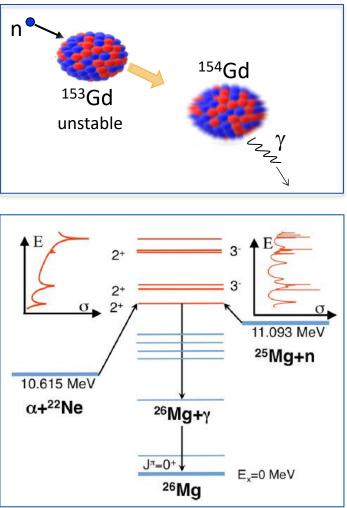
The last decade has seen much progress in the development of theory tools that allow us to achieve more accurate calculations for both direct and compound (statistical) nuclear reactions. Integrated nuclear structure and reaction descriptions provide the basis for making cross-section predictions and enable indirect determination of cross sections that are difficult to measure directly. This is particularly important for applications involving reactions with unstable nuclei, such as astrophysics simulations.

I will discuss recent advances at the intersection of direct and compound-nuclear reactions. I will give examples where progress in theory has enabled indirect (surrogate) measurements of compound-nuclear reactions, including both low-energy neutron capture and other desired reactions. I will also comment on efforts underway to measure reactions in inverse-kinematics experiments at radioactive-beam facilities.

*This work is performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Support from the LDRD Program, Projects 19-ERD-017, 20-ERD-030, 21-LW-032, 22-LW-029, 23-SI-004, and 24-ERD-023 is acknowledged.



Nuclear astrophysics requires information on multiple types of reactions

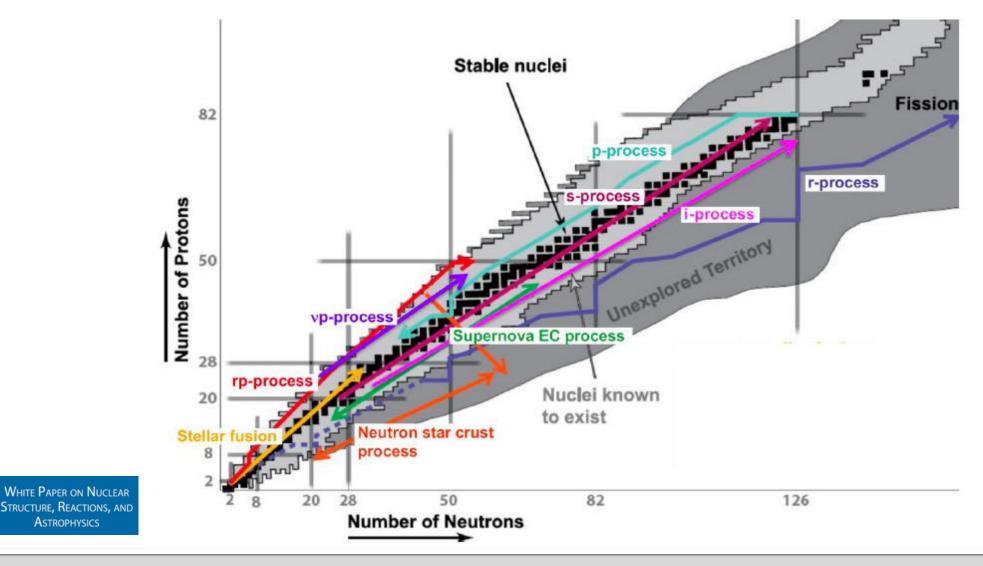


Massimi et al, PLB (2017)

- Many low-energy reactions of interest are compound reactions
 - Cross sections can exhibit resolved resonances
 - Cross sections may be dominated by smooth averages over dense, overlapping resonances
- Direct reactions typically play a smaller role



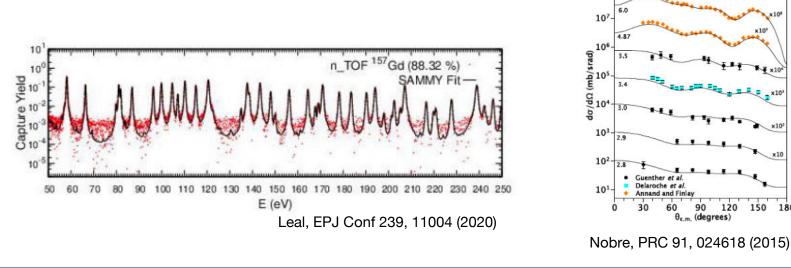
Nuclear astrophysics requires information on multiple types of reactions for a wide range of isotopes

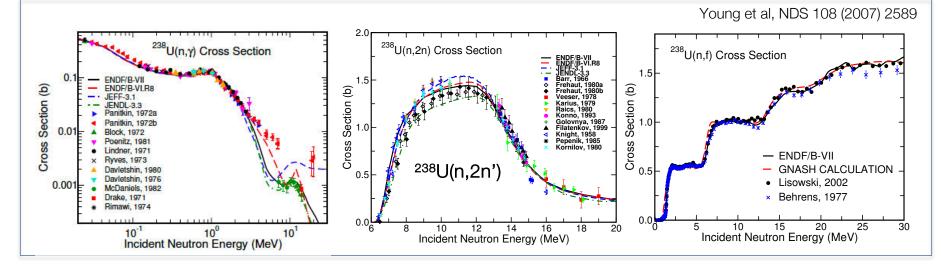




We have robust reaction theories and flexible data evaluation tools to describe a wide variety of reactions

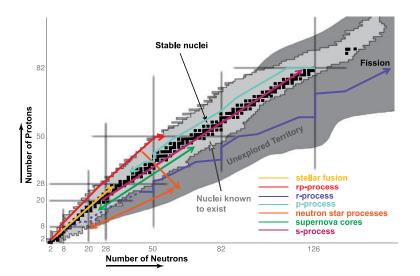
- Multiple reaction mechanism & types
 - Direct, resonance, compound (overlapping resonances)
 - n-induced, charged-particle
 - $-\gamma$ emission, particle emission, fission
- Evaluations
 - Tools: coupled-channels, R-matrix,
 - Hauser-Feshbach codes
 - RIPL-3 parameters
 - Covariances
- Reaction theories
 - Contain simple nuclear structure description
 - Adjust parameters to experimental data





'Simple' descriptions require data to adjust parameters in phenomenological models

- Challenges:
 - Ambiguous model combinations, large parameter uncertainties, and multiple reaction channels produce large uncertainties in reaction calculations
 - Away from stability, where few/no constraints are known, minor processes may become significant
- Needed a multipronged approach:
 - development of predictive microscopic structure and reaction theories
 - direct measurements (where possible) to validate theory
 - indirect measurements to constrain theory





Substantial progress in integrating nuclear structure & reaction theory for light nuclei

Successful ab initio reaction descriptions

- Treat structure and reactions simultaneously (NCSM/RGM approach)
- State-of-the-art NN+3N nuclear interactions
- Computationally challenging
- Restricted to selected area(s) of nuclear chart

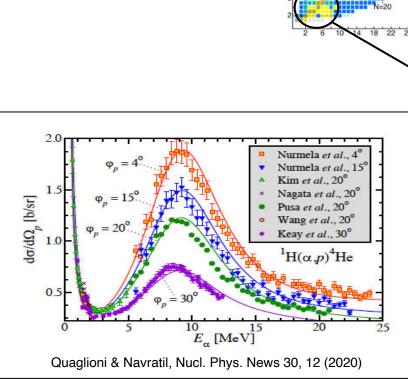
Resonating Group Method (RGM):

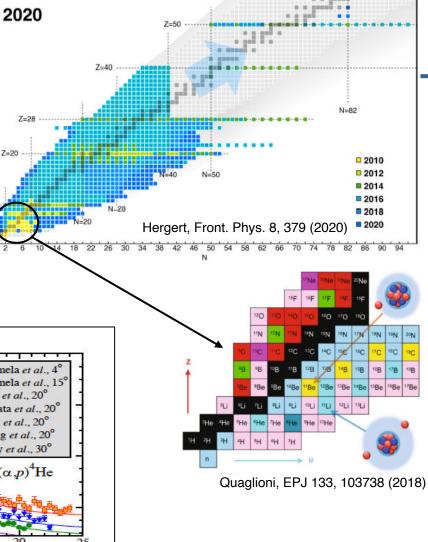
Ansatz:

$$|\Psi\rangle = \sum_{\nu} \int_{r} \mathrm{d}r \ r^{2} \frac{g_{\nu}(r)}{r} \hat{\mathcal{A}} |\Phi_{\nu r}\rangle$$

