Interplay of Direct, Pre-Equilibrium, and Compound Processes in Nuclear Reactions

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Reactions & Structure of Exotic Nuclei
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Structure and reactions of unstable isotopes

… are important for addressing basic science questions and for applications.

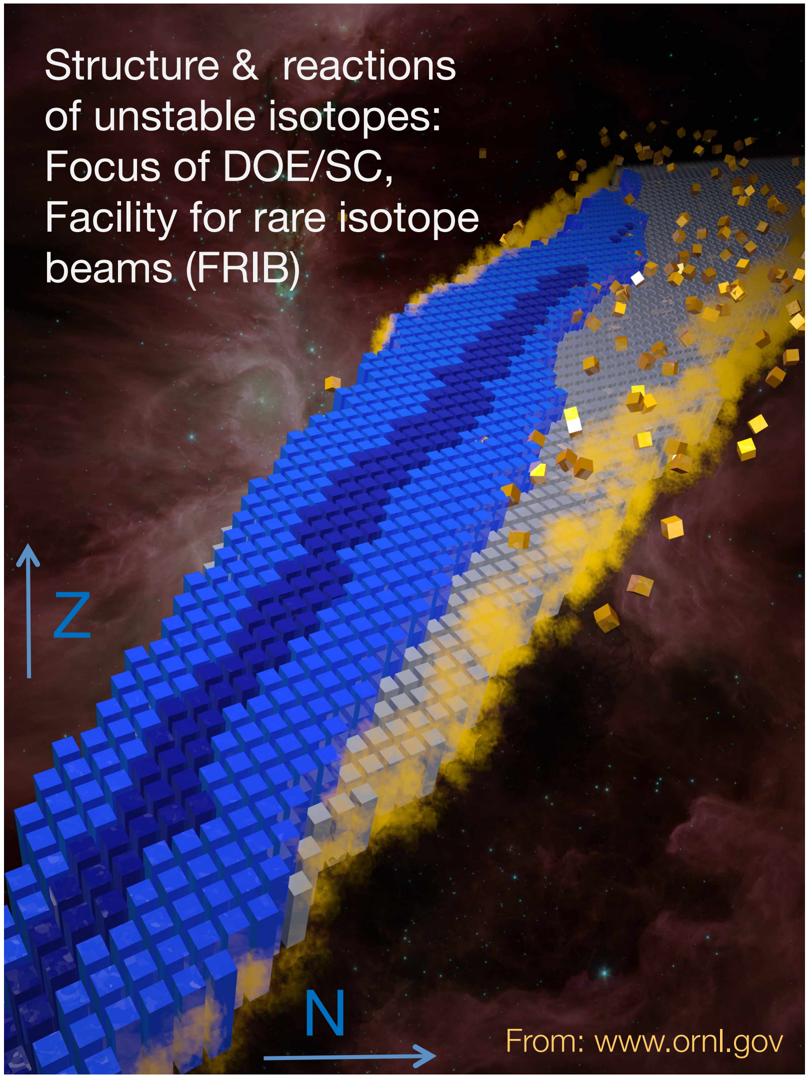
Reaction cross sections are important for nuclear astrophysics, nuclear energy, and national security.

Challenge: Many important nuclear reaction cross sections cannot be measured directly

Needed:

- Reliable structure & reaction theory to predict cross sections
- Theory-experiment collaborations for indirect determination of desired cross sections -> Reaction-theory development to plan and interpret experiments.

This talk: Focus on challenges for determining cross sections for compound-nuclear reactions



Structure & reactions of unstable isotopes: Focus of DOE/SC, Facility for rare isotope beams (FRIB)

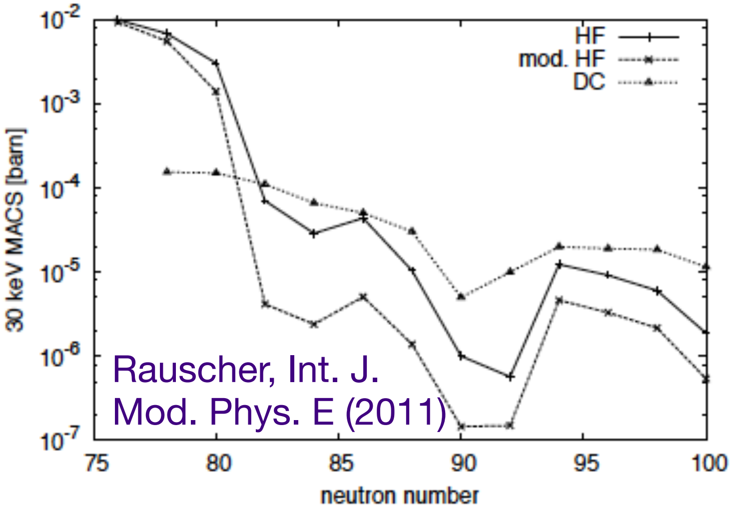
From: www.ornl.gov

Modeling of astrophysical processes and general neutron-rich enviroments requires cross sections for exotic nuclei

Astrophysics: (n,γ) cross sections required for understanding synthesis of heavy elements via *r* process

National security: cross sections for many n-induced reactions on unstable isotopes required

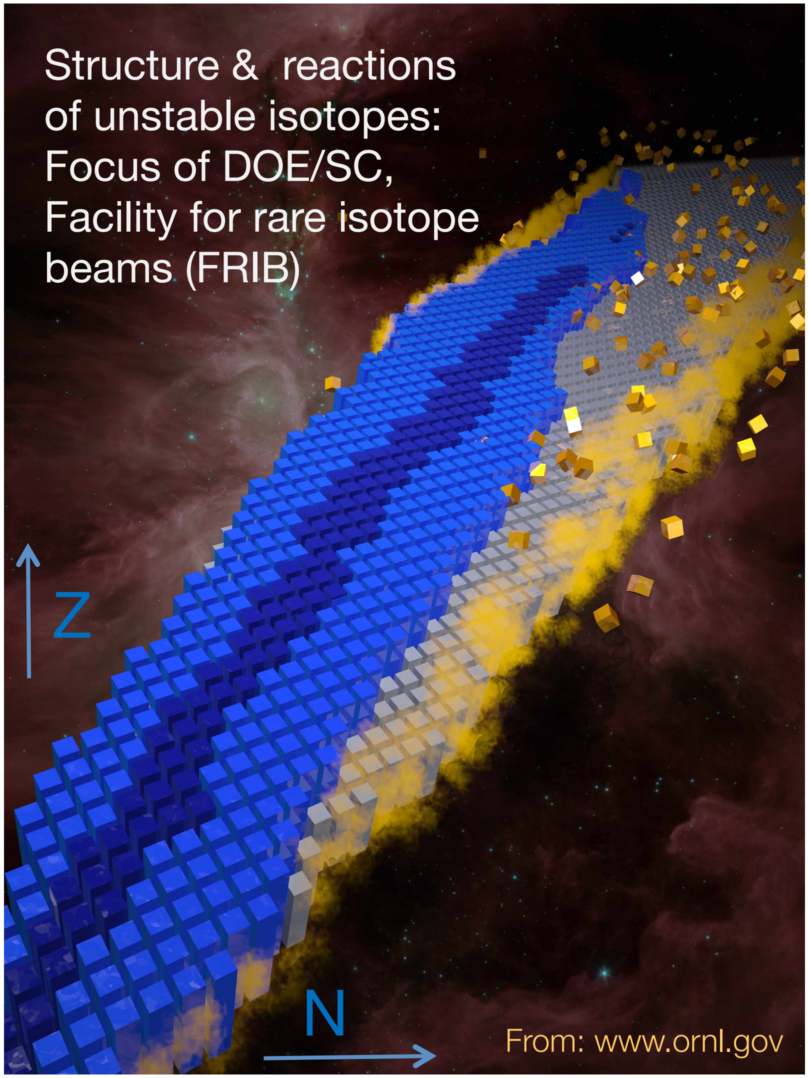
Calculated (n,γ) cross sections for Sn isotopes



Rauscher, Int. J. Mod. Phys. E (2011)

Types of reactions: primarily compound reactions, but direct reactions may contribute as well

Theory: uncertainties in cross sections increase dramatically with distance from stability



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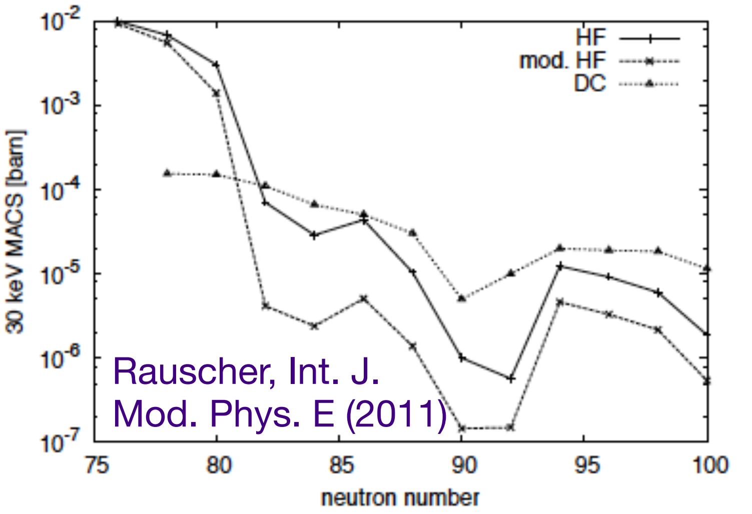

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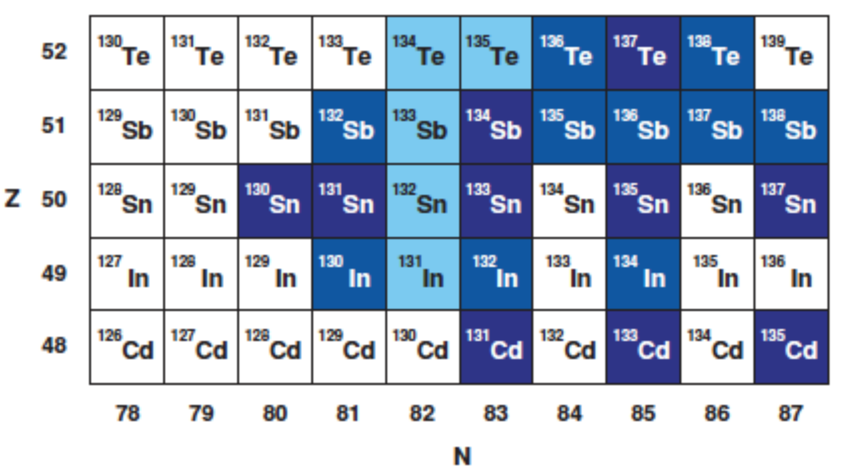
Impact of cross section uncertainties on predicted r-process abundances



	52	^{130}Te	^{131}Te	^{132}Te	^{133}Te	^{134}Te	^{135}Te	^{136}Te	^{137}Te	^{138}Te	^{139}Te
	51	^{129}Sb	^{130}Sb	^{131}Sb	^{132}Sb	^{133}Sb	^{134}Sb	^{135}Sb	^{136}Sb	^{137}Sb	^{138}Sb
Z	50	^{128}Sn	^{129}Sn	^{130}Sn	^{131}Sn	^{132}Sn	^{133}Sn	^{134}Sn	^{135}Sn	^{136}Sn	^{137}Sn
	49	^{127}In	^{128}In	^{129}In	^{130}In	^{131}In	^{132}In	^{133}In	^{134}In	^{135}In	^{136}In
	48	^{126}Cd	^{127}Cd	^{128}Cd	^{129}Cd	^{130}Cd	^{131}Cd	^{132}Cd	^{133}Cd	^{134}Cd	^{135}Cd
		78	79	80	81	82	83	84	85	86	87

N

>5% change in the overall abundance pattern caused by cross section variation

- by factor of 10/50/100-1000
- for dark/medium/light

blue cases.

Effect is compounded (>40%) when multiple rates are changed.

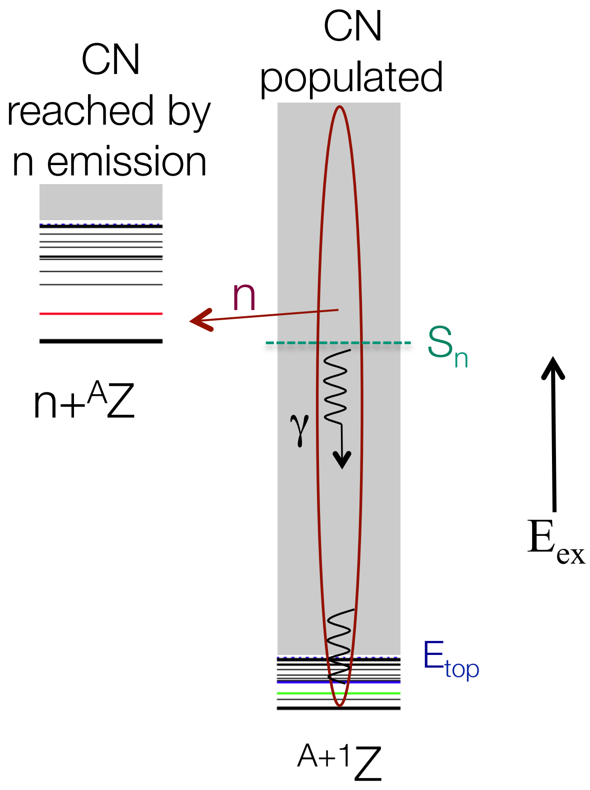
Surman et al, PRC (2009)

Where's the challenge in calculating $^{A}Z(n,\gamma)$?

