First principles calculations of light-ion reactions as a tool for nuclear data.

Nuclear Data for the Next Decade

9-13 March 2025

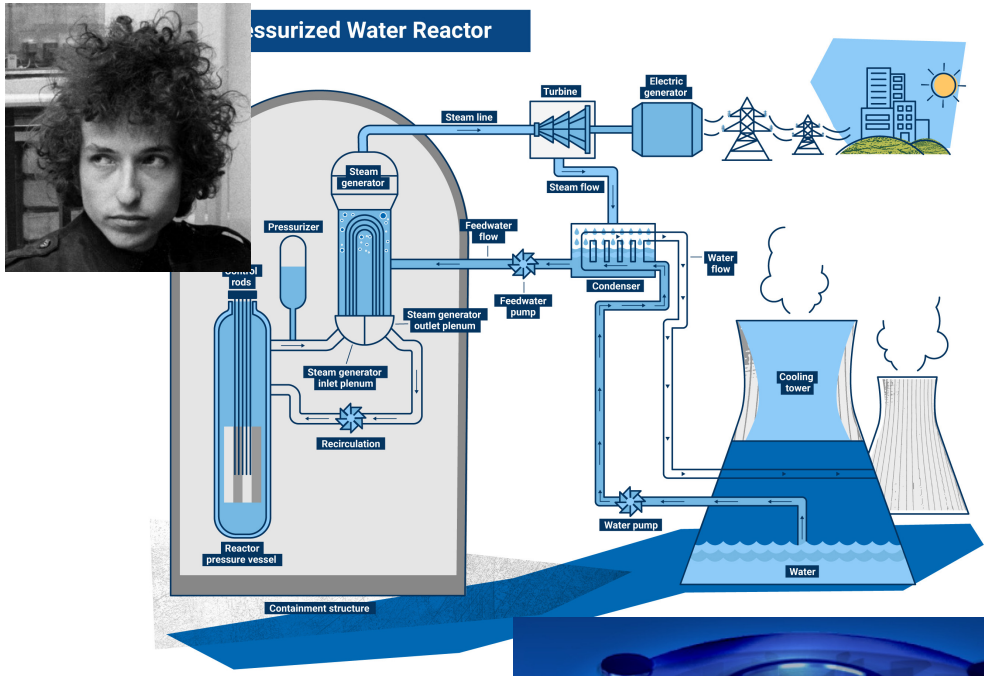
Konstantinos Kravvaris

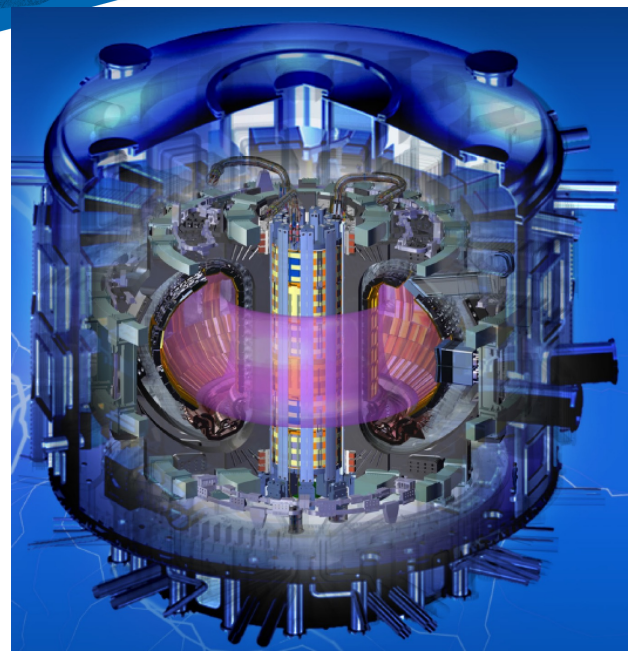
Prepared by LLNL under Contract DE-AC52-07NA27344.