• Solve Hill-Wheeler eqn to obtain amplitude $g_{\nu}(r)$: $\sum_{\nu} \int dr \ r^2 \left[H_{\nu'\nu}(r',r) - EN_{\nu'\nu}(r',r) \right] \frac{g_{\nu}(r)}{r} = 0.$

Johnson et al, J. Phys.G 47, 123001 (2020)





Mercenne, Launey, Dytrych, Escher, et al, CPC 280, 108476 (2022) Launey, Dytrych, Mercenne, Ann. Rev. Nucl. Part. Sci. 71, 253 (2021) Dreyfuss, Launey, Escher, Sargsyan, et al., PRC 102, 044608 (2020)

Resonating Group Method (RGM):

• Ansatz:

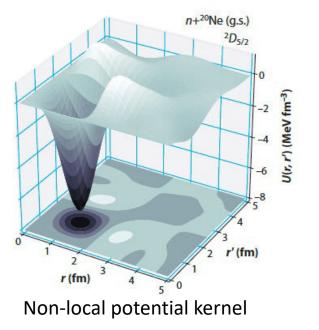
$$\Psi^{J^{\pi}M}\rangle = \sum_{c} \int_{z} dr r^2 \frac{g_c^{J^{\pi}M}(r)}{r} \mathcal{A}_c |\Phi_{cr}^{J^{\pi}M}\rangle$$

• Solve Hill-Wheeler eqn to obtain amplitude $g_{\nu}(r)$:

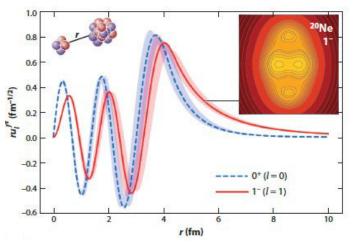
 $\sum_{c} \int dr r^2 \left[H_{c'c}(r',r) - E N_{c'c}(r',r) \right] \frac{g_c^{J^{\pi}M}(r)}{r} = 0.$

- Norm and potential kernels expressed in terms of SU(3) re-coupling coefficients and one-body (and two-body) density matrix elements
- Advantages:
 - Triple-reduced matrix elements
 - Block-diagonal norm kernel
 - Proton-neutron formalism

Initial steps for calculating phase shifts and N+A scattering



Overlaps for $\alpha\text{-induced}$ reactions



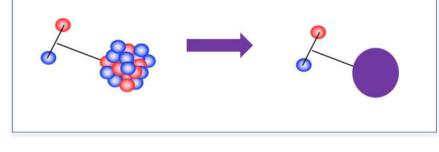
 $\alpha\text{+}^{16}\text{O}$ /=0 and 1 relative wave functions (ab initio SA-NCSM)

Initial results are promising. More development needed to predict reactions like $^{22}Ne(\alpha,n)^{25}Mg$

What about reaction theory for medium-mass and heavy nuclei?

Direct reactions

- Reduction to few-body problems with effective interactions
- Mechanisms: transfer, inelastic scattering, breakup
- Higher-order processes: multi-step, coupled-channels, breakup-fusion,...
- Efforts underway to integrate nuclearstructure descriptions



Compound-nuclear (CN) reactions

R-matrix regime

resonances

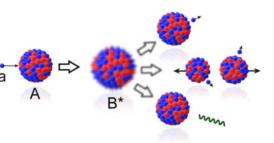
data or fully microscopic

calculation

Assumes isolated

Requires measured

- R-matrix theory describes CN reactions through isolated resonances
- Hauser-Feshbach (HF) theory describes CN reactions that can be statistically averaged
- Both are essential for nuclear data evaluations and calculating astrophysical reaction rates





- Assumes strongly overlapping resonances
- Requires structure models
 and parameters

ZERO

ENERGY

FOR a+A

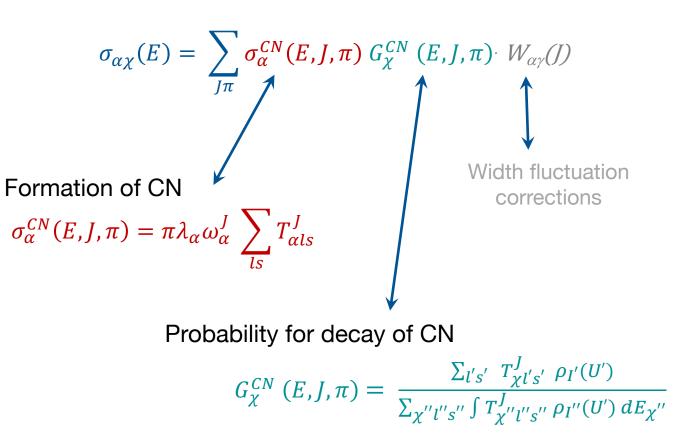
ENERGY LEVELS

$$\sigma_{\alpha\chi} = \sum_{J,\pi} \sigma_{\alpha}^{CN} (E, J, \pi) \cdot G^{CN}_{\chi} (E, J, \pi)$$

*WFC omitted here to simplify notation.



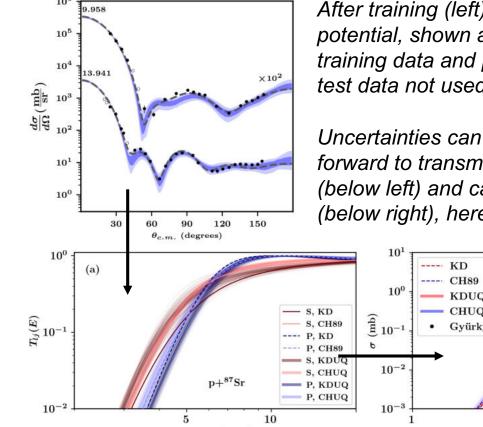
- Inputs needed:
 - Optical-model potentials
 - Level densities (LDs)
 - $-\gamma$ -ray strength functions (γ SF)
 - Constraints: D_0 , $<\Gamma_\gamma>$, cross section data
- Challenges:
 - Ambiguous model combinations, large parameter uncertainties, and multiple reaction channels
 - Uncertainty quantification
 - Away from stability there are few/no known constraints





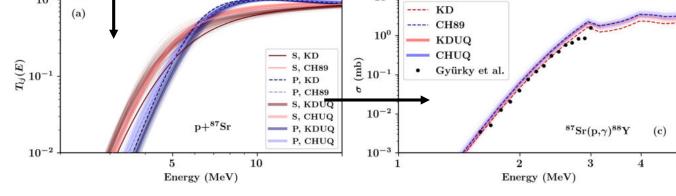
Uncertainty-Quantified (UQ) Optical Potentials for isotopes near stability: KDUQ and CHUQ

- We developed *well-calibrated uncertainties* for two widely used optical potentials
- Advances include outlier identification, assessment of *unaccounted-for uncertainty*
- We can now pinpoint how optical-potential uncertainties impact compound (low-energy) and direct (higher energy) reactions within a self-consistent framework
- Parameters provided with uncertainty ranges and as posterior collection - see PRC supplement.



After training (left), the UQ optical potential, shown as blue bands, spans its training data and performs well against test data not used in training (not shown).

Uncertainties can then be propagated forward to transmission coefficients (below left) and capture cross sections (below right), here for 87 Sr(p,y) 88 Y.



A global phenomenological dispersive OMP is under development.

Dispersive OMPs connect to bound-state properties - which helps address the lack of data for exotic nuclei.

- Expected influx of data for reactions on unstable isotopes from FRIB requires developing new OMPs for neutron-rich isotopes, including fission fragments.
- The status of OMPs was reviewed at a Topical Program at FRIB and findings were published in a review paper:
 - C. Hebborn *et al*, "Optical potentials for the rare-isotope beam area," J. Phys. G. 50, 060501 (2023).

https://arxiv.org/abs/2210.07293

 The publication discusses state-of-the-art potentials, identifies shortcomings, and charts a path for future theoretical and experimental work.