Anatomy of a capture reaction

n+target ➔ population of CN

Subsequent decay by competition of γ emission, neutron evaporation



Theoretical description

Hauser-Feshbach (HF) formalism:

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

Cross section is a sum of products

σ_{α}^{CN} : formation of CN, from optical model

$G^{CN}{}_{\gamma}$: decay of CN, contains info on competing decay channels

α = n+target

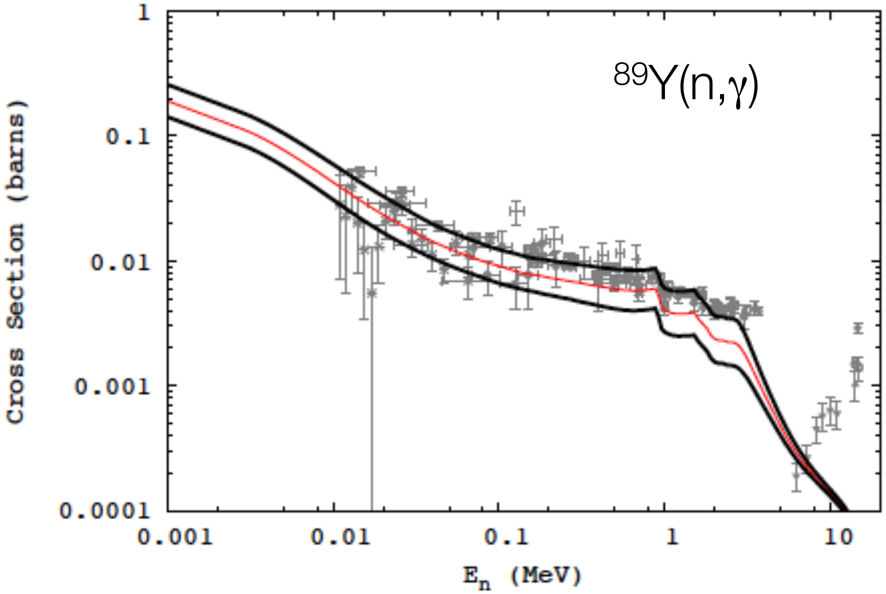
Challenge for calculations

Accurate description of competition requires:

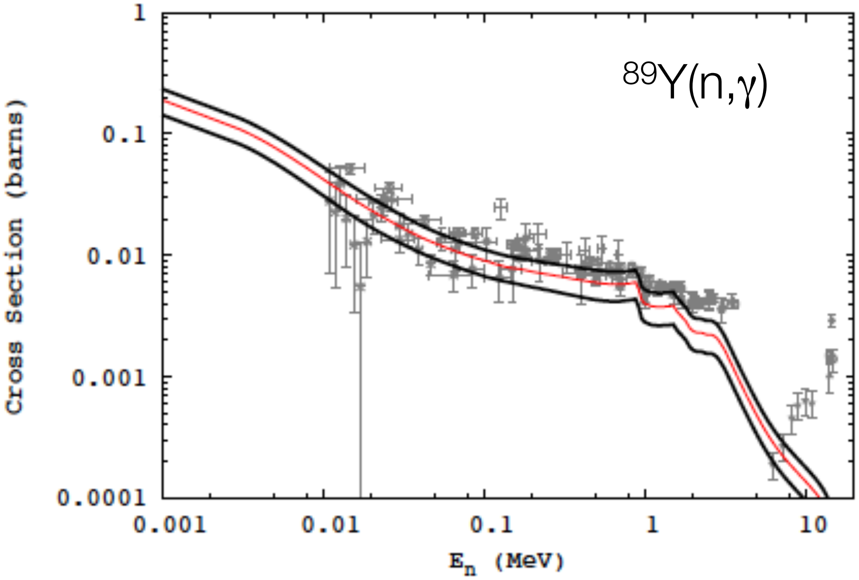
- γ–ray strength function (γSF)
- level densities (LD) in $^{A,A+1}Z$
- discrete low-lying levels with J^{π}, branching ratios – esp. important for isomers!
- optical model for n+target: in decent shape near stability
- width fluctuation corrections

Sensitivity of HF calculations to γSF and LD

Example: variation of LD parameter δW



Example: variation of γSF normalization



For details see:
R.D. Hoffman et al, UCRL-TR-222275 (2006)

Reasonable parameter variations lead to significant uncertainties. Extrapolations increase the uncertainties.

Strategies for constraining HF inputs

I. **Determine ingredients γSF & LD**:

- Theory challenging, not all nuclei covered, but progress is being made
- Experiments need to ‘de-convolute’ γSF & LD, not all nuclei can be reached

II. **Cross section constraints from neighbors**:

- Measure (n,γ) cross sections in other nuclei & do regional fits
- Extrapolations required

III. **Constraints from surrogate observables**:

- Surrogate approach: use charged-particle transfer or inelastic scatering to create CN of interest and observe decay
- Use measurement to constrain calculation of desired cross section
- Theory needed to relate measurement to desired cross section
- Measure quantities in **actual nuclei of interest**

Surrogate Reactions 101

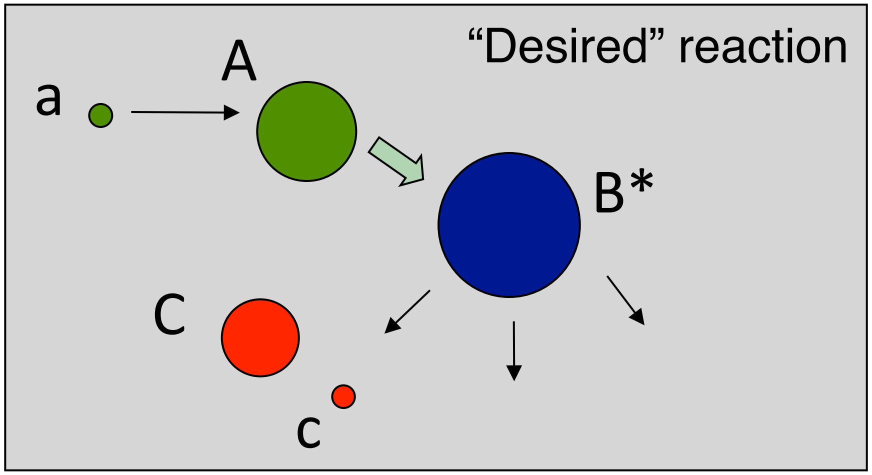
Compound reaction

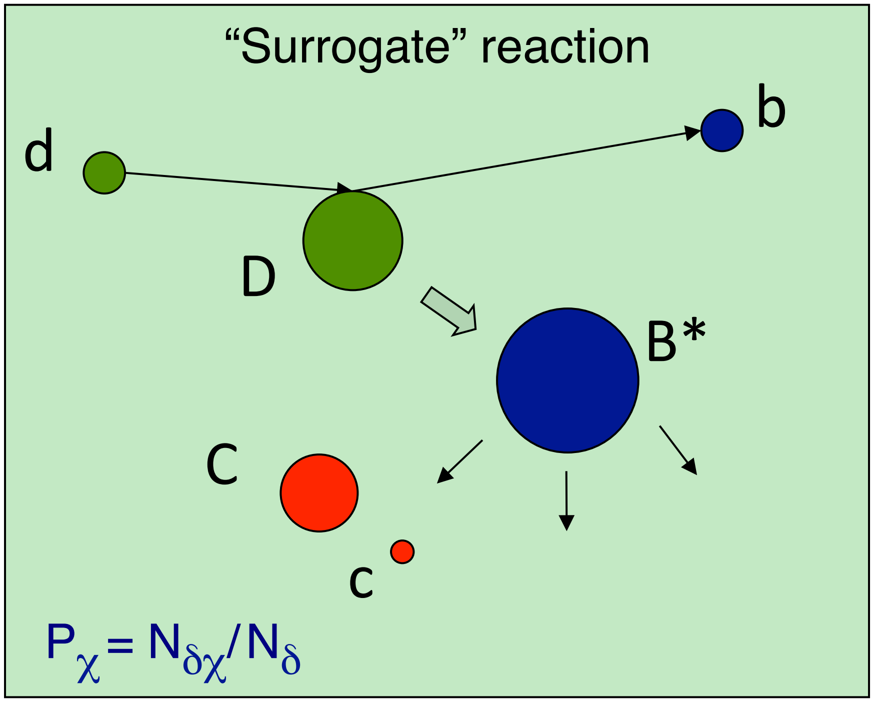
A reaction that proceeds in two stages: formation of a compound-nucleus (CN) and decay

Surrogate approach

An indirect method for obtaining cross sections for compound-nucleus (CN) reactions

Using an intial direct reaction, a CN is formed and its decay is observed. Theory is used to extract the desired reaction.


“Desired” reaction

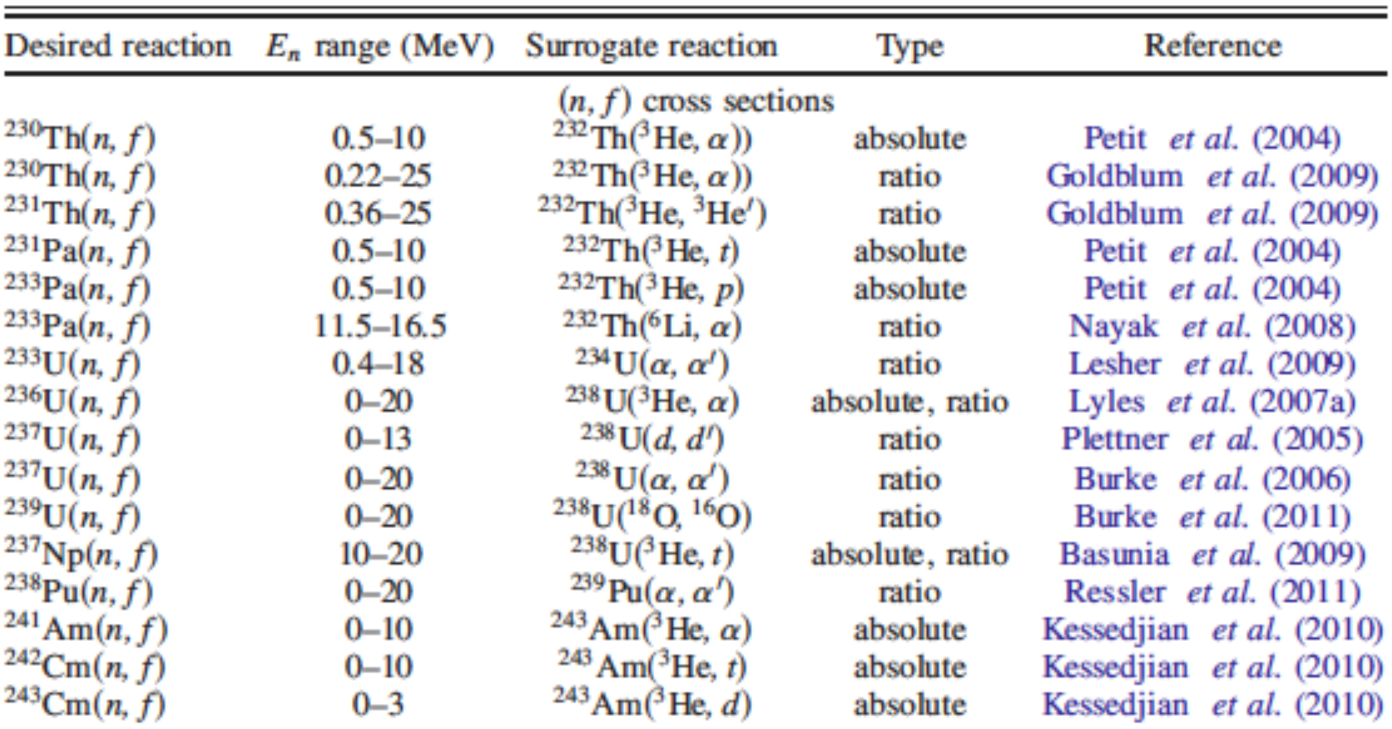

“Surrogate” reaction

$P_\chi = N_{\delta\chi}/N_\delta$

Surrogate Reactions 101

History

- The surrogate method was introduced in the 1970s by Britt, Cramer, Wilhelmy, *et al*, to determine (n,f) cross sections.
- In the last 10 years, the method has been revived, primarily for (n,f).
- Most applications use approximate treatments, ignoring the difference in the reaction mechanisms that lead to the CN (aka Weisskopf-Ewing approximation)