The times they are a-changin’

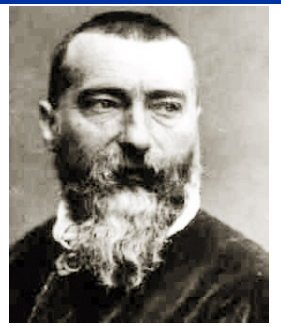
–Bob Dylan

- V&V for fusion
- Improved lithium cross sections for T-breeding
- T transport
- Exotic fusion energy approaches
- Neutron multiplication from beryllium
- Interactions with tritium breeding blanket materials
- Improved neutron standards
- Predictive nuclear data

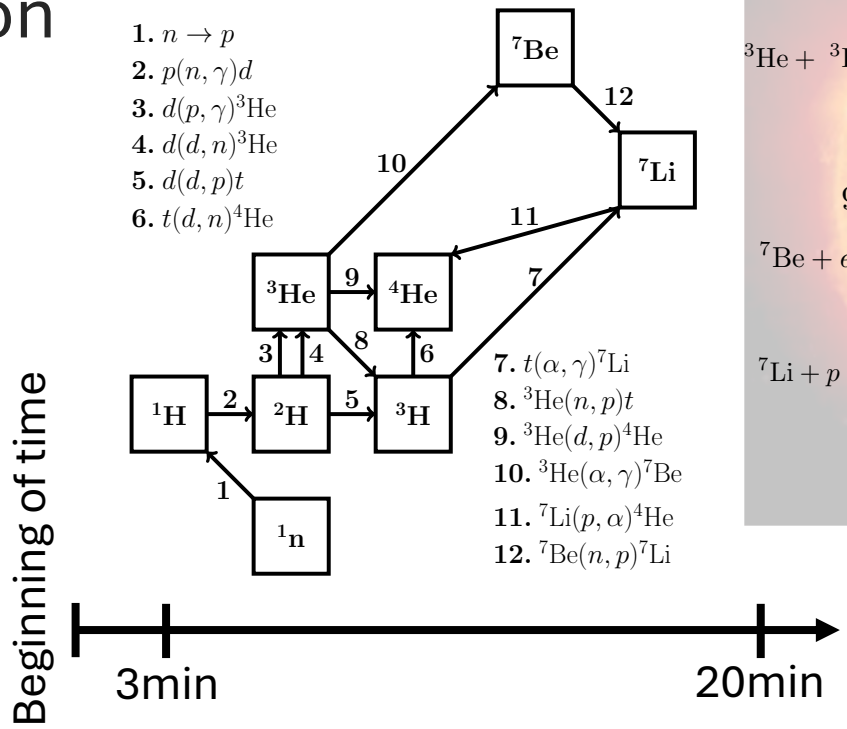


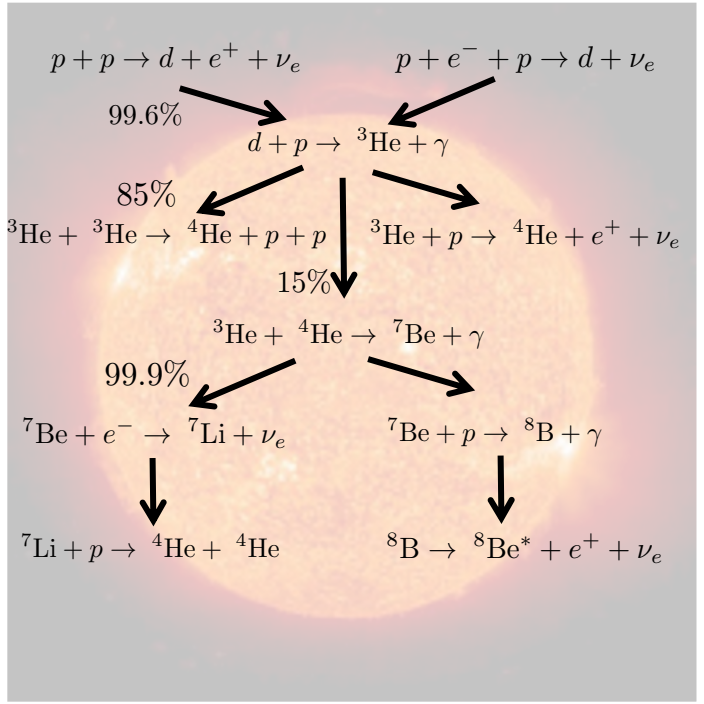


“The more things change, the more they stay the same” –Jean-Baptiste Alphonse Karr



- Light-ion cross sections relevant to big bang nucleosynthesis/solar fusion
- Light-ion reaction networks
- Improved modeling for stockpile stewardship applications





Currently, the phenomenological R-matrix provides the backbone for such evaluations.