	Mass	Energy	D.	Mic.	UQ
KD	$24 \le A \le 209$	$1~{\rm keV} \le E \le 200~{\rm MeV}$	×	×	×
KDUQ	$24 \le A \le 209$	$1~{\rm keV} \le E \le 200~{\rm MeV}$	×	×	1
DOM (STL)	C, O, Ca, Ni, Sn, Pb isotopes	$-\infty < E < 200~{\rm MeV}$	1	×	1
MR	12 < Z < 83	$E < 200 { m ~MeV}$	1	×	X
MBR	12 < Z < 83	$E < 200 { m ~MeV}$	1	×	X
NSM	40 Ca, 48 Ca, 208 Pb	$E < 40 { m MeV}$	1	1	X
SCGF	O, Ca, Ni isotopes	$E < 100 { m ~MeV}$	1	1	×
MST-B	$A \le 20$	$E\gtrsim70~{ m MeV}$	×	1	×
MST-V	$4 \le A \le 16$	$E\gtrsim 60~{ m MeV}$	×	1	×
WLH	$12 \leq A \leq 242$	$0 \le E \le 150 \text{ MeV}$	×	1	1
JLMB	A > 30	$1~{\rm keV} < E < 340~{\rm MeV}$	x	1	×



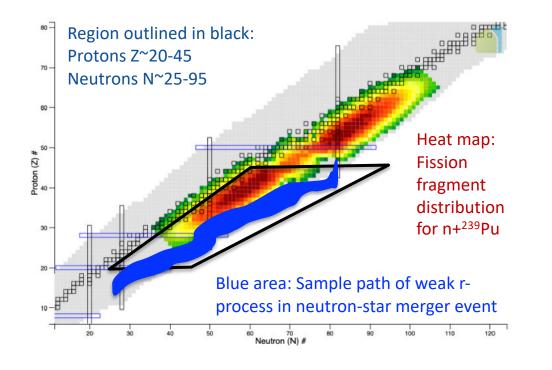
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 - Uncertainty quantification
 - Away from stability there are few/no known constraints
- Needed a multipronged approach:
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 $\sigma_{\alpha\chi}(E) = \sum_{J\pi} \sigma_{\alpha}^{CN}(E, J, \pi) G_{\chi}^{CN}(E, J, \pi) W_{\alpha\gamma}(J)$ Width fluctuation Formation of CN corrections $\sigma_{\alpha}^{CN}(E,J,\pi) = \pi \lambda_{\alpha} \omega_{\alpha}^{J} \sum T_{\alpha ls}^{J}$ Probability for decay of CN $G_{\chi}^{CN}(E,J,\pi) = \frac{\sum_{l's'} T_{\chi l's'}^{J} \rho_{I'}(U')}{\sum_{\chi'' I''s''} \int T_{\chi'' I''s''}^{J} \rho_{I''}(U') dE_{\chi''}}$



Are we ready to predict neutron capture cross sections for unstable nuclei relevant to the r process? What does it take? Escher, Kravvaris, Potel, Pruitt, Berryman, Gorton (wip)

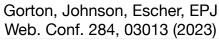
- Opportunity: Advances in nuclear theory place region of the weak r-process (light fission fragments) within striking distance
- Goal: Develop capability to predict neutron capture reactions for weak r-process isotopes
 - Systematically replace 3 key ingredients by newlydeveloped quantities: LDs, gSFs, optical model
 - Develop optical model (*aka* effective nucleon-nucleus interaction) for weak r-process region
 - Perform statistical reaction calculations with YAHFC and provide capture rates with UQ
 - Benchmark calculations and assess uncertainties (UQ)

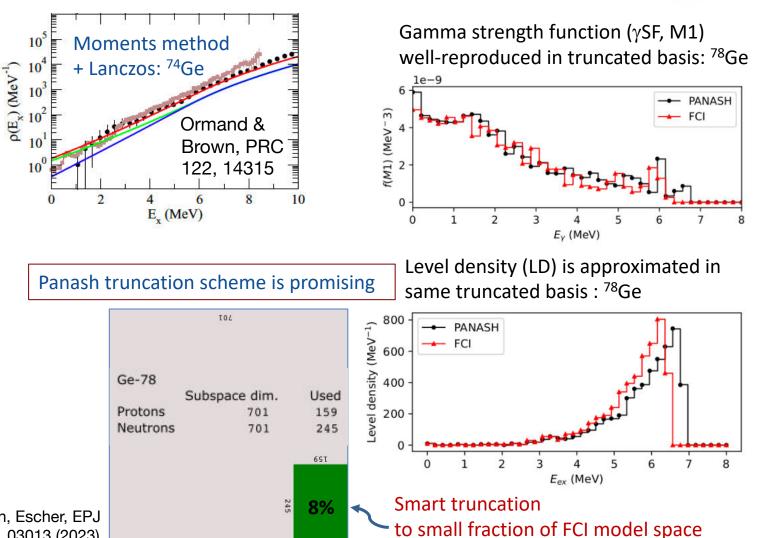


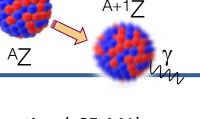


Extending nuclear shell model to predict static properties of relevant nuclei

- The shell model provides a microscopic predictions for LDs and γSFs
- Smart truncations and modern computers increase reach of shell model
- Innovative combination of moments method with Lanczos algorithm enable new LD calculations
- Shell-model advantages:
 - Includes important correlations
 - Yields total and partial level densities
 - Gives low-energy γSF
 - Provides insights into structure
- Challenges:
 - Model space sizes for very heavy nuclei
 - Interactions needed







National Action



- Inputs needed:
 - Optical-model potentials
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Indirect measurements using the Surrogate Reactions Method

- Concept
- (p,d) as a surrogate reaction mechanism
- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism



Surrogate reactions method combines theory and experiment to constrain cross section calculations for compound reactions Escher et al, RI

Escher et al, RMP 84, 353 (2012)

Producing a CN in a surrogate reaction:

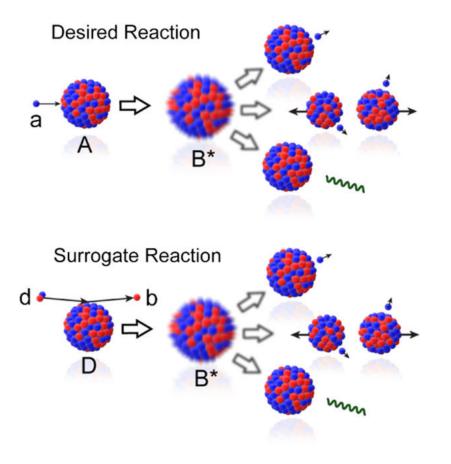
- Starts with a 'direct' reaction to produce a 'doorway state' at E_{ex} > several MeV
- Doorway evolves into a CN
- Spin distribution of doorway state = spin distribution of the CN

Observe the decay of the CN:

- Measure coincidence probability of outgoing surrogate particle with decay into channel of interest
- Model HF decay and fit parameters to measured surrogate probability

Obtain desired cross section:

 Calculate desired reaction cross section using inferred parameters



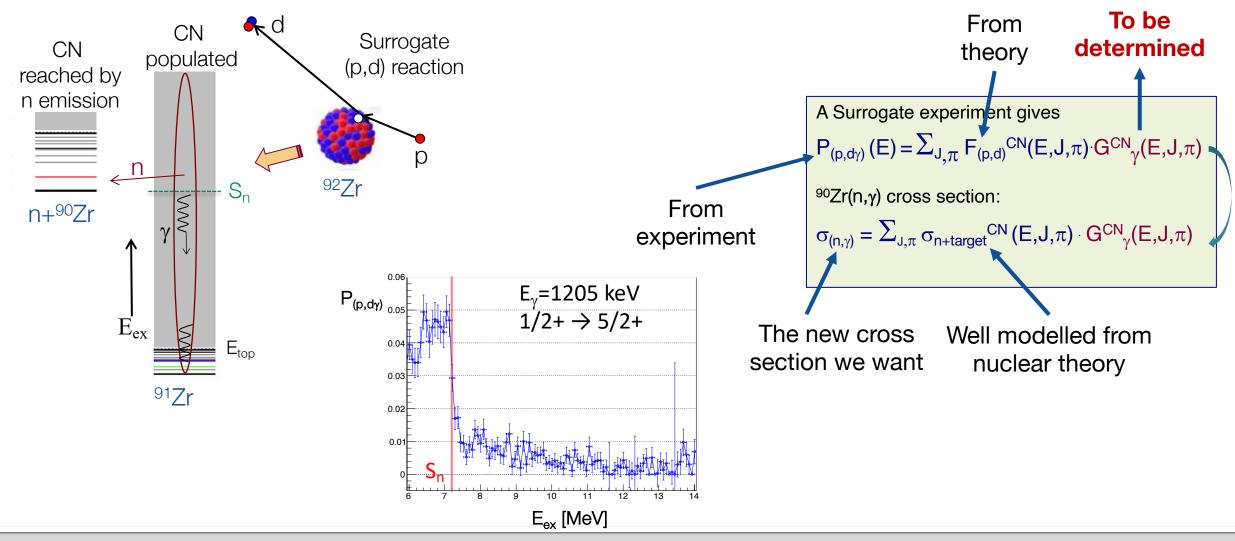


Concept

• (p,d) as a surrogate reaction mechanism

- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism

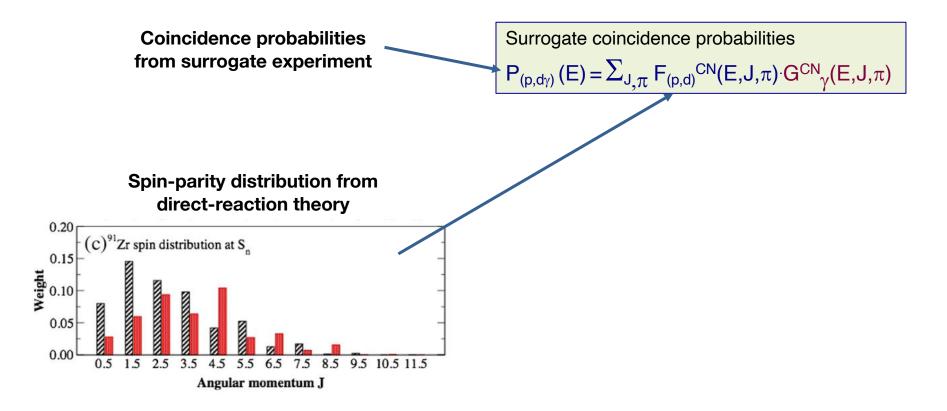




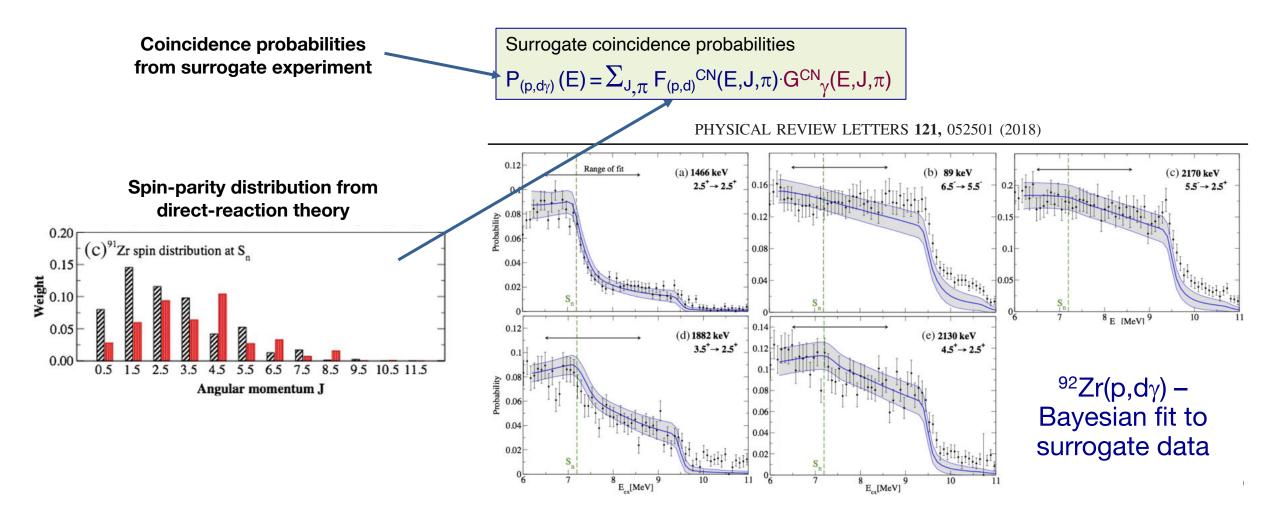
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*Width fluctuation corrections are omitted here, but accounted for in applications.





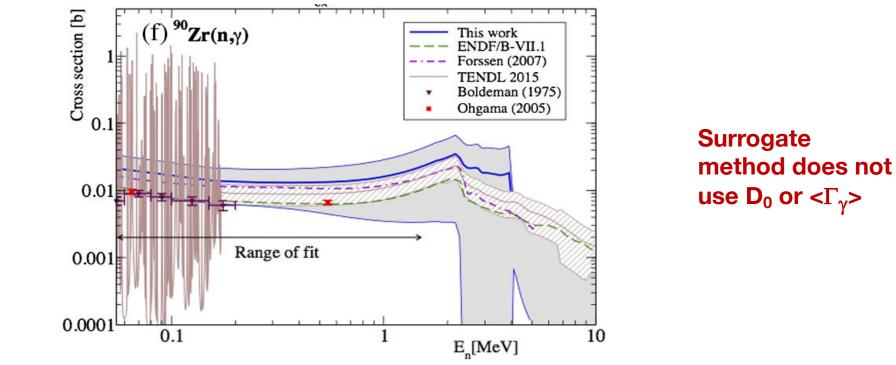






Surrogate (p,d) transfer reactions enable determination of unknown (n, γ) cross sections - benchmark ⁹⁰Zr(n, γ)

Escher et al, PRL 121, 052501 (2018)



Procedure

- Measure the surrogate reaction coincidence probability
- Calculate the spin-parity distribution of the doorway state = spin-parity of the CN
- > Model CN decay and perform Bayesian parameter fit to surrogate coincidence probabilities
- Sample posterior HF parameter distributions to obtain neutron-capture cross section