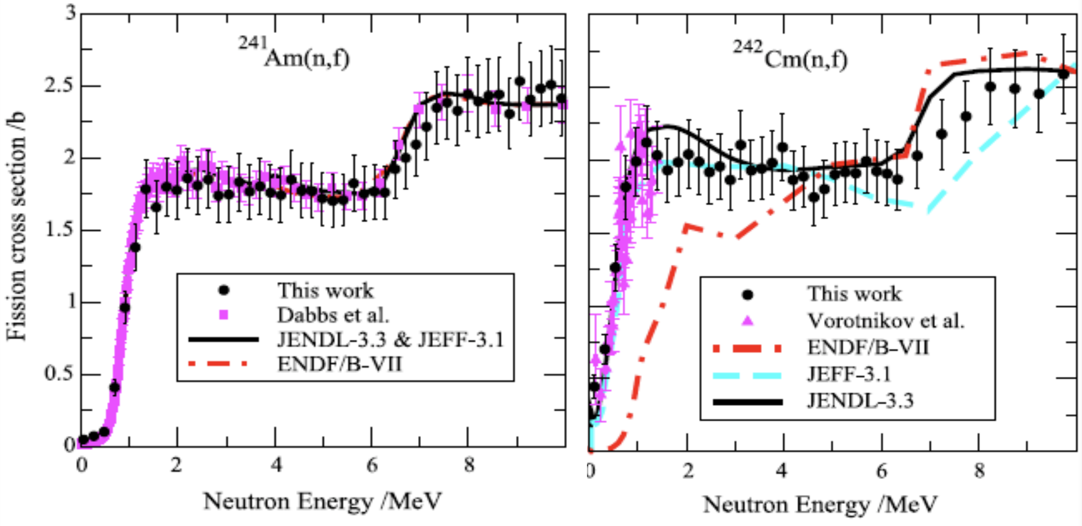
Desired reaction	E_n range (MeV)	Surrogate reaction	Type	Reference
		(n, f) cross sections		
$^{230}\mathrm{Th}(n, f)$	0.5–10	$^{232}\mathrm{Th}(^3\mathrm{He}, \alpha))$	absolute	Petit *et al.* (2004)
$^{230}\mathrm{Th}(n, f)$	0.22–25	$^{232}\mathrm{Th}(^3\mathrm{He}, \alpha))$	ratio	Goldblum *et al.* (2009)
$^{231}\mathrm{Th}(n, f)$	0.36–25	$^{232}\mathrm{Th}(^3\mathrm{He}, ^3\mathrm{He}')$	ratio	Goldblum *et al.* (2009)
$^{231}\mathrm{Pa}(n, f)$	0.5–10	$^{232}\mathrm{Th}(^3\mathrm{He}, t)$	absolute	Petit *et al.* (2004)
$^{233}\mathrm{Pa}(n, f)$	0.5–10	$^{232}\mathrm{Th}(^3\mathrm{He}, p)$	absolute	Petit *et al.* (2004)
$^{233}\mathrm{Pa}(n, f)$	11.5–16.5	$^{232}\mathrm{Th}(^6\mathrm{Li}, \alpha)$	ratio	Nayak *et al.* (2008)
$^{233}\mathrm{U}(n, f)$	0.4–18	$^{234}\mathrm{U}(\alpha, \alpha')$	ratio	Lesher *et al.* (2009)
$^{236}\mathrm{U}(n, f)$	0–20	$^{238}\mathrm{U}(^3\mathrm{He}, \alpha)$	absolute, ratio	Lyles *et al.* (2007a)
$^{237}\mathrm{U}(n, f)$	0–13	$^{238}\mathrm{U}(d, d')$	ratio	Plettner *et al.* (2005)
$^{237}\mathrm{U}(n, f)$	0–20	$^{238}\mathrm{U}(\alpha, \alpha')$	ratio	Burke *et al.* (2006)
$^{239}\mathrm{U}(n, f)$	0–20	$^{238}\mathrm{U}(^{18}\mathrm{O}, ^{16}\mathrm{O})$	ratio	Burke *et al.* (2011)
$^{237}\mathrm{Np}(n, f)$	10–20	$^{238}\mathrm{U}(^3\mathrm{He}, t)$	absolute, ratio	Basunia *et al.* (2009)
$^{238}\mathrm{Pu}(n, f)$	0–20	$^{239}\mathrm{Pu}(\alpha, \alpha')$	ratio	Ressler *et al.* (2011)
$^{241}\mathrm{Am}(n, f)$	0–10	$^{243}\mathrm{Am}(^3\mathrm{He}, \alpha)$	absolute	Kessedjian *et al.* (2010)
$^{242}\mathrm{Cm}(n, f)$	0–10	$^{243}\mathrm{Am}(^3\mathrm{He}, t)$	absolute	Kessedjian *et al.* (2010)
$^{243}\mathrm{Cm}(n, f)$	0–3	$^{243}\mathrm{Am}(^3\mathrm{He}, d)$	absolute	Kessedjian *et al.* (2010)

J. Escher *et al*, RMP 84 (2012) 353

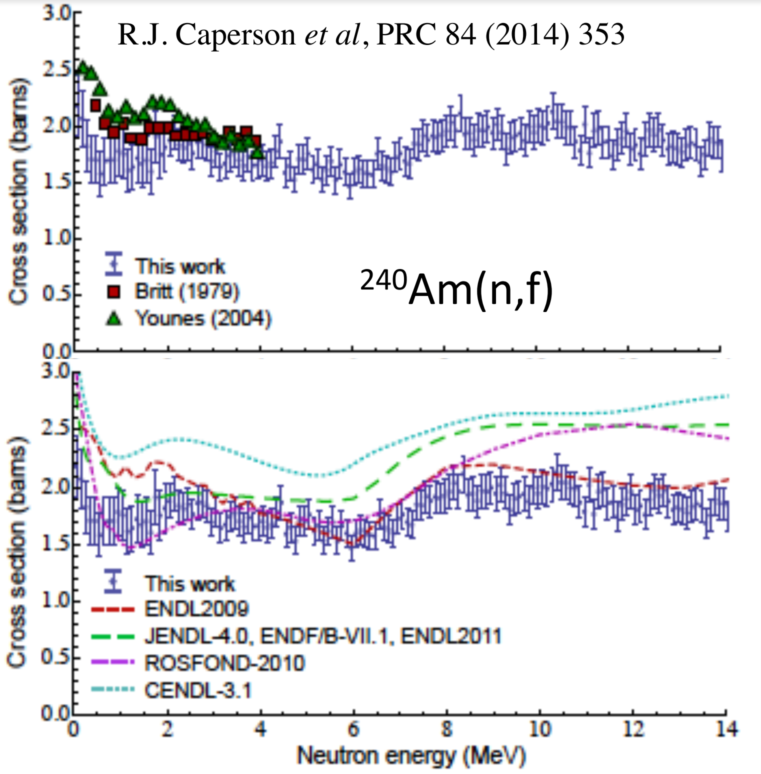
(n,f) cross sections from surrogate measurements

- ✓ Complement and extend indirect and direct measurements
- ✓ Typically agree within 10-15% with benchmarks
- ✓ Make use of approximation schemes

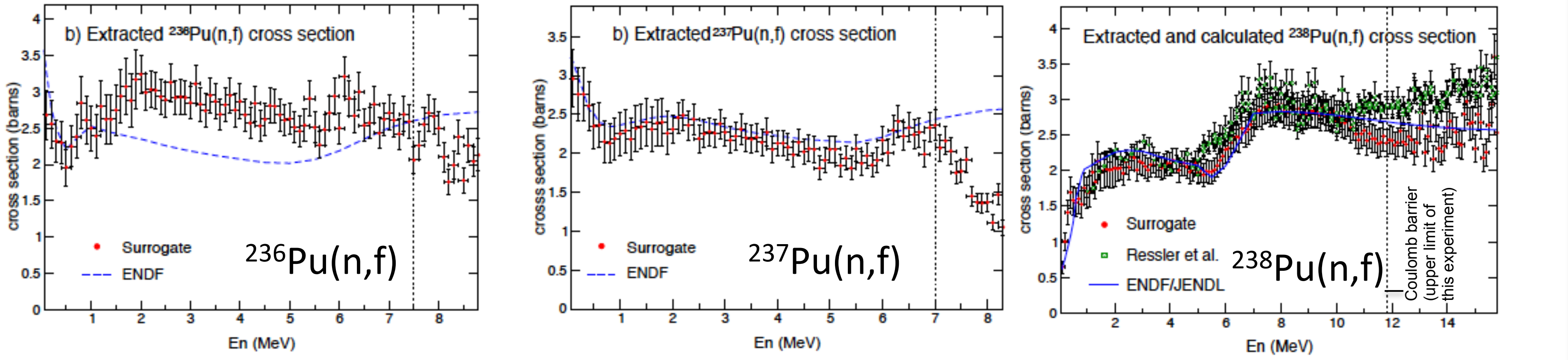
Kessedjian *et al*. (CENBG), PLB 692 (2010) 297



R.J. Caperson *et al*, PRC 84 (2014) 353



R.O. Hughes *et al*, PRC 90 (2014) 014304

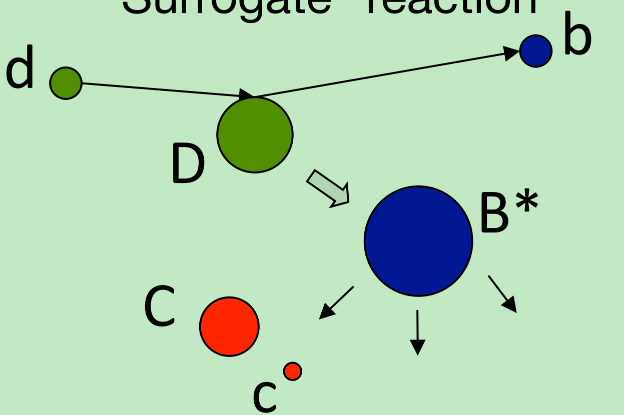


Previous work used a number of approximations

Prevailing assumptions

1. Weisskopf-Ewing approximation valid
2. No ‘pre-equilibrium’ contributions

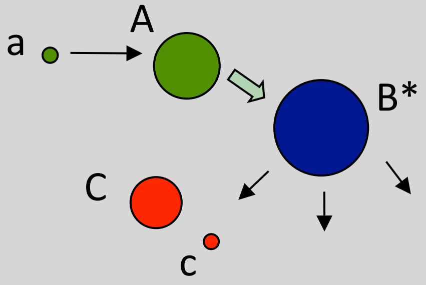
“Surrogate” reaction



$P_{\chi} = N_{\delta\chi}/N_{\delta}$

Weisskopf-Ewing description of the “desired” reaction:

$$\sigma_{\alpha\chi}^{WE}(E) = \sigma_{\alpha}^{CN}(E) \cdot \mathcal{G}^{CN}_{\chi}(E)$$



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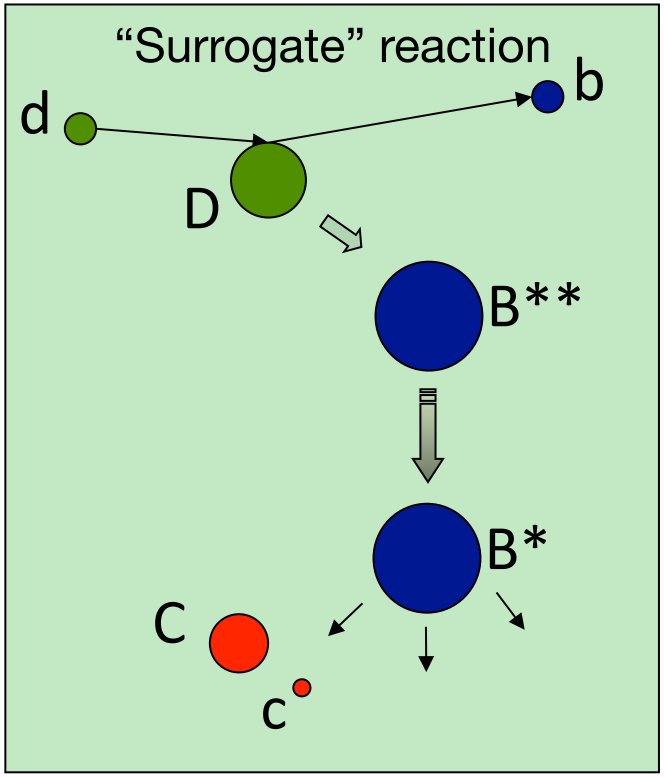
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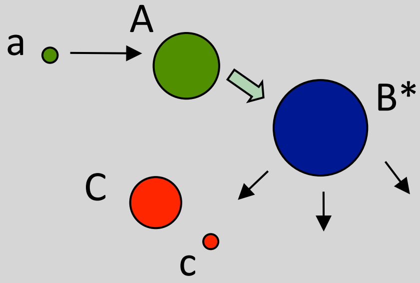
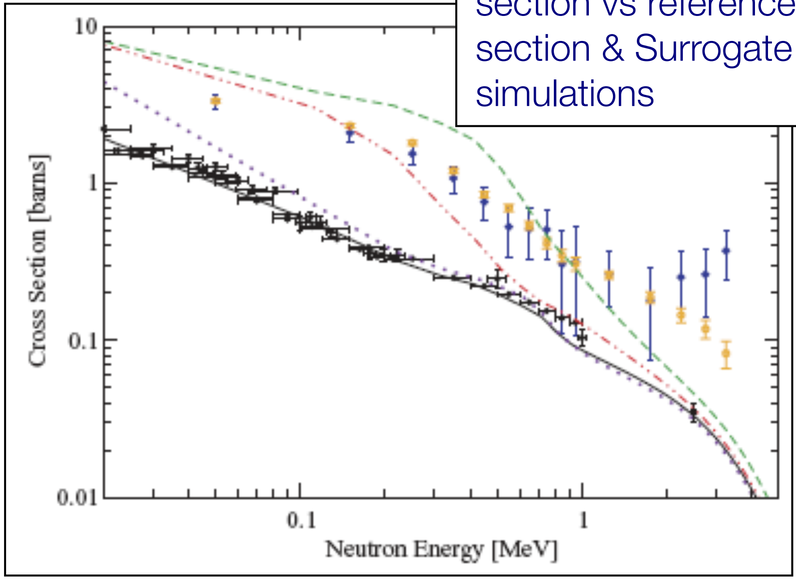