- Concerns:
  - It only gets as good as the data you use to fit to—predictiveness is limited
  - Consequently, model error is difficult to quantify (including ad hoc choices, channel radius)
  - Treatment of non-resonant processes may require non-observables as input.

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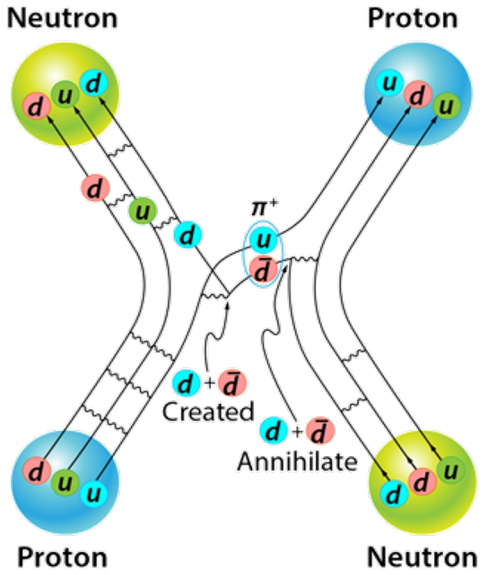
Shameless plug:

How low can you go? Ab initio theory removes quite a few (if not all) the assumptions made in modeling.

Quantum Chromodynamics



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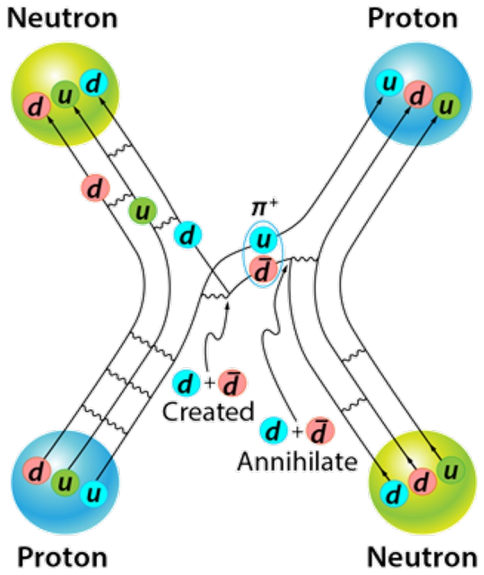
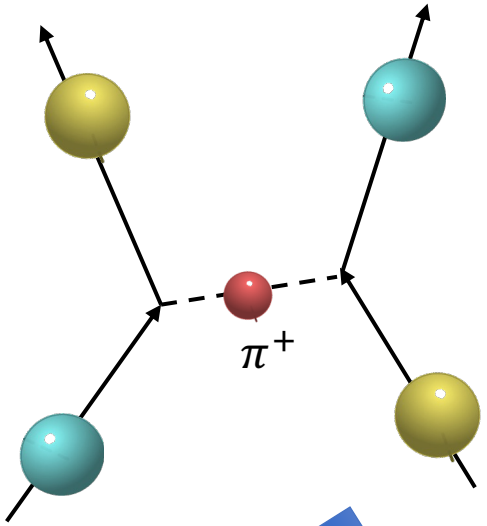


Chiral Effective Field Theory



Two & three-nucleon (NN+3N) forces

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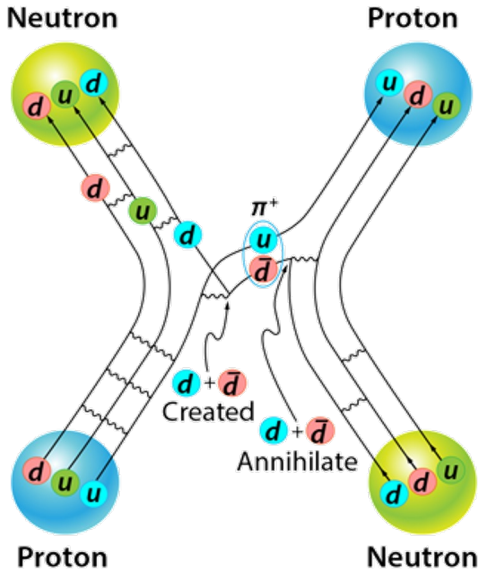