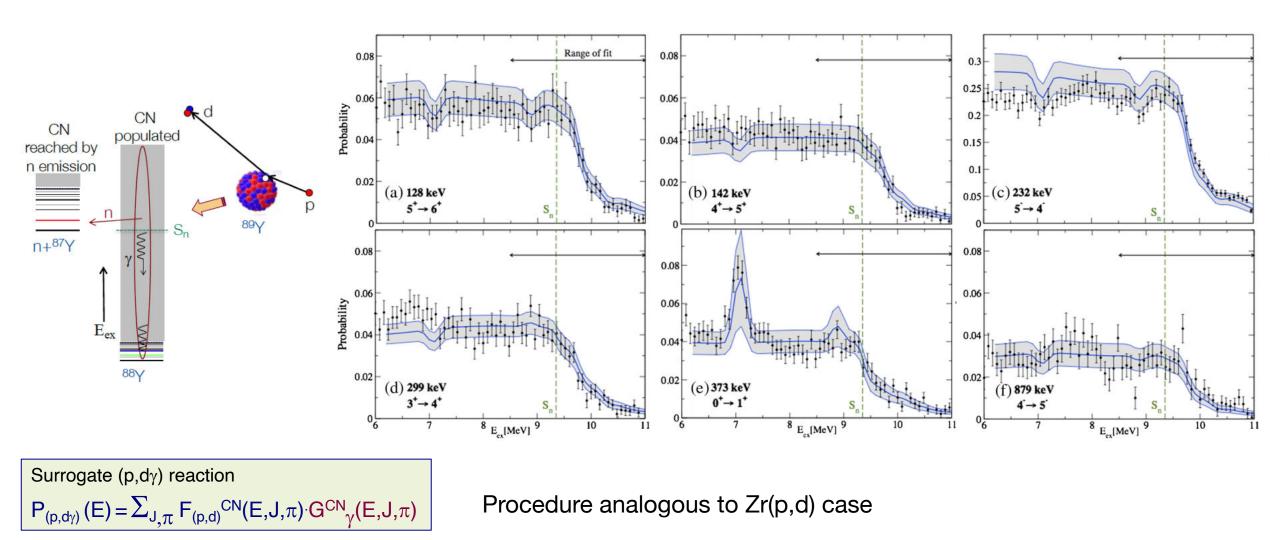


D ₀ [keV]	Reference		
10	This work	Extracted E1, M1 strengths	
6.89 (0.53)	Mughabghab, 2006	1e-05 $= E1 (This work)$ $= - M1 (this work)$ $= - E1 + M1$ $= Utsunomiya (2008)$	
6.00 (1.40)	RIPL-3	1e-06 – O Berman (1967) Guttormsen (2017)	
7.18 (23)	Guttormsen, PRC 2017		urrogate iethod does no
<Γγ> [meV]	Reference		se D_0 or $<\Gamma_{\gamma}>$
185	This work		
170 (20)	Mughabghab, 2006	$1e-09 \begin{pmatrix} -& -& -& -& -& -& -& -& -& -& -& -& -& $	
130 (40)	RIPL-3		
180 (137) 130 (40)	Guttormsen, PRC 2017	Oslo data from: Guttormsen et al, PRC 96, 024313 (2017)	



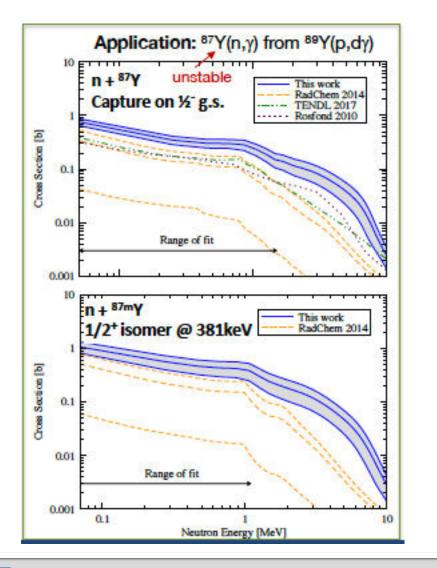
Application to neutron capture on unstable target: ⁸⁷Y(n, γ) cross sections from ⁸⁹Y(p,d γ) surrogate reaction data

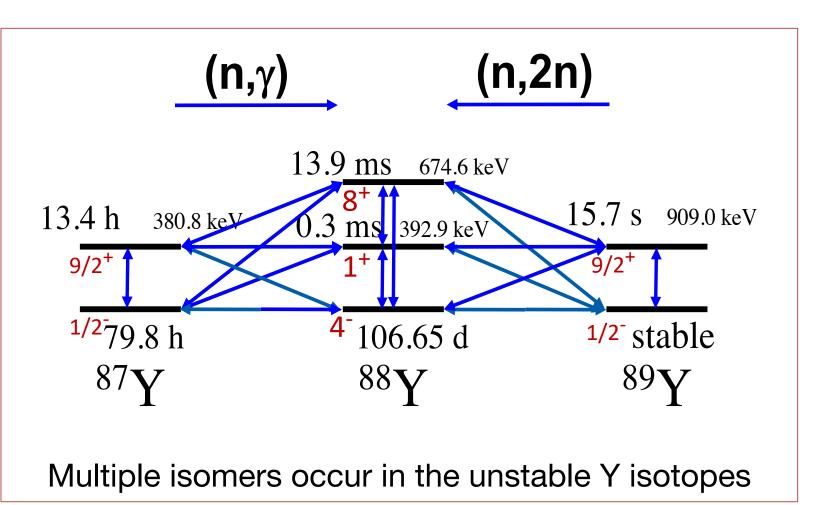
Escher et al, PRL 121, 052501 (2018)





Application to neutron capture on unstable target: We also obtained cross sections for reactions involving isomers





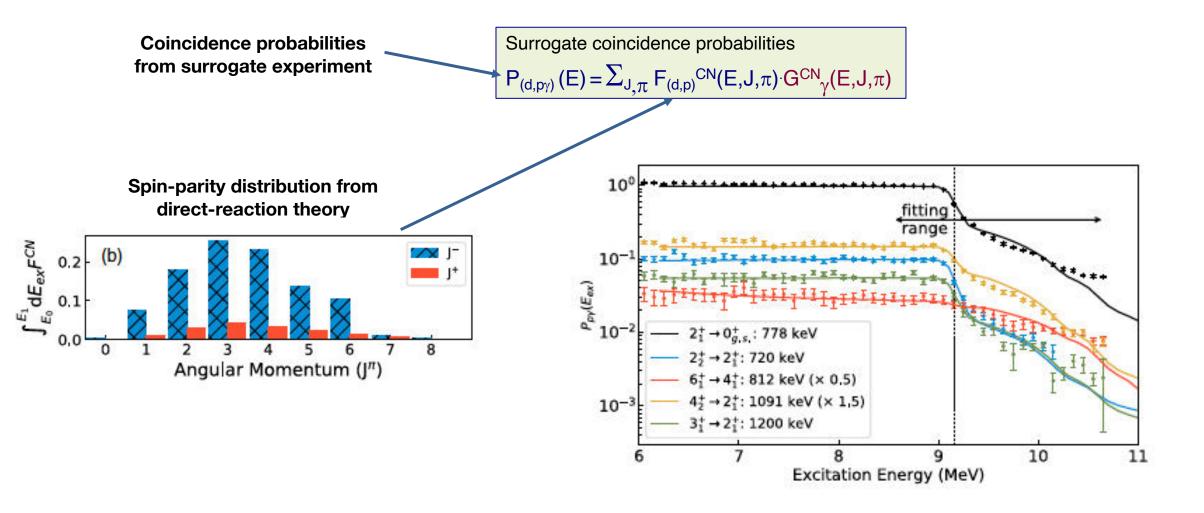


- Concept
- (p,d) as a surrogate reaction mechanism
- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism



Surrogate (d,p) transfer reactions enable determination of (n,γ) cross sections benchmark ⁹⁵Mo(n,γ)

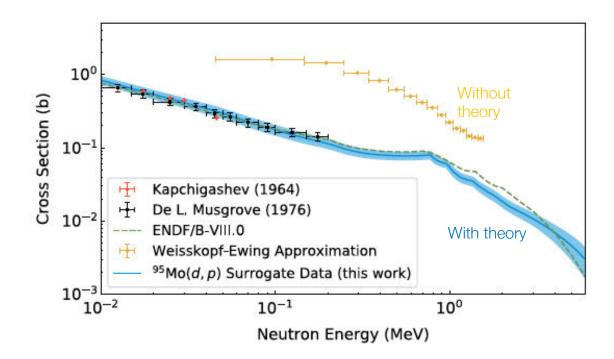
Ratkiewicz, Cizewski, JE, Potel, et al, PRL 122, 052502 (2019)





Surrogate (d,p) transfer reactions enable determination of (n, γ) cross sections benchmark ⁹⁵Mo(n, γ)

Ratkiewicz, Cizewski, JE, Potel, et al, PRL 122, 052502 (2019)