Current implementations of surrogate method are insufficient

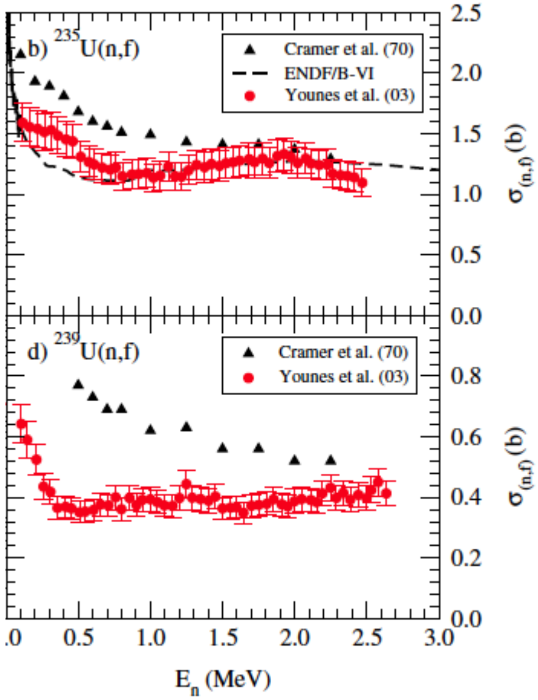
Known limitations

1. WE approximation fails for (n,γ) and (n,p)
2. Limitations visible in low-E regime, e.g. in (n,f) reactions

Extracted ^{157}Gd(n,γ) cross section vs reference cross section & Surrogate simulations



J. Escher and F.S. Dietrich, PRC 81 (2010) 024612
N. Scielzo, J. Escher, et al., PRC 81 (2010) 034608



Younes & Britt, PRC (2003)

Suspect assumption

`Pre-equilibrium effects' are non-existent or can be ignored

Need to move beyond 'Surrogates 101'

Surrogate Reactions – next level….

Objective

Apply the surrogate method to wider range of reactions, such as (n,γ) and (n,2n)

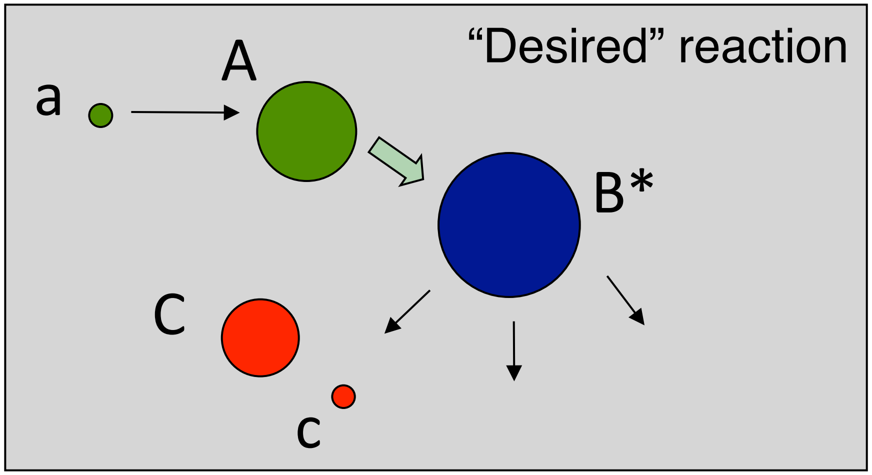
Needed:

Improved treatment of the reaction mechanisms:

- descriptions of the formation of the CN via transfer or inelastic scattering reactions
- descriptions of the competition between damping and ‘pre-equilibrium’ decay processes.

New strategy for using surrogate data.

Experiments to shed light on the processes.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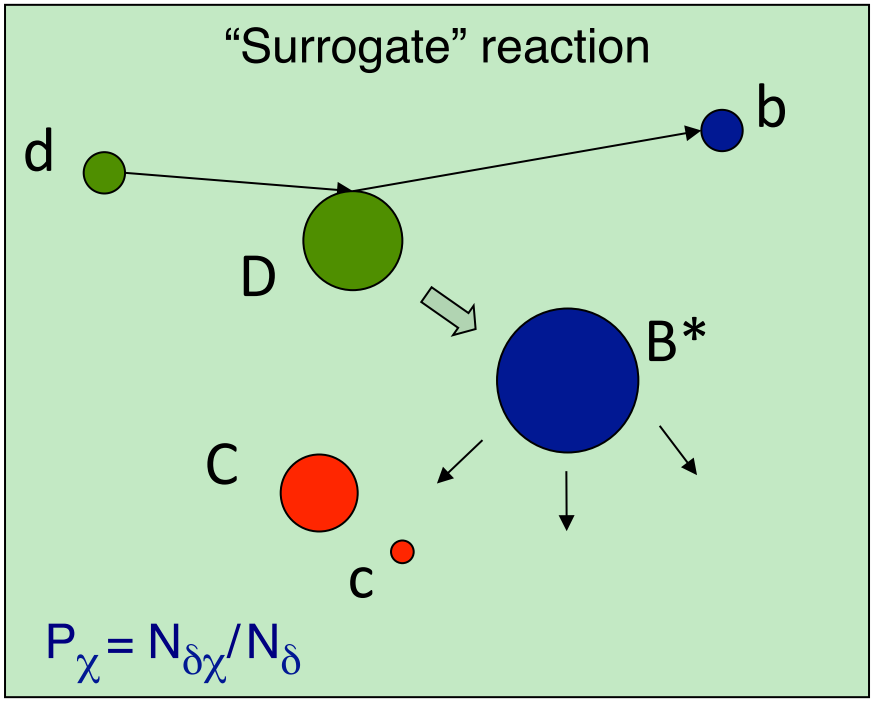
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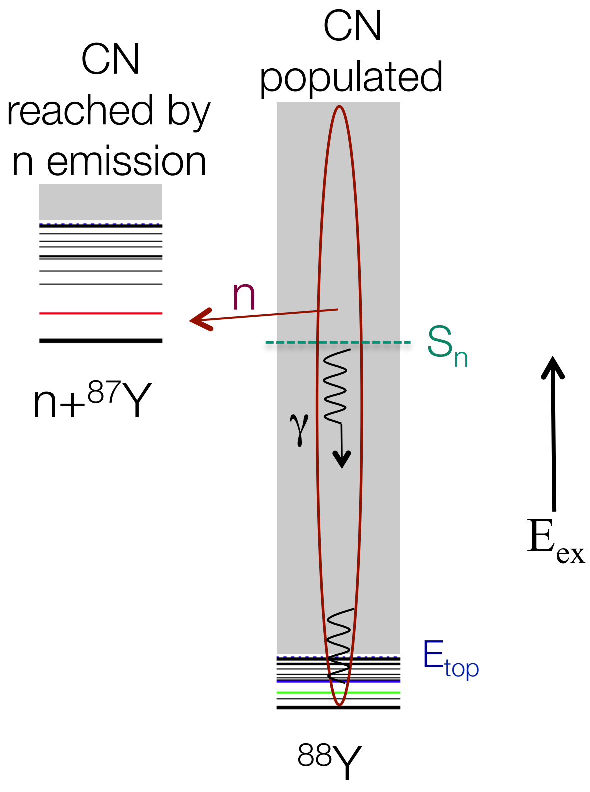
Implementing a new strategy: Surrogate approach beyond WE

Desired reaction: ^{87}Y(n,g)^{88}Y



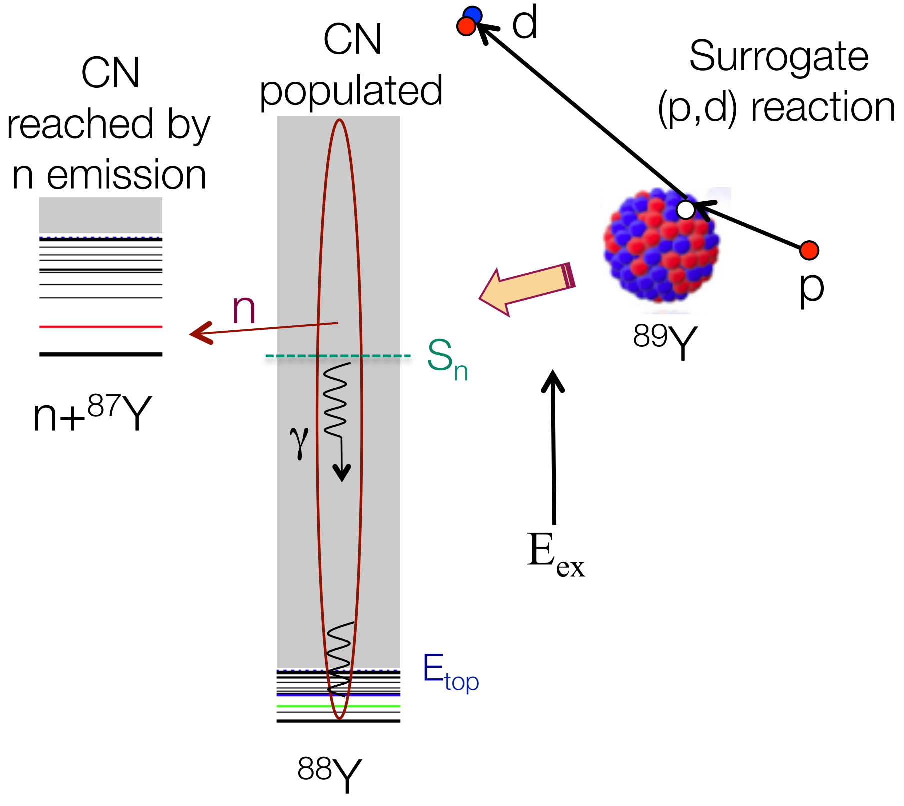
Hauser-Feshbach description of “desired” CN reaction

$$\sigma_{(n,\gamma)} = \sum_{J,\pi} \sigma_{n+target}^{CN}(E,J,\pi) \cdot G^{CN}_{\gamma}(E,J,\pi)$$

Implementing a new strategy: Surrogate approach beyond WE

Surrogate experiment

- Produce CN ^{88}Y via alternative **p + ^{89}Y -> d + ^{88}Y** involving stable ^{89}Y
- Measure outgoing surrogate particle **d** in coincidence with observables indicative of relevant decay channel ➔ $P_{\delta\gamma}(E)$



A Surrogate experiment gives

$$P_{(p,d\gamma)}(E) = \Sigma_{J,\pi}\, F_{(p,d)}^{CN}(E,J,\pi)\cdot G^{CN}_{\gamma}(E,J,\pi)$$

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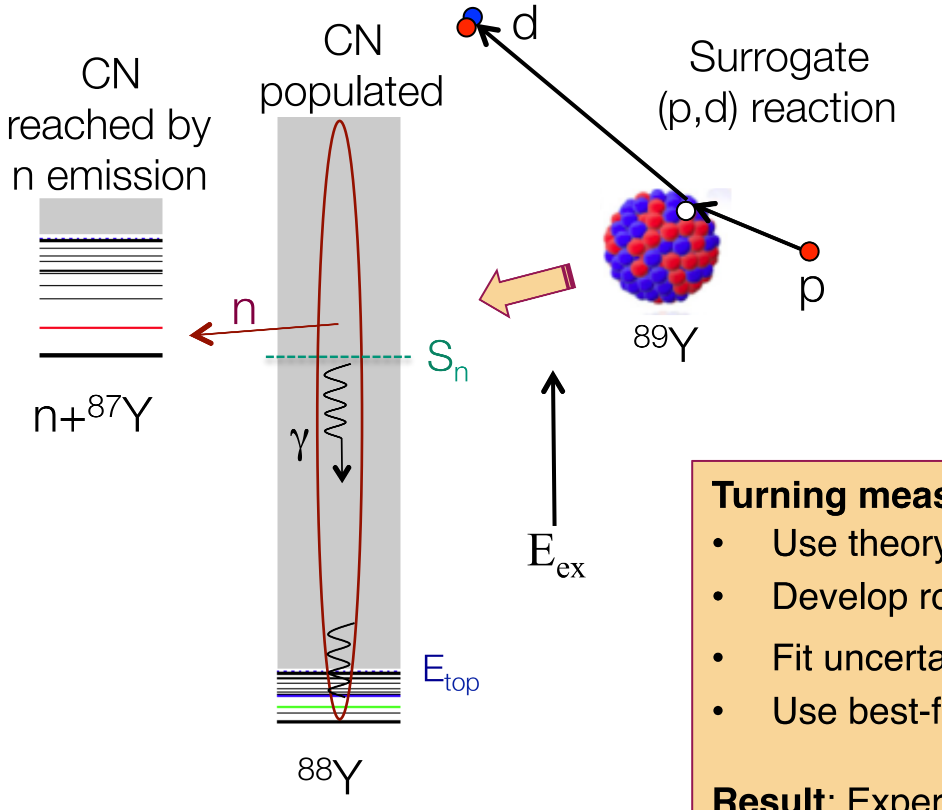