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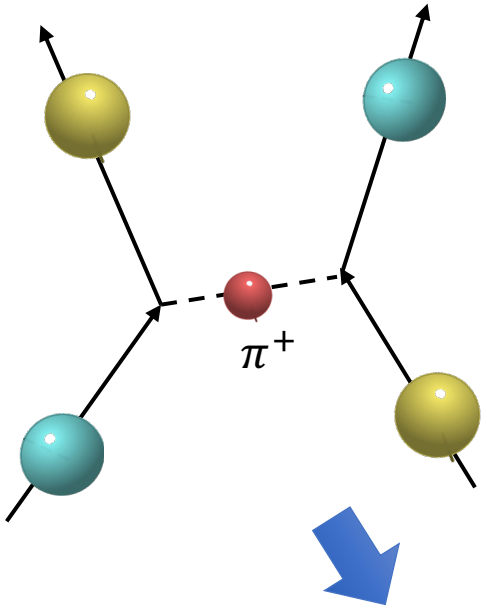
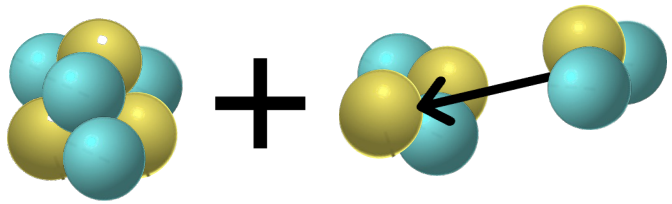


Two & three-nucleon (NN+3N) forces

Unified ab initio many-body approach to structure and reactions



All active (point-like) nucleons, non-relativistic quantum mechanics

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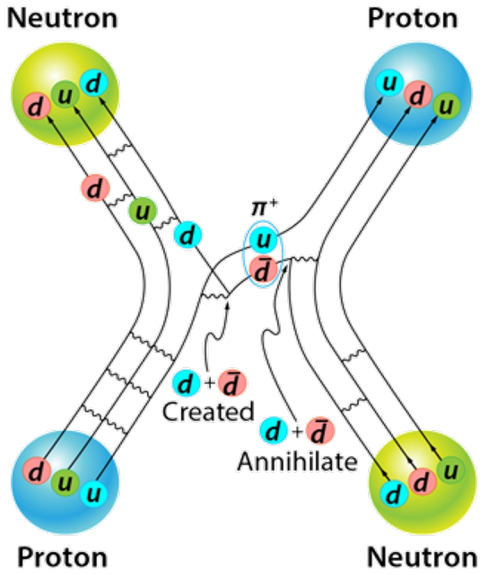
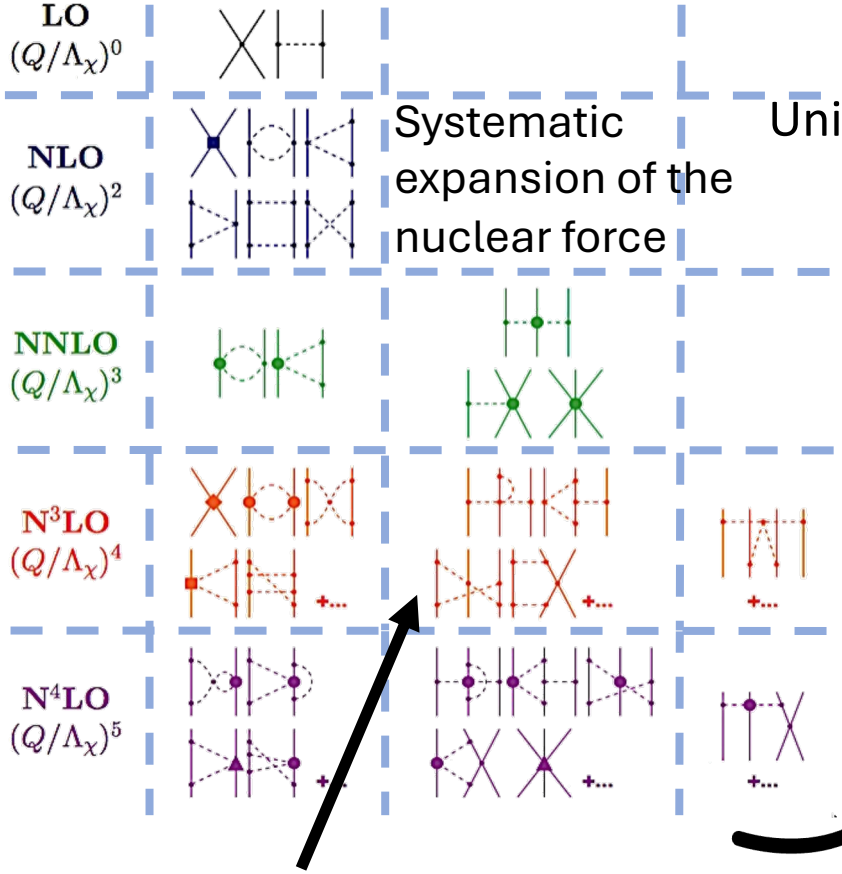
Quantum Chromodynamics