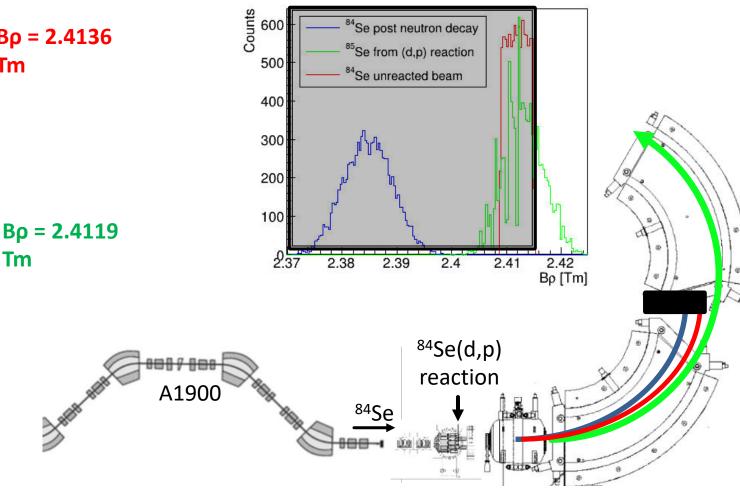


Procedure

- Measure the surrogate reaction coincidence probability
- Calculate the spin-parity distribution of the doorway state = spin-parity of the CN
- > Model CN decay and perform Bayesian parameter fit to surrogate coincidence probabilities
- Sample posterior HF parameter distributions to obtain neutron-capture cross section



We are developing the surrogate reactions method in inverse kinematics **Experiments performed at ANL, TRIUMF, and FRIB**



Slide from A. Ratkiewicz

Here recoils are utilized instead of gammas

- 2. ⁸⁴Se undergoes (d,p) reaction at CD_2 target to form ⁸⁵Se above the neutron separation. Nucleus gammadecays to ground state.
- S800 FP is rate-limited to ~6 kHz, so we use the "soap-on-a-rope" to block the beam.
 - Use the recoils to determine whether CN decay channel (⁸⁴Se/⁸⁵Se) – by tagging on ⁸⁵Se

Three scenarios:

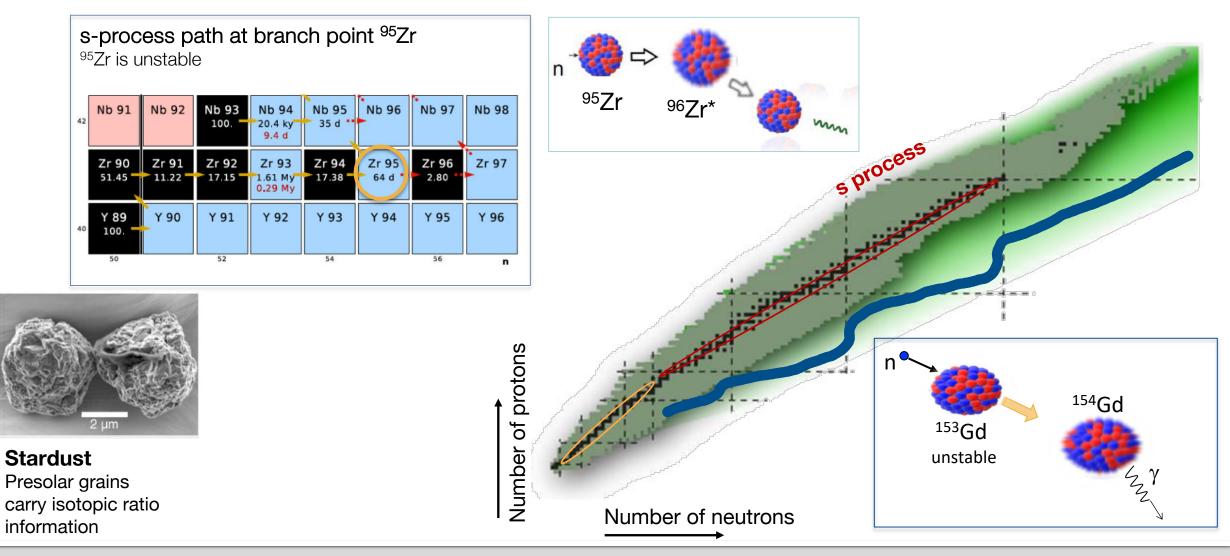
- 1. ⁸⁴Se does not react with CD₂ target, continues with same momentum distribution as determined by slits in A1900.
- $B\rho = 2.4136$ – Tm

Tm

- Concept
- (p,d) as a surrogate reaction mechanism
- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism

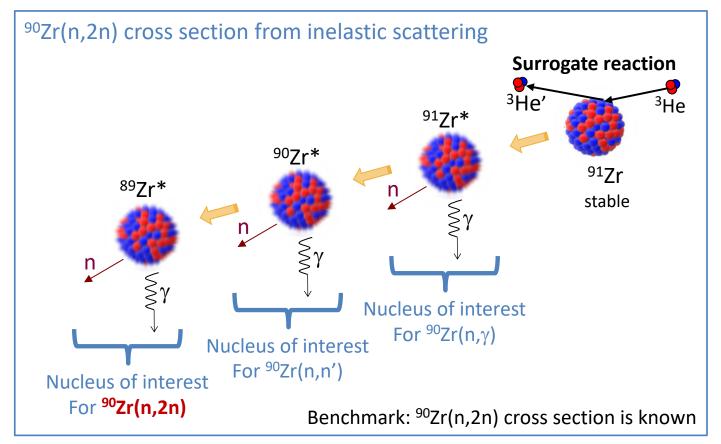


Using inelastic scattering as a surrogate mechanism provides new opportunities: Applications to s process



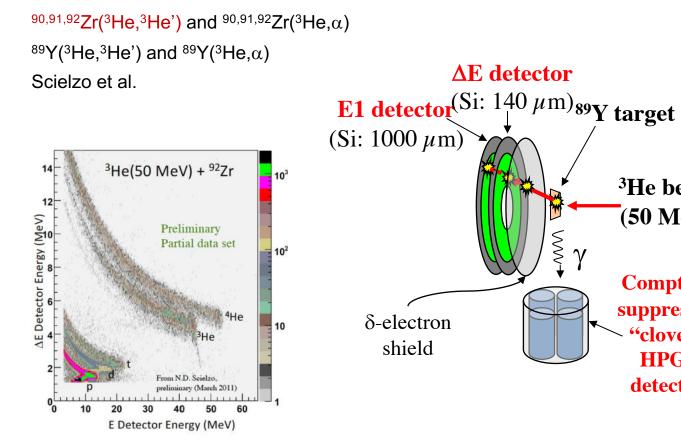


- Opportunities:
 - Unknown (n,n') and (n,2n) reactions become accessible. Examples: ⁸⁸Y(n,2n), ¹⁶⁸Tm(n,2n)
 - Obtain multiple desired reaction cross sections simultaneously
 - Inverse-kinematics experiments at radioactive beam facilities
- Challenges:
 - Compound nucleus highly excited
 - Multiple intermediate nuclei involved
 - Non-statistical effects expected

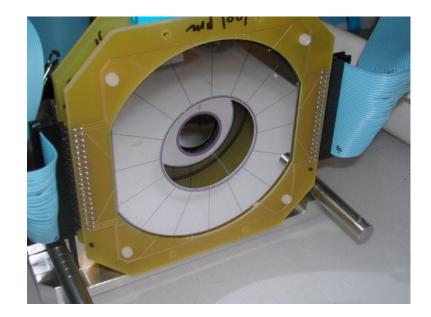




STARS/LiBerACE experiments at LBNL







³He beam

(50 MeV)

Compton-

suppressed

"clover"