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Turning measurement into cross section

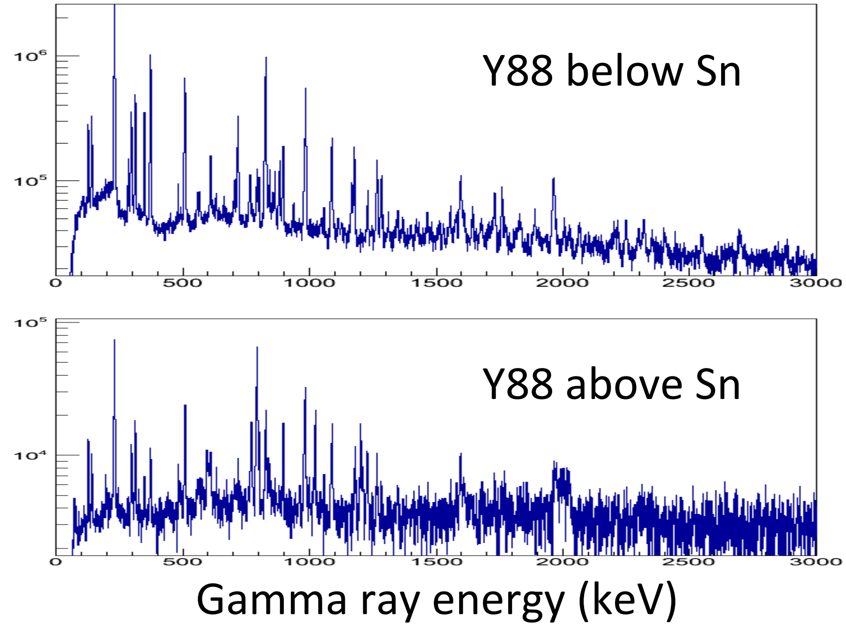
- Use theory to describe Surrogate reaction, predict $F_{(p,d)}^{CN}$
- Develop rough decay model G^{CN}_{γ}
- Fit uncertain parameters in G^{CN}_{γ} to reproduce $P_{(p,d\gamma)}$
- Use best-fit parameters to calculate desired $\sigma_{(n,\gamma)}$

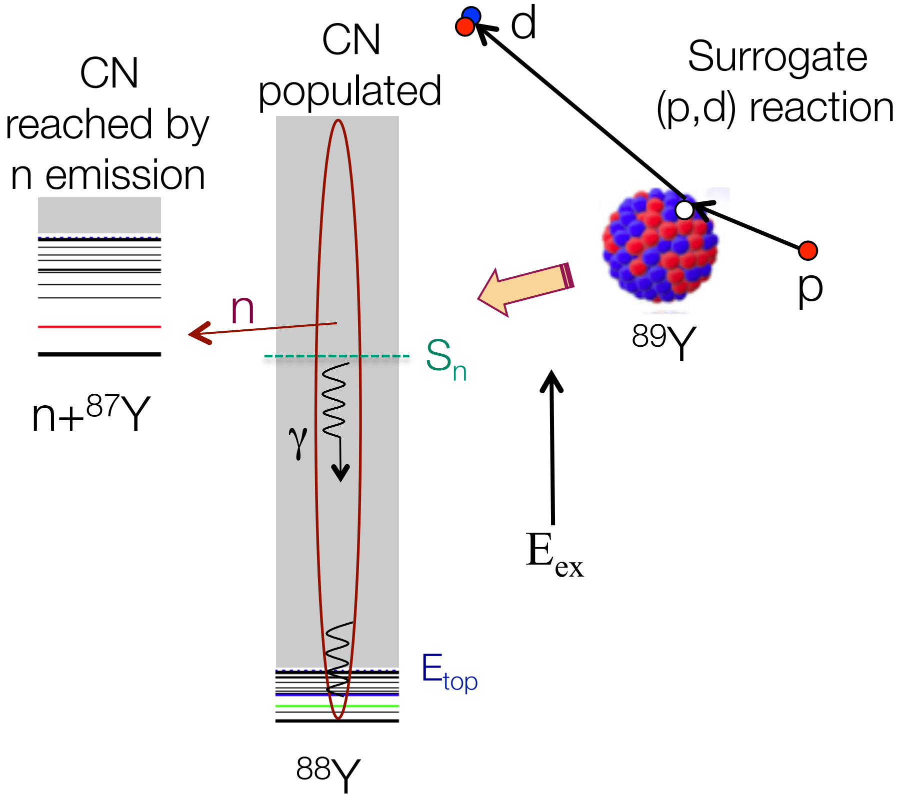
Result: Experimentally constrained cross section calculation.

^{89}Y(p,d)^{88}Y experiment to constrain ^{87}Y(n,γ)

Experiment at Texas A&M Cyclotron
^{89}Y(p,d) and ^{90,91,92}Zr(p,d)

γ-ray cascade in coincidence with outgoing surrogate particle (deuteron)



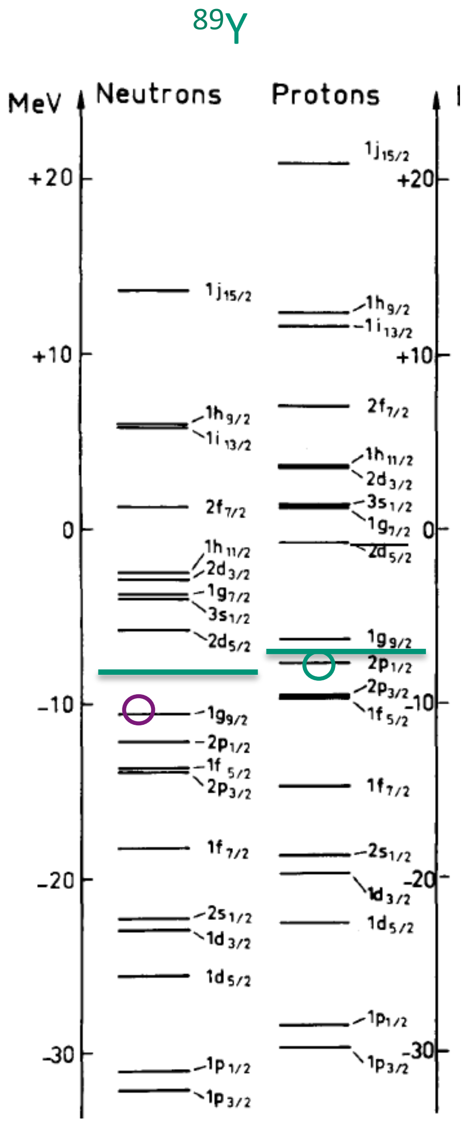


Burke, Casperson, Scielzo et al.

Describing CN formation in ^{89}Y(p,d) reaction

^{89}Y(p,d)^{88}Y:

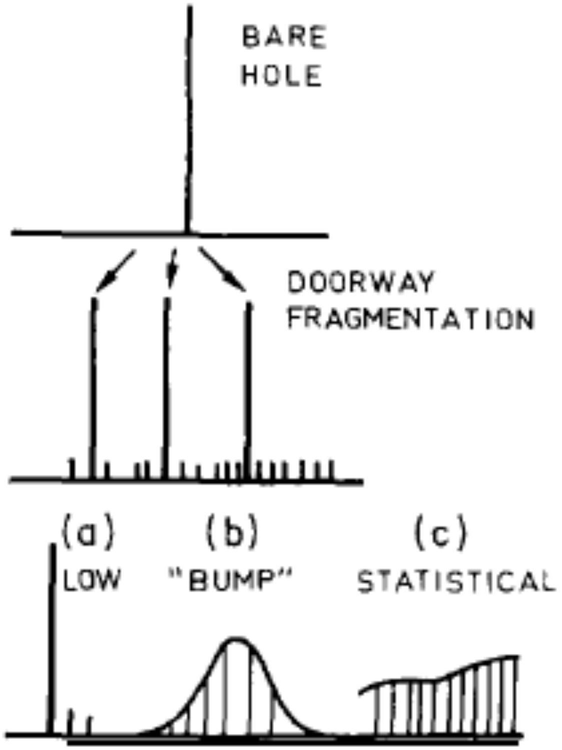
- Remove neutron from ^{89}Y (n:$J^{\pi}=0^{+}$ × p:$J^{\pi}=1/2^{-}$). Treat proton hole as spectator.



○ neutron hole made in reaction

Fragmentation of single-hole states: transfer reaction populates doorway states, which couple to more complex configurations

-> damping to CN occurs



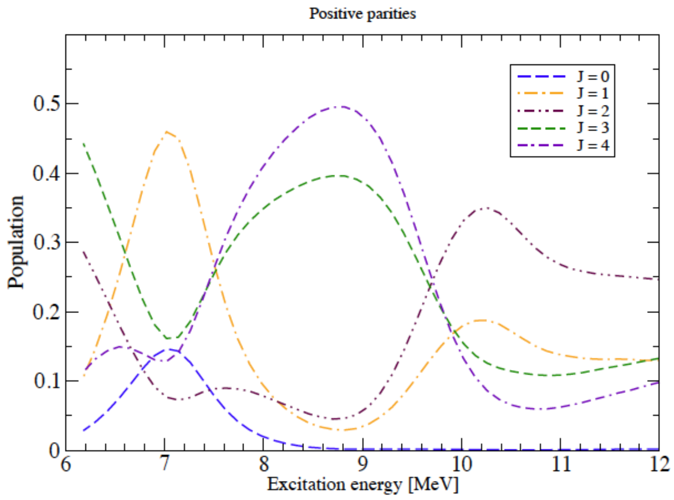
From Gales et al, Phys. Rep. 166 (1988) 125

Describing CN formation in ^{89}Y(p,d) reaction

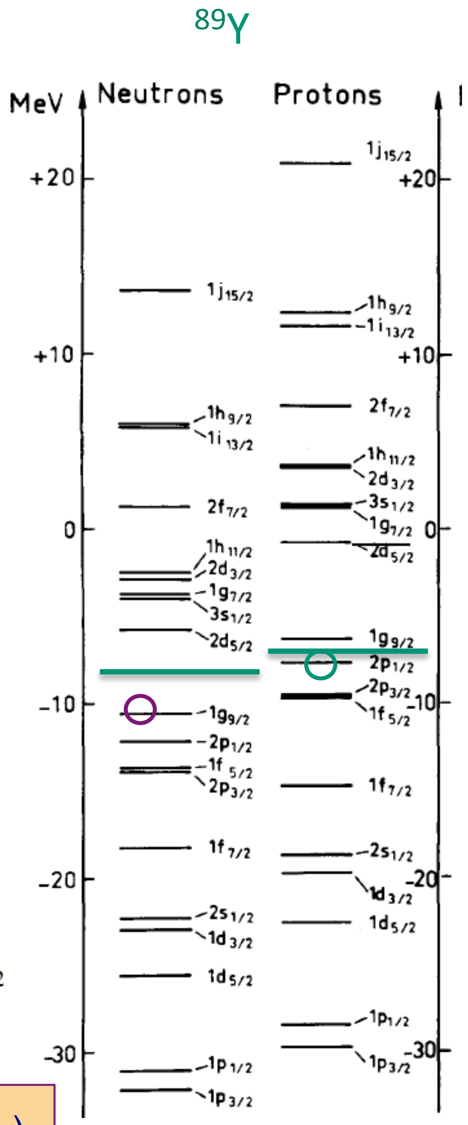
^{89}Y(p,d)^{88}Y:

- Remove neutron from ^{89}Y (n:$J^{\pi}=0^{+}$ × p:$J^{\pi}=1/2^{-}$). Treat proton hole as spectator.
- Apply damping & add all J^{π} contributions
- Extract spins, determine J^{π} distribution of ^{88}Y as function of E.