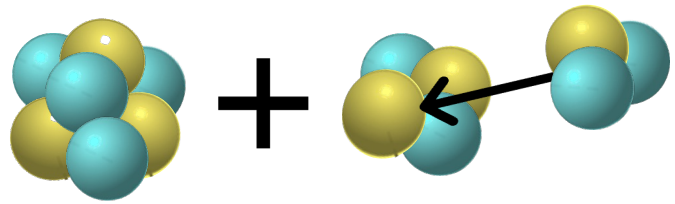




Systematic expansion of the nuclear force

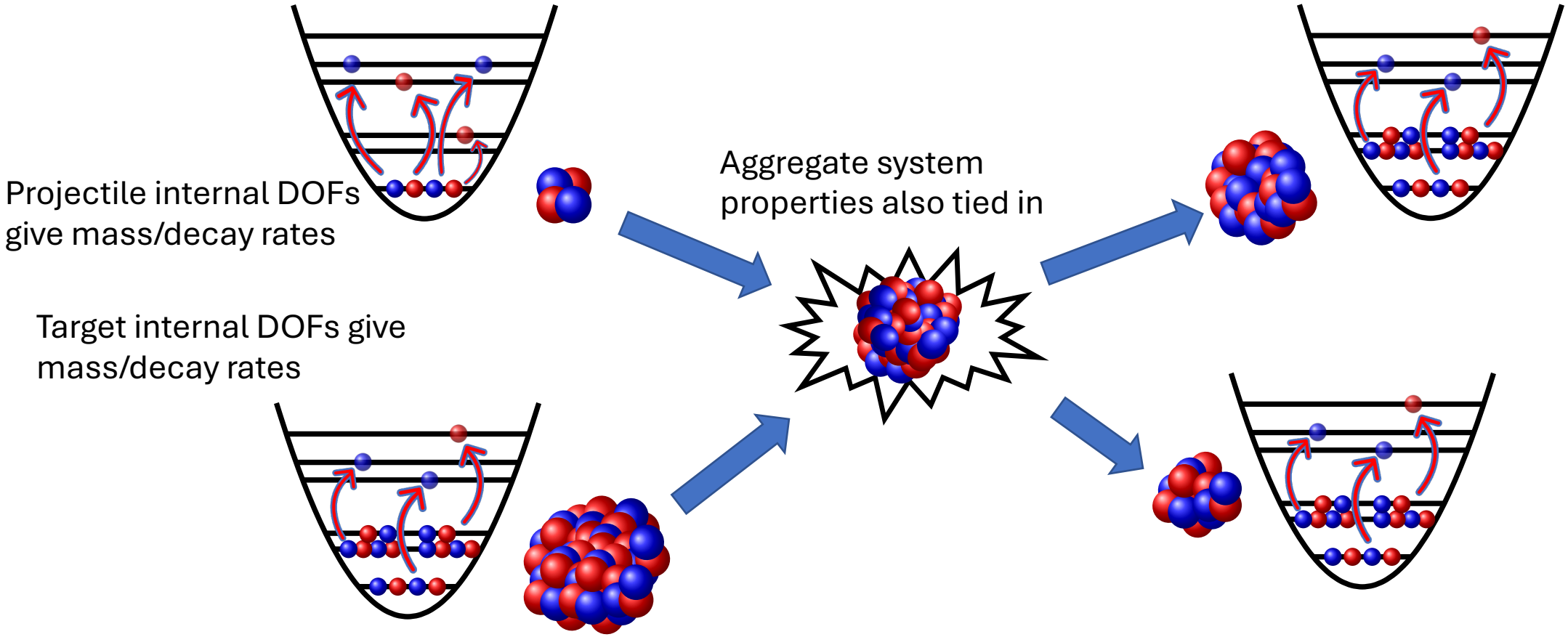
Fit to few-body observables (masses, decay rates)