HPGe

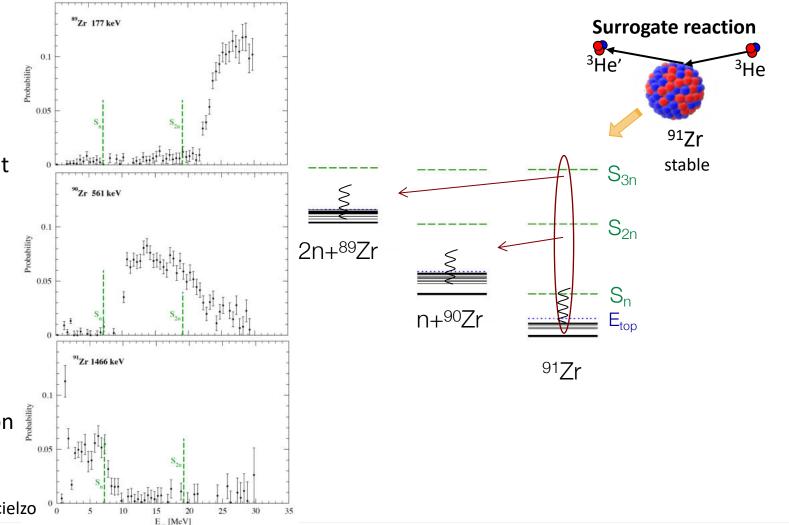
detector



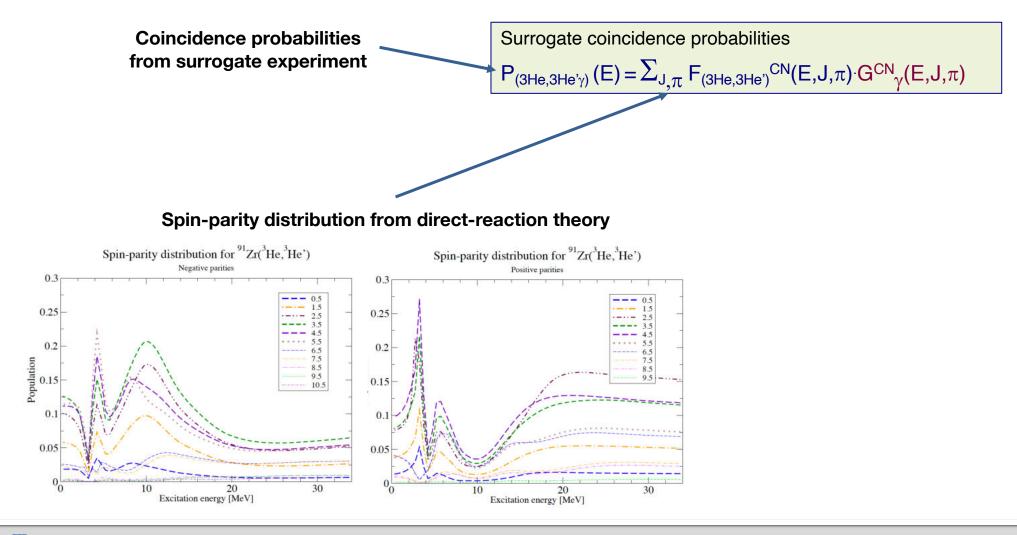
Surrogate reactions method for (n,n') and (n,2n) The Zr case provides a benchmark for the method

- Experiment provides:
 - ⁹¹Zr(³He,³He') 'singles' cross section as function of E_{ex} and ejectile angle
 - Coincidence probabilities $P_{(3He,3He')\gamma}(E_{ex})$ for γ -transitions in 3 different nuclei
- Theory must:
 - Calculate ⁹¹Zr(³He, ³He') 'singles' cross section and determine spin-parity distribution
 - Model ⁹¹Zr decay into 3 final nuclei and fit decay parameters
 - Sample posterior HF parameter distribution and calculate desired cross sections

Surrogate data from N. Scielzo

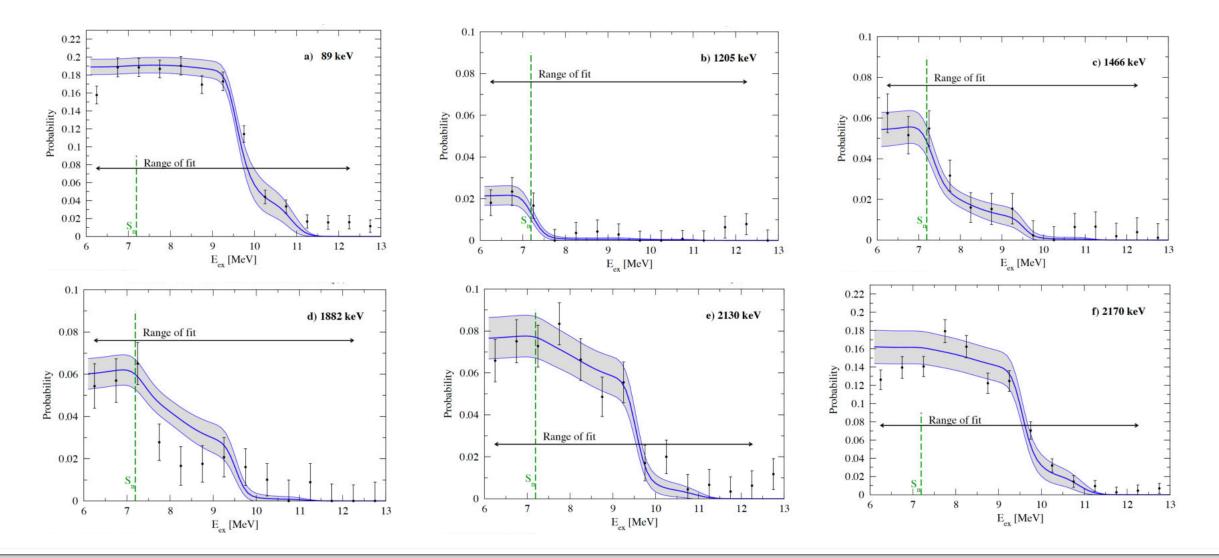








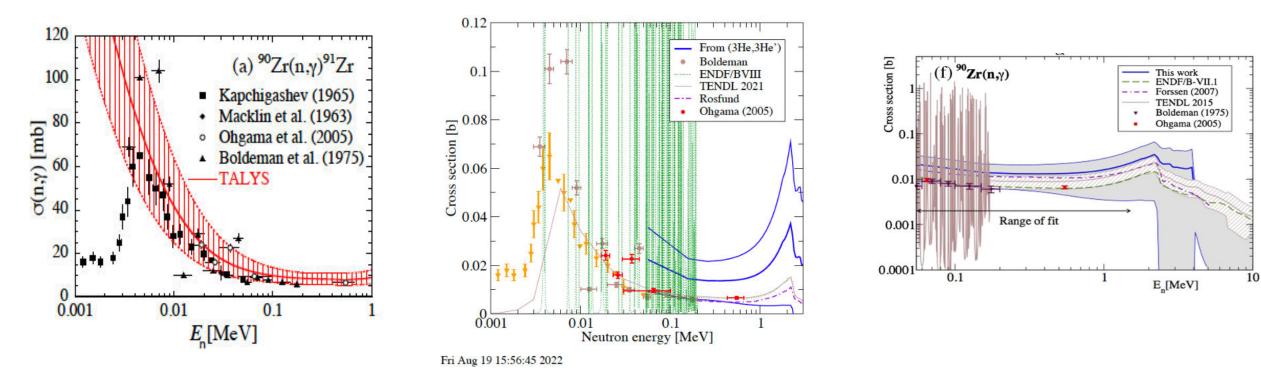
Fits to gamma transitions in 91 Zr \rightarrow constrain LDs and γ SF in 91 Zr



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Escher et al., WIP (2023)