Spin-parity population $F_{(p,d)}^{CN}(E,J,\pi)$



$$P_{(p,d\gamma)}(E)=\Sigma_{J,\pi}\, F_{(p,d)}^{CN}(E,J,\pi)\cdot G^{CN}_{\gamma}(E,J,\pi)$$



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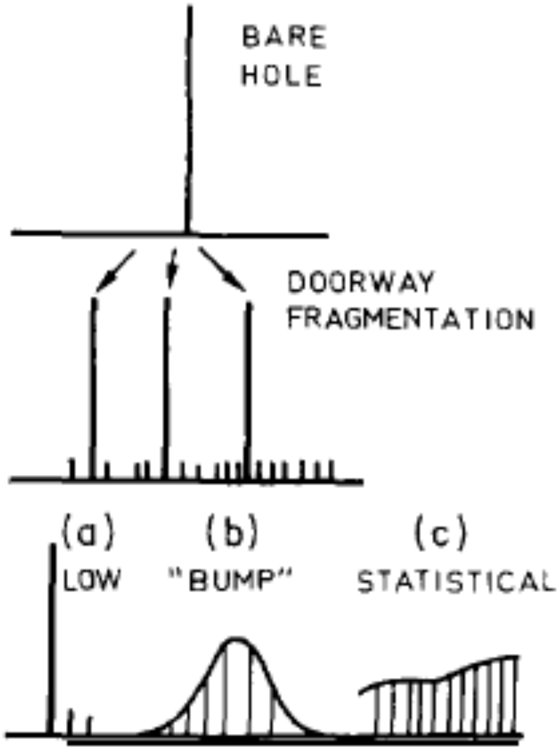

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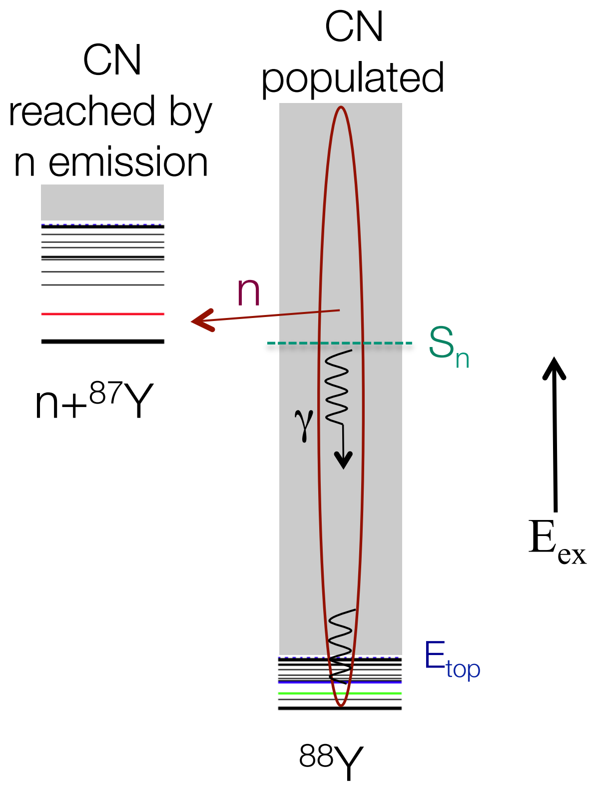
Modeling CN decay

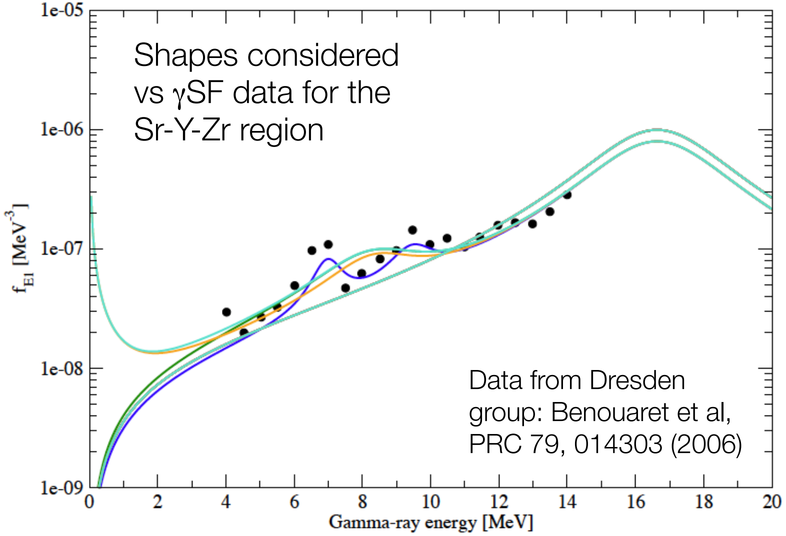
Develop rough decay model for ^{88}Y*:

- Literature values for energies + spins of low-lying states
- Literature values for branchings between low states
- LDs of Gilbert-Cameron form w/variable parameters
- γSF: various possibilities based on recent measurements & theory for the region



Example γSF:

Considering 5 shapes, w and w/o upturn and/or extra strength around 8 MeV.



Shapes considered vs γSF data for the Sr-Y-Zr region

Data from Dresden group: Benouaret et al, PRC 79, 014303 (2006)

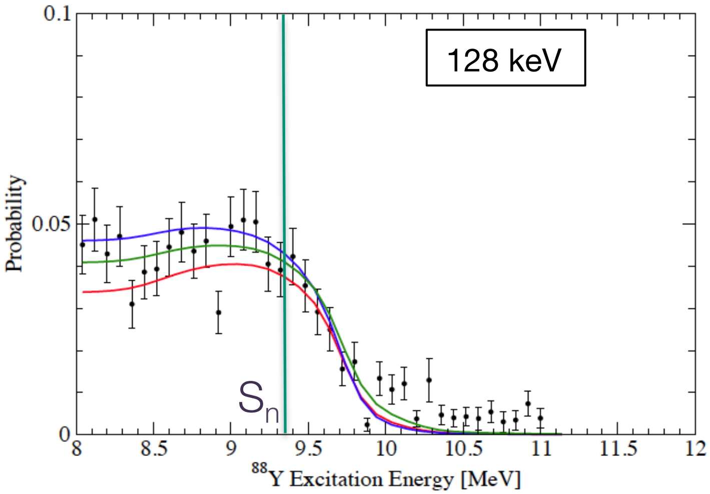
Decay model gives $G^{CN}_{\gamma}(E,J,\pi)$ for range of LD and γSF parameters.

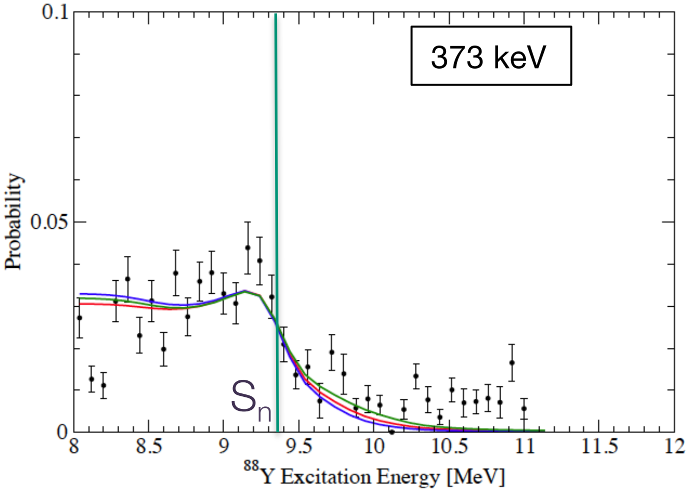
$$P_{(p,d\gamma)}(E)=\Sigma_{J,\pi}\, F_{(p,d)}^{CN}(E,J,\pi)\cdot G^{CN}_{\gamma}(E,J,\pi)$$

Fitting model parameters to multiple surrogate observables provides constraints on $G^{CN}_{\gamma}(E,J,\pi)$.

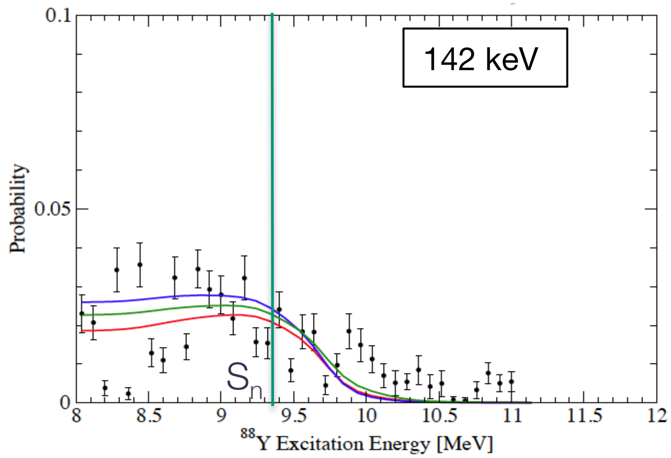
Fitting decay model to surrogate data

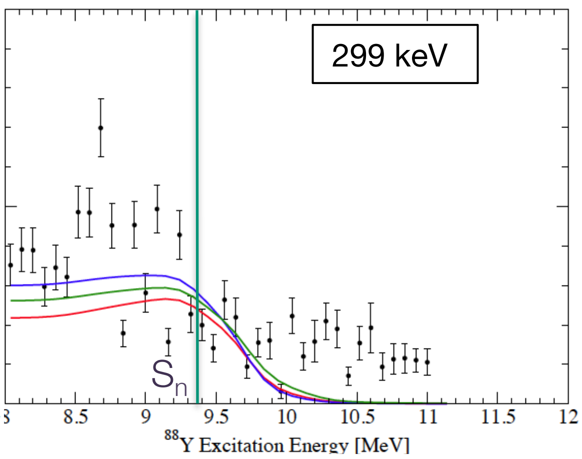
Fitting HF inputs to
reproduce surrogate
observables

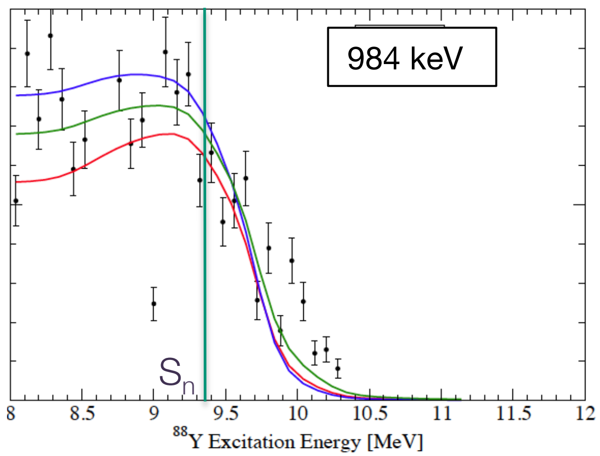




Preliminary



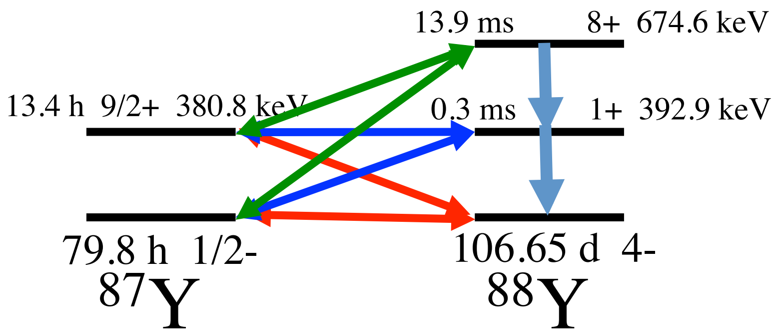


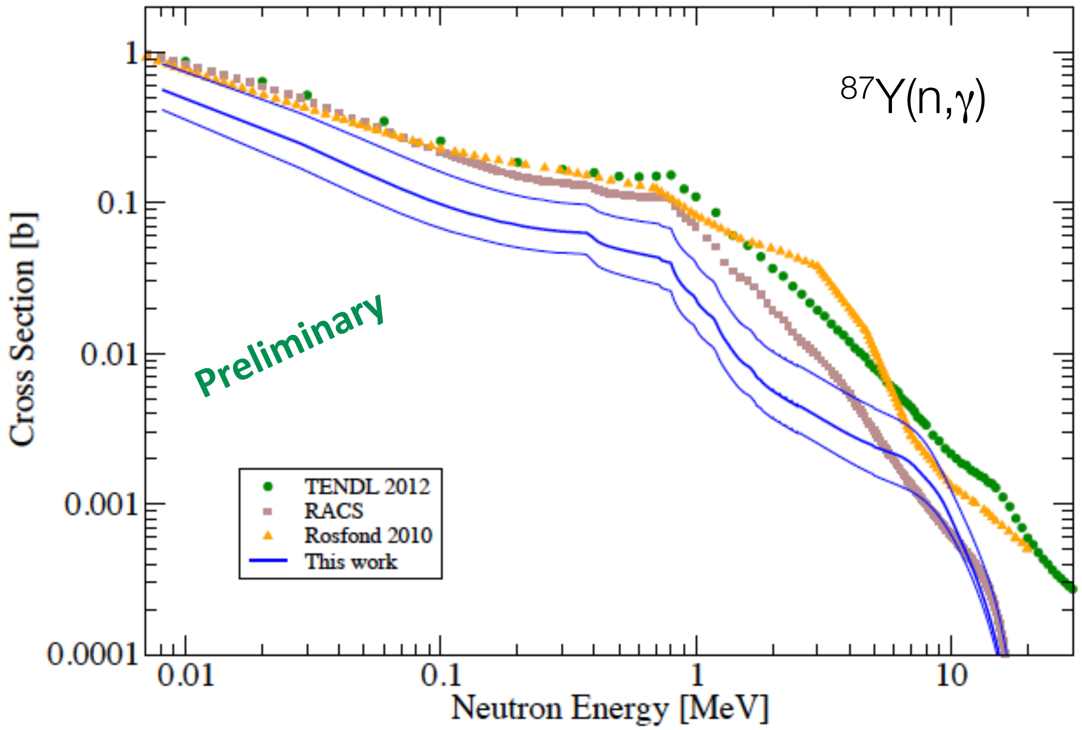


Fit yields best set of parameters & uncertainty estimate.