Unified ab initio many-body approach to structure and reactions



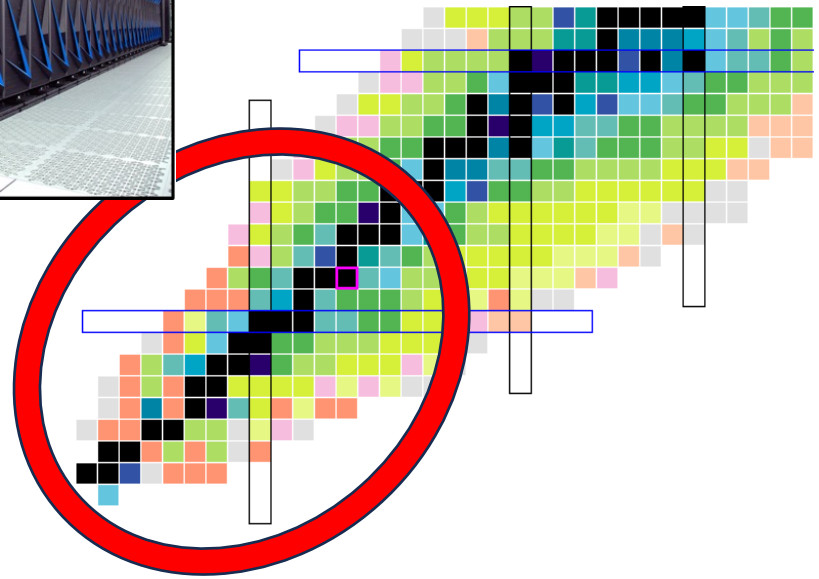
All active (point-like) nucleons, non-relativistic quantum mechanics

Describing the dynamical reaction process maintains the internal degrees of freedom of the nucleus