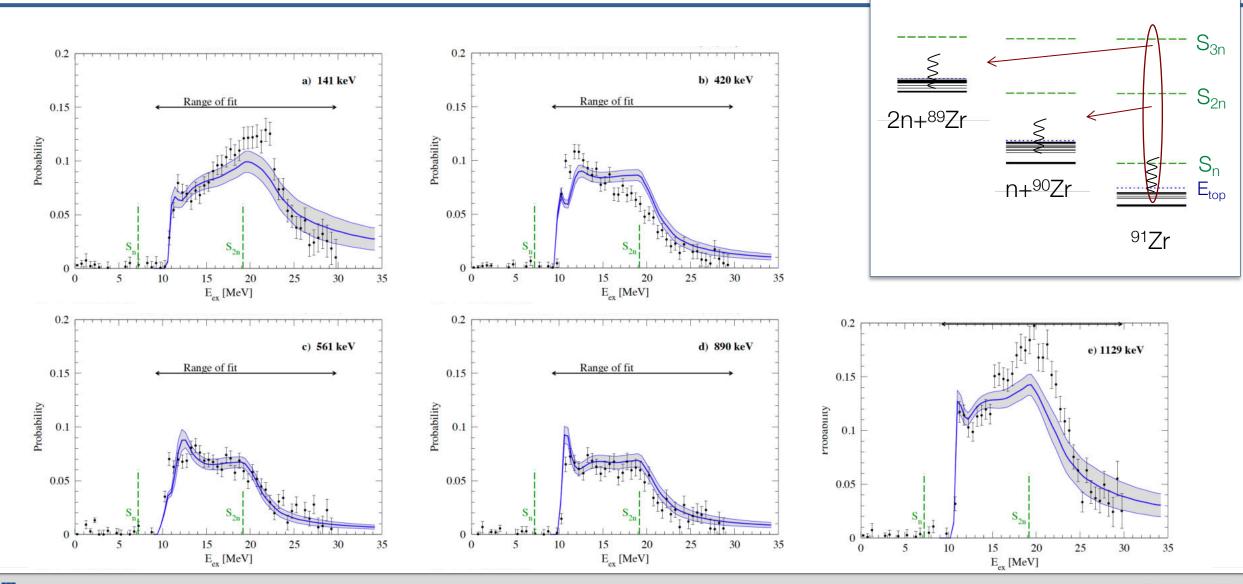
Guttormsen et al, PRC 2019 Oslo method, ⁹²Zr(p,d) This work (preliminary) Escher et al, PRL 2019 Surrogate method, ⁹²Zr(p,d)

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Simultaneous fit to gammas in ⁹⁰Zr and ⁸⁹Zr

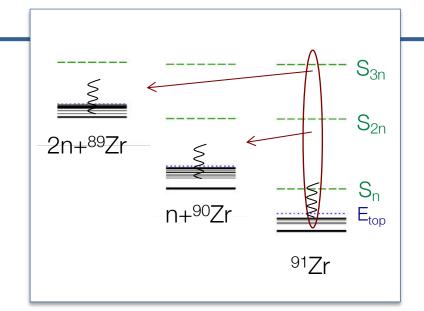
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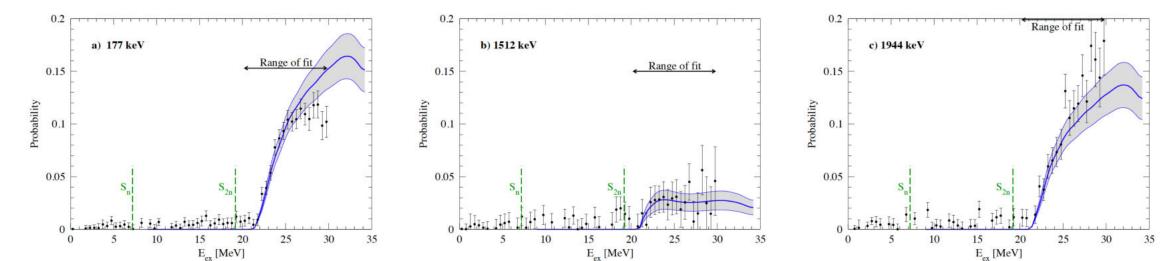


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Escher et al., WIP (2023)



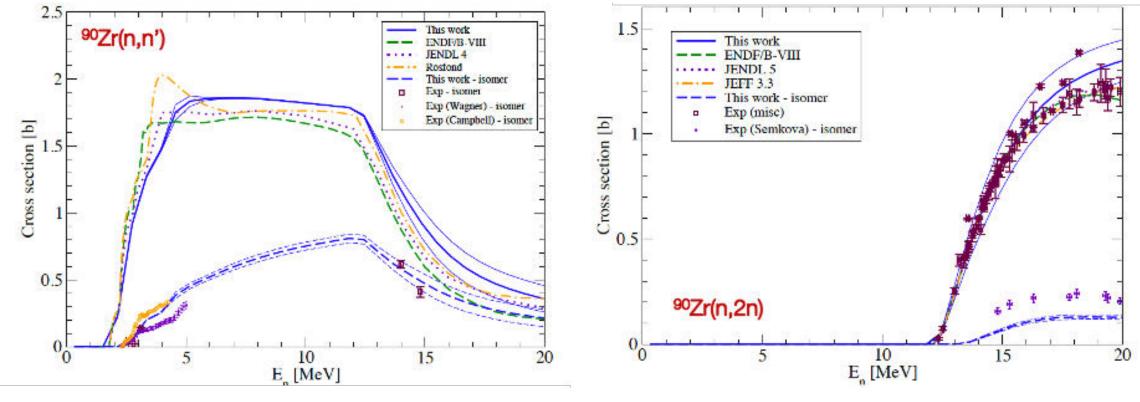


Simultaneous fit to gammas in ⁹⁰Zr and ⁸⁹Zr

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Escher et al., WIP (2023)



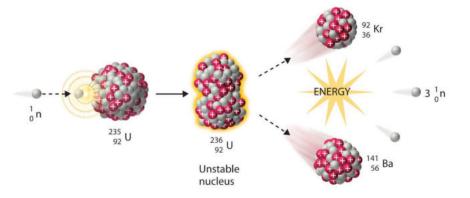
(preliminary)



Full circle: We plan to revisit the surrogate reactions method to obtain (n,f) cross sections and insights into the fission process

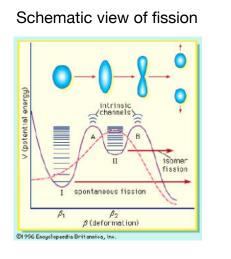
Describing fission challenges theory (and experiment)

- Descriptions range from phenomenological to microscopic
- Lots of data needed to provide constraints

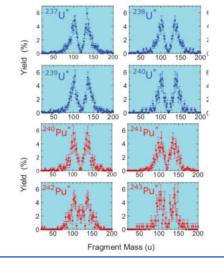


Opportunity: Surrogate fission measurements

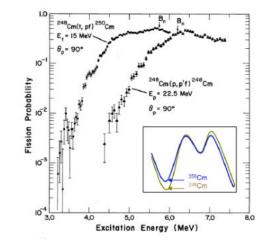
- Observe fission properties in coincidence with surrogate ejectile
- Control over energy of fissioning nucleus, including sub-threshold
- Multiple surrogate reactions in one experiment

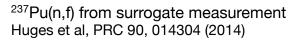


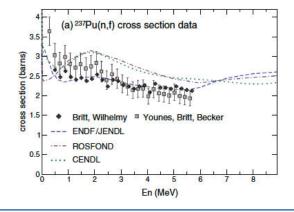
Fragment mass distributions Chiba et al, NDS 119, 229 (2014)



Fission barriers from surrogate data Back, EPJConf. 232, 03002 (2020)









Concluding remarks

- 1. Nuclear astrophysics requires information on multiple reaction types for many isotopes. We will not be able to measure all. Predictive theory is indispensable.
- Substantial progress has been made integrating structure and reaction theory for light nuclei.
 Symmetry-adapted bases promise to extend advances to medium-mass nuclei.
- 3. For heavy nuclei, efforts are underway to integrate sophisticated structure theory into reaction calculations:
 - Optical models are being extended off-stability
 - Shell-model and DFT-based theories are used to calculate LDs and γSFs
 - Consistency and UQ need to be implemented

- 4. Measurements are needed to validate and complement theory
- 5. Surrogate reactions method constrains cross section calculations for compound reactions by combining an indirect measurement with theory
 - Method uses inelastic scattering or transfer reactions in regular or inverse kinematics
 - Theory provides important information on population of doorway states and extracts desired cross section

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This summer in Vienna.....



Compound-Nuclear Reactions and Related Topics (CNR*24)

- Nuclear reaction mechanisms (direct, compound, pre-equilibrium, other)
- Nuclear fission
- Statistical Hauser-Feshbach theory
- Surrogate methods
- Optical model
- Level densities and photon strength functions
- R-matrix theory
- Nuclear structure for nuclear reactions
- · Measurements relevant to compound-nuclear reactions (direct and indirect)
- Nuclear data evaluation and dissemination (including Machine Learning, Statistics, Bayesian Inference)
- Applications in nuclear astrophysics, energy, waste management, nonproliferation, medical physics, etc.
- Experimental facilities

Jul 8–12, 2024 Vienna International Centre

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Abstract/Registration deadline: March 31

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