$$P_{(p,d\gamma)}(E)=\Sigma_{J,\pi}\, F_{(p,d)}^{CN}(E,J,\pi)\cdot G^{CN}_{\gamma}(E,J,\pi)$$

Results





Notes

- Cross section lower than previous evaluations
- Theory work underway to improve the J^{π} predictions
- Exp. work underway to reduce data scatter and to provide better constraints for theory
- Approach to be validated with ^{90}Zr(n,γ) benchmark

Using best set of parameters to calculate ^{87}Y(n,γ) and ^{87m}Y(n,γ)

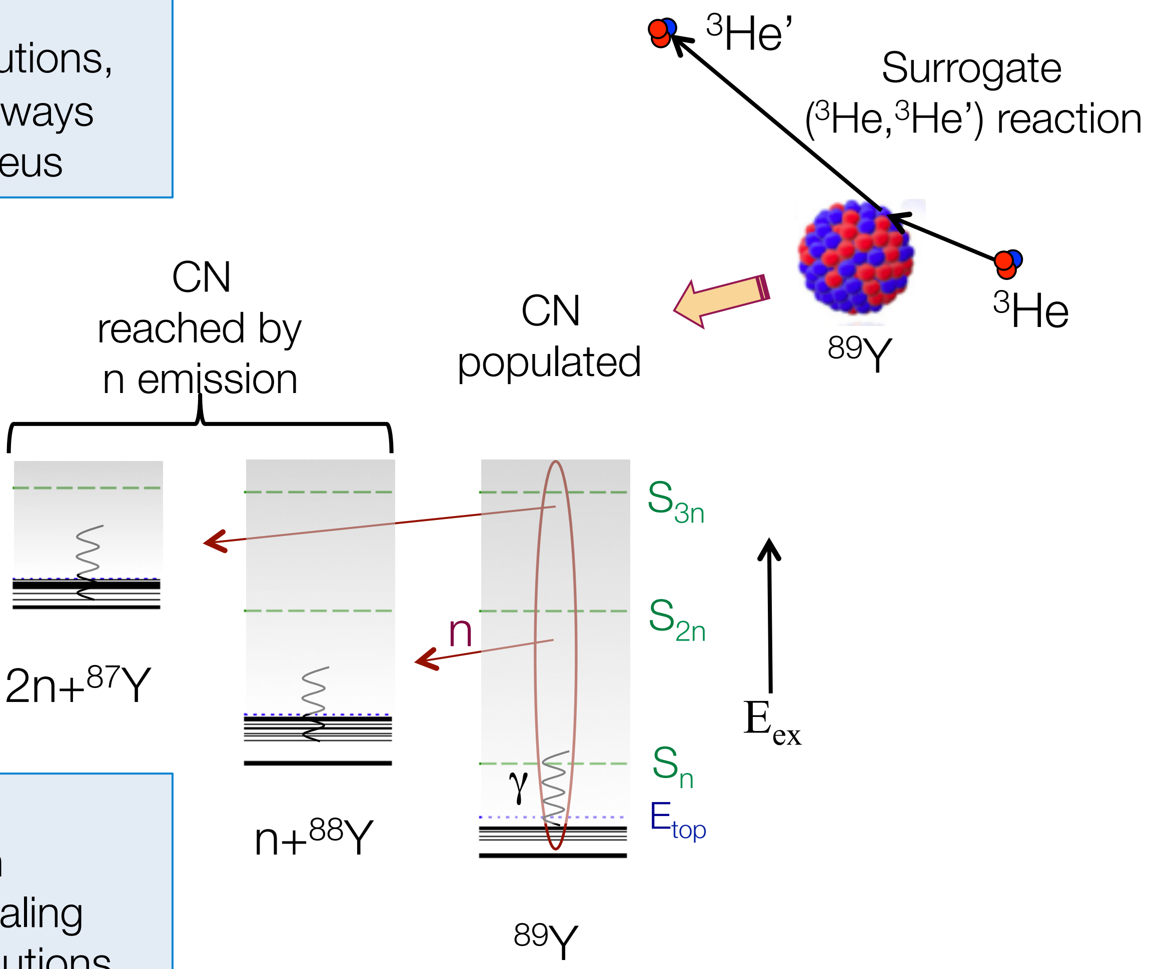
$$\sigma_{(n,\gamma)} = \sum_{J,\pi} \sigma_{n+target}^{CN}(E,J,\pi) \cdot G^{CN}_{\gamma}(E,J,\pi)$$

Is there ‘pre-equilibrium’ decay in surrogate reactions? How can we deal with it?

^{88}Y(n,2n): $t_{1/2}(^{88}Y)$=105d

Prevailing assumption:

No ‘pre-equilibrium’ contributions, i.e. the surrogate reaction always produces a compound nucleus



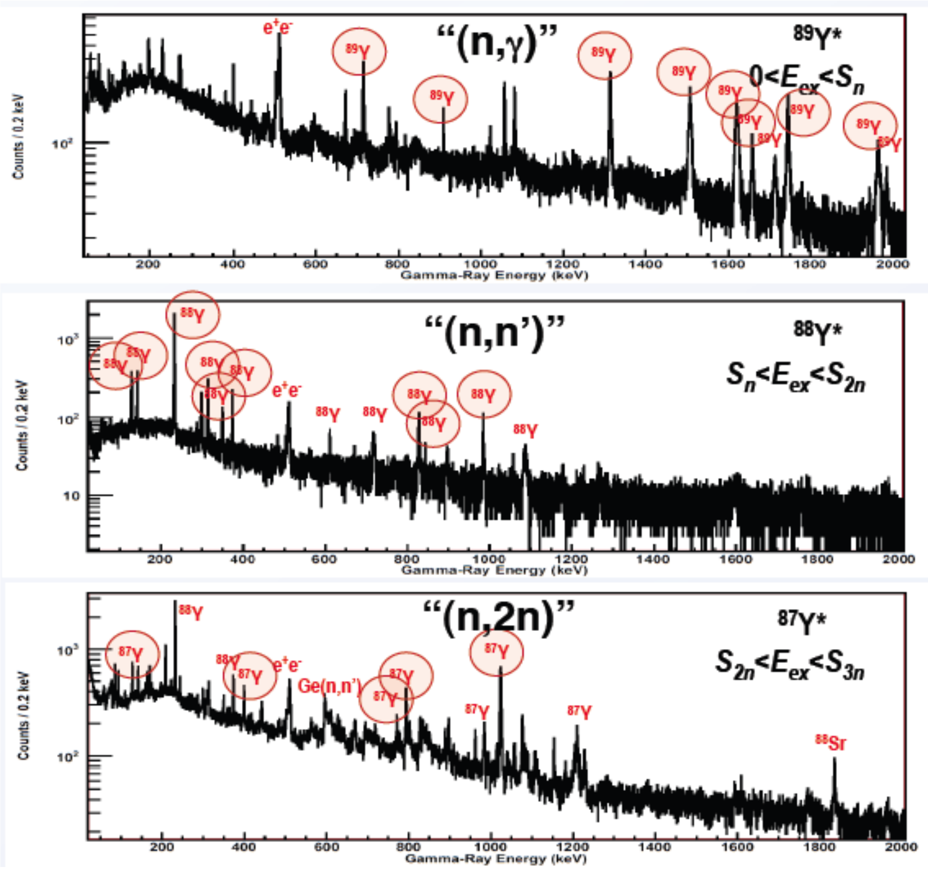
We need to…
1. Question this assumption
2. Develop a strategy for dealing with ‘pre-equilibrium contributions

CN formation via inelastic scattering

Experiment at LBNL:

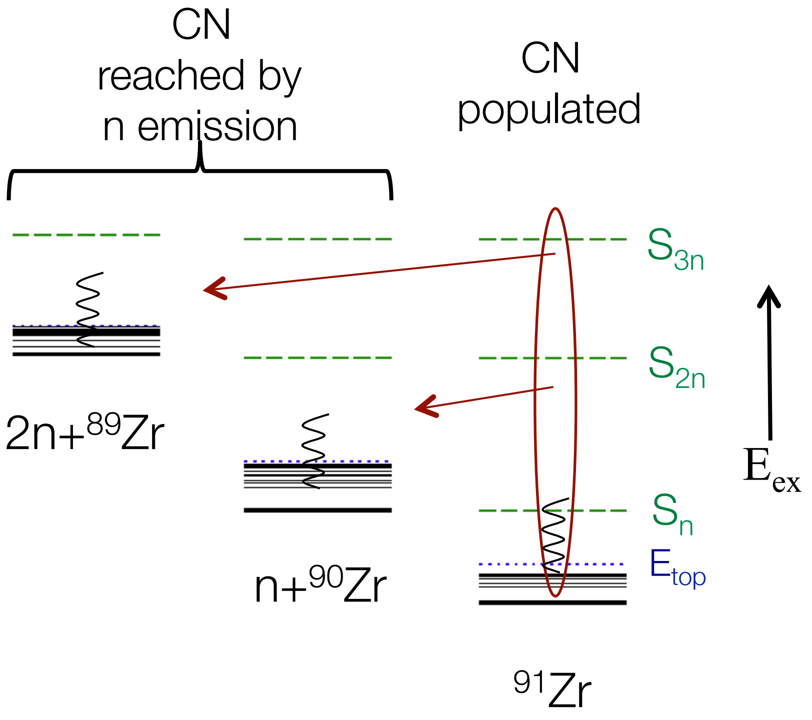
- ^{90,91,92}Zr(^{3}He,^{3}He’) and ^{89}Y(^{3}He,^{3}He’)

γ-ray cascade in coincidence with outgoing surrogate particle (^{3}He’)



$E_\gamma \longrightarrow$

Data from N.D. Scielzo



CN reached by n emission

CN populated

Describing CN formation via inelastic scattering

Structure theory for ^{90}Zr(^{3}He,^{3}He')

- QRPA with Skyrme SLy4
- (Alternative: RPA with Gogny D1N)
- Description of states to 30 MeV

Reaction theory for ^{90}Zr(^{3}He,^{3}He')

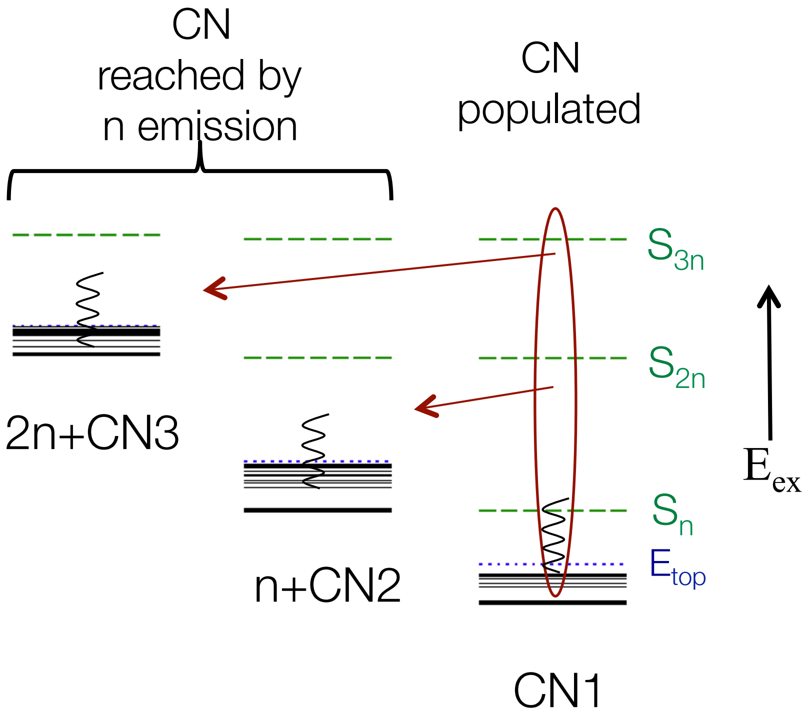
- DWBA description (Fresco code)
- Calculations up to J=9

Treatment of damping (CN formation)

- Phenomenological spreading width
- Accounts for higher-order couplings
- Energy-dependent width