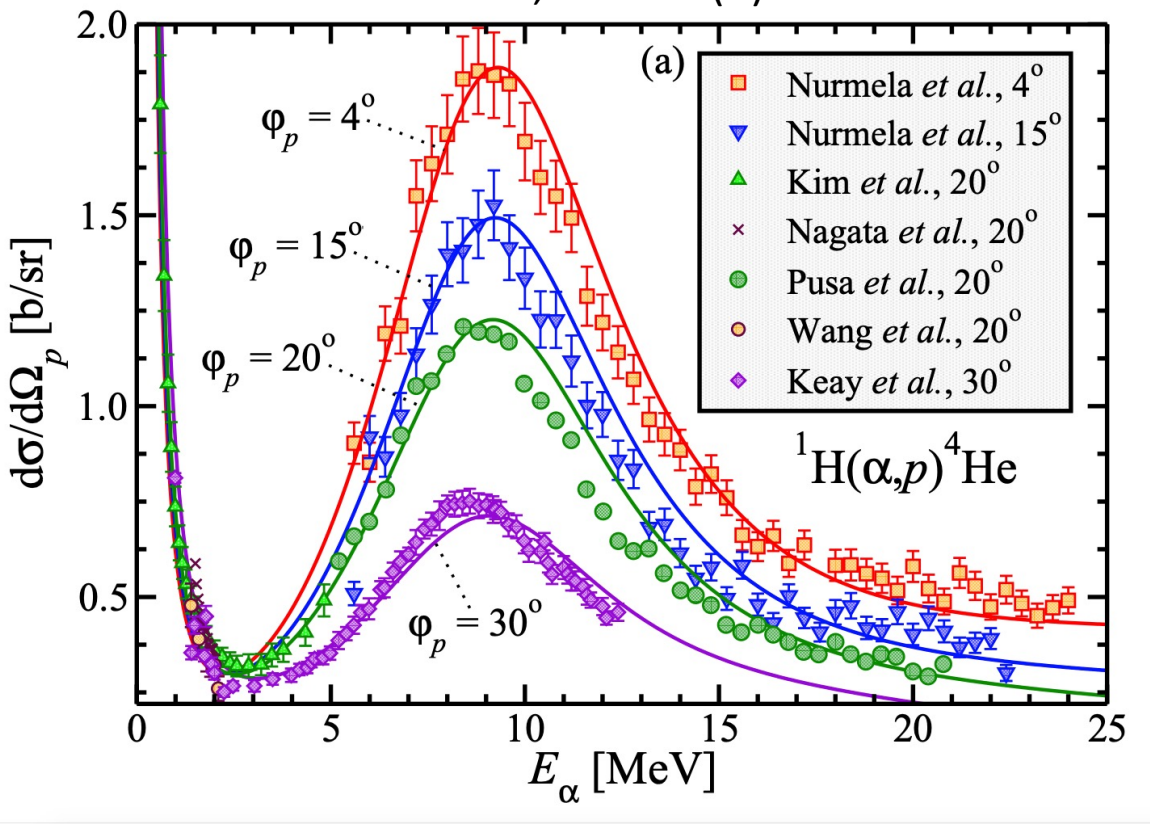
The full quantum-mechanical treatment of a reaction at the many-body level is computationally expensive

- Ab initio single-nucleon reaction calculations for nuclei beyond oxygen are prohibitive
- Composite incoming nuclei are significantly more challenging
- Look into low-fidelity approaches to extend the reach--not evaluation quality but insights can be gained

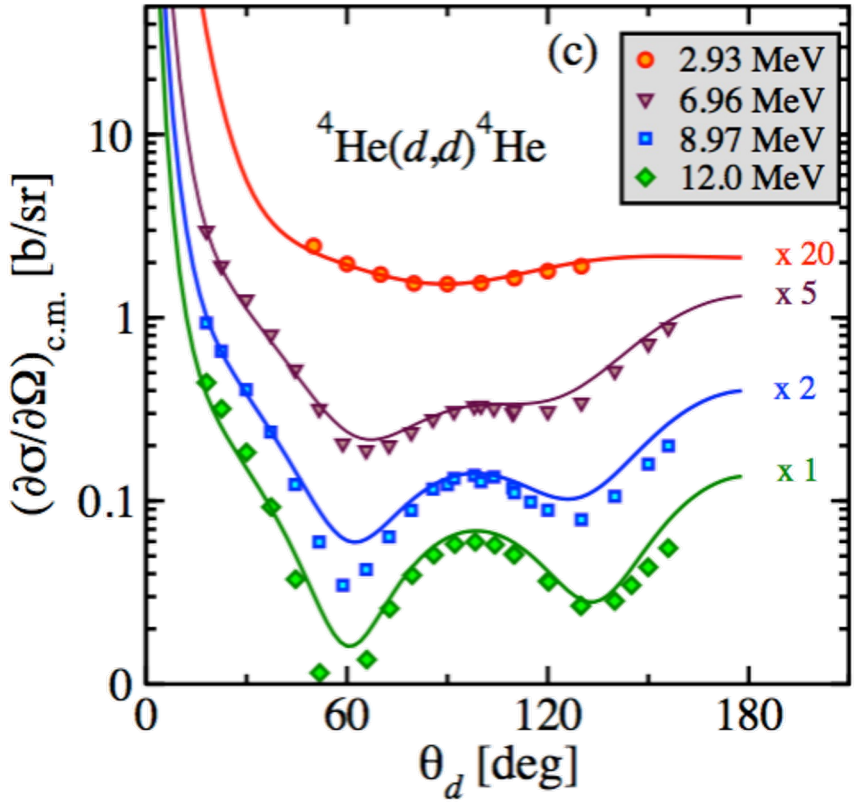


Making accurate predictions begs the question of the impact of parametric uncertainties