Spin-parity distribution in CN

- Determined from relative contributions of xsecs



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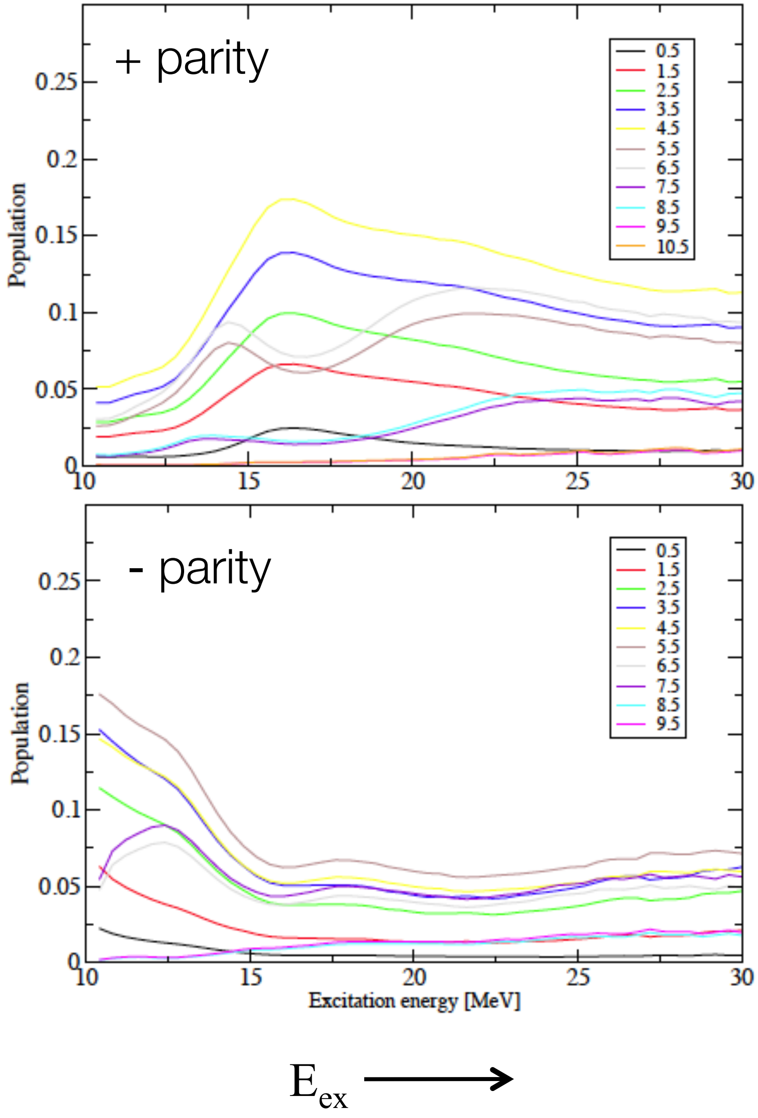


Comparison with experiment

Procedure:

- Calculate $F_{\delta}^{CN}(E,J,\pi)$
- Model CN decay
- Adjust HF parameters to reproduce measured $P_{\chi}(E)$, here γ-transitions
- Use best-fit HF parameters to obtain G^{CN}_{χ}
- Calculate desired cross section

A Surrogate experiment gives

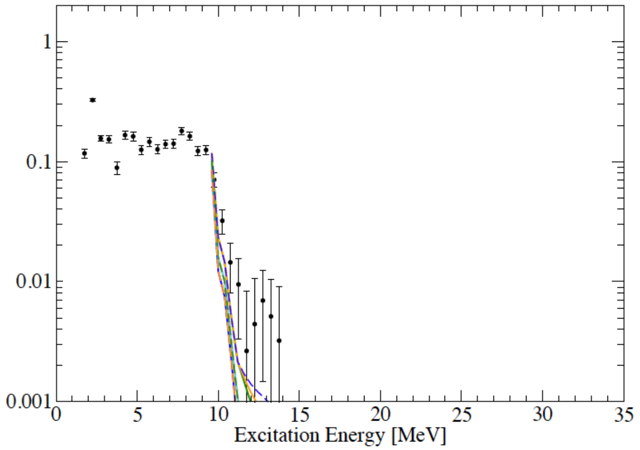
$$P_{\chi}(E) = \Sigma_{J,\pi}\, F_{\delta}^{CN}(E,J,\pi) \cdot G^{CN}_{\chi}(E,J,\pi)$$

Hauser-Feshbach description of “desired” CN reaction

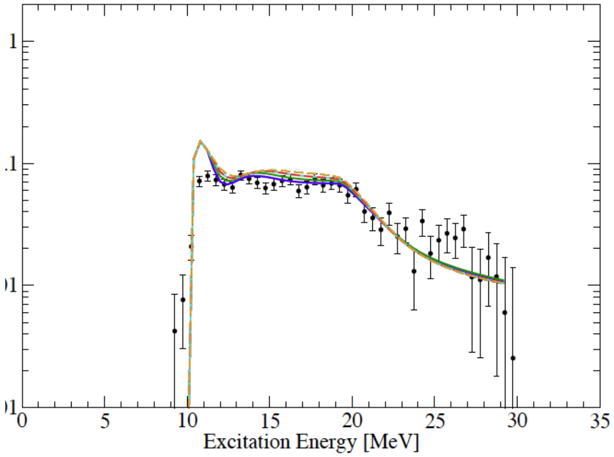
$$\sigma_{\alpha\chi} = \Sigma_{J,\pi}\, \sigma_{\alpha}^{CN}(E,J,\pi) \cdot G^{CN}_{\chi}(E,J,\pi)$$

Preliminary

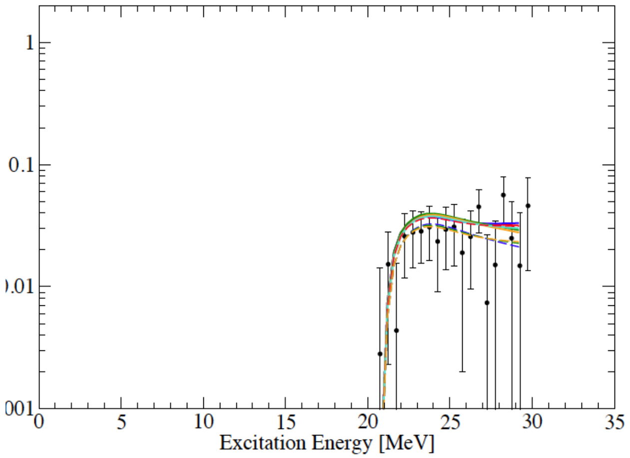
$P_{\gamma}(E)$ for 2170 keV in ^{91}Zr
Predictions vs. data



$P_{\gamma}(E)$ for 890 keV in ^{90}Zr
Predictions vs. data

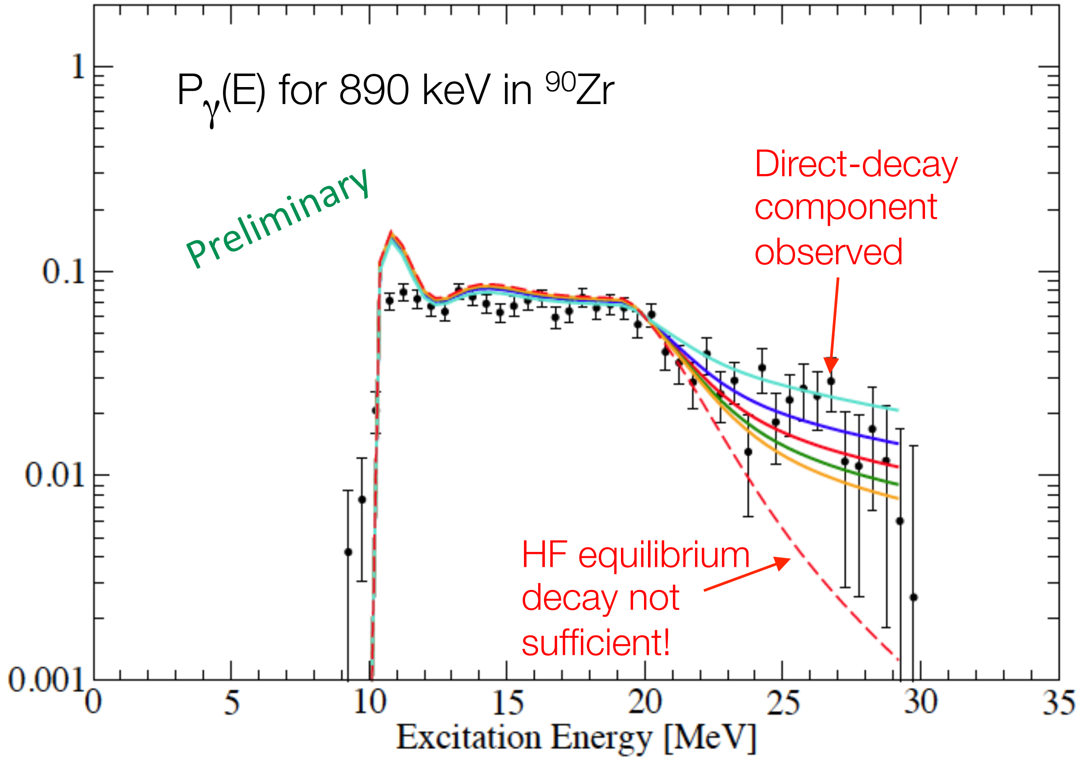


$P_{\gamma}(E)$ for 1512 keV in ^{89}Zr
Predictions vs. data



…and similarly for Y

Comparison with experiment

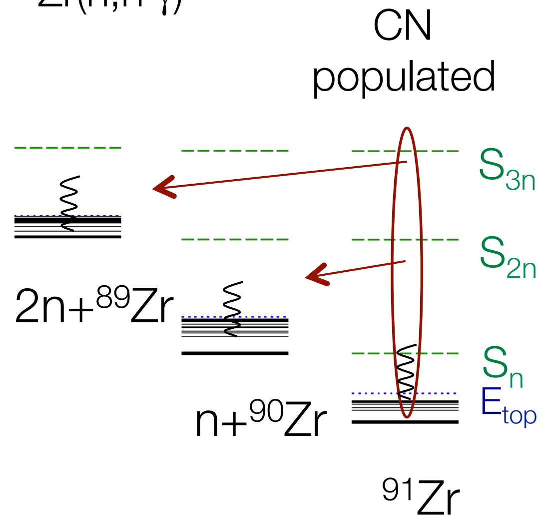

$P_\gamma(E)$ for 890 keV in ^{90}Zr

Preliminary

Direct-decay component observed

HF equilibrium decay not sufficient!

^{91}Zr(^{3}He,^{3}He' n'γ)
~ ^{90}Zr(n,n'γ)



Insights:

- Reproducing Surrogate coincidence probability requires ‘pre-equilibrium’ contribution
- Neutron emission prior to equilibration sets in around E_n=7 MeV
- Modeling this contribution is relevant for describing 2n emission
- γ-ray measurements provide useful information

Insights

- Cross section calculations for compound reactions: Require reliable structure input (which is often not available)
- Indirect cross section approaches: Require a solid understanding of the reaction processes involved
- Pickup reactions: A good description of the fragmentation of hole states is needed
- Inelastic scattering: To include pre-equilibrium decay in the description, (Q)RPA is not sufficient. An exciton description is useful, explicit coupling to the continuum would be a plus
- Stripping reactions: Will play a prominent role at FRIB and other RIB facilities. Breakup and breakup-fusion needs to be included in the description -> see G. Potel's talk
- Low level density situations: require additional thought, as the statistical assumptions are no longer valid.
- High-quality experimental data is needed to constrain the theory and to produce cross section results. Benchmarks are valuable.

Thanks to my Collaborators

Surrogate Reactions

Theory

Frank Dietrich, Daniel Gogny, Ian Thompson, Walid Younes (LLNL)

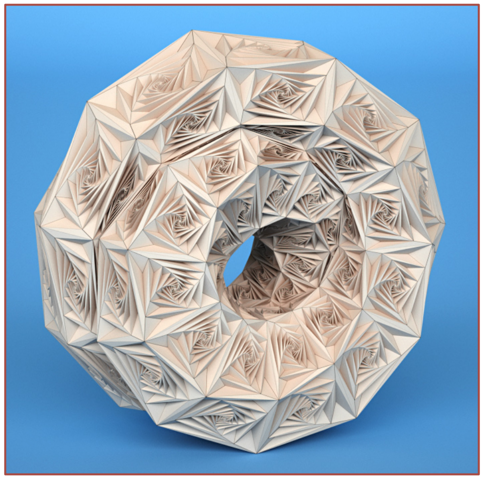
Experiment

J. Burke, R. Casperson, R. Hughes,
J.J. Ressler, N.D. Scielzo (LLNL)
C. Beausang, T. Ross (U Richmond)
J. Cizewski et al (Rutgers)

ReactionTheory.org

TORUS: Theory of Reactions for Unstable iSotopes
A Topical Collaboration for Nuclear Theory

www.reactiontheory.org



TORUS collaborators

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Charlotte Elster, OU
Goran Arbanas, ORNL

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

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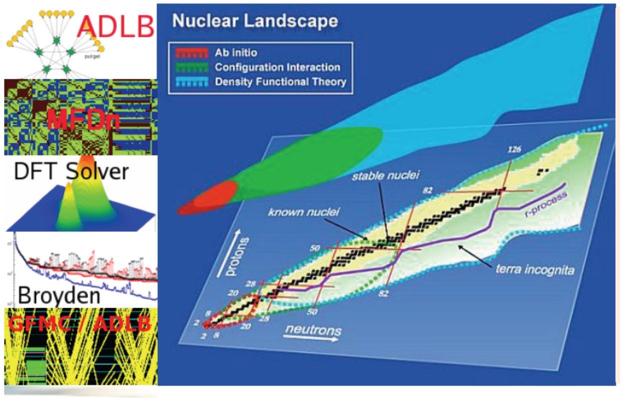

SciDAC collaborators

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I.J. Thompson (LLNL)
G. Nobre (BNL)
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J. Terasaki (UNC)
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Capture-γ Project

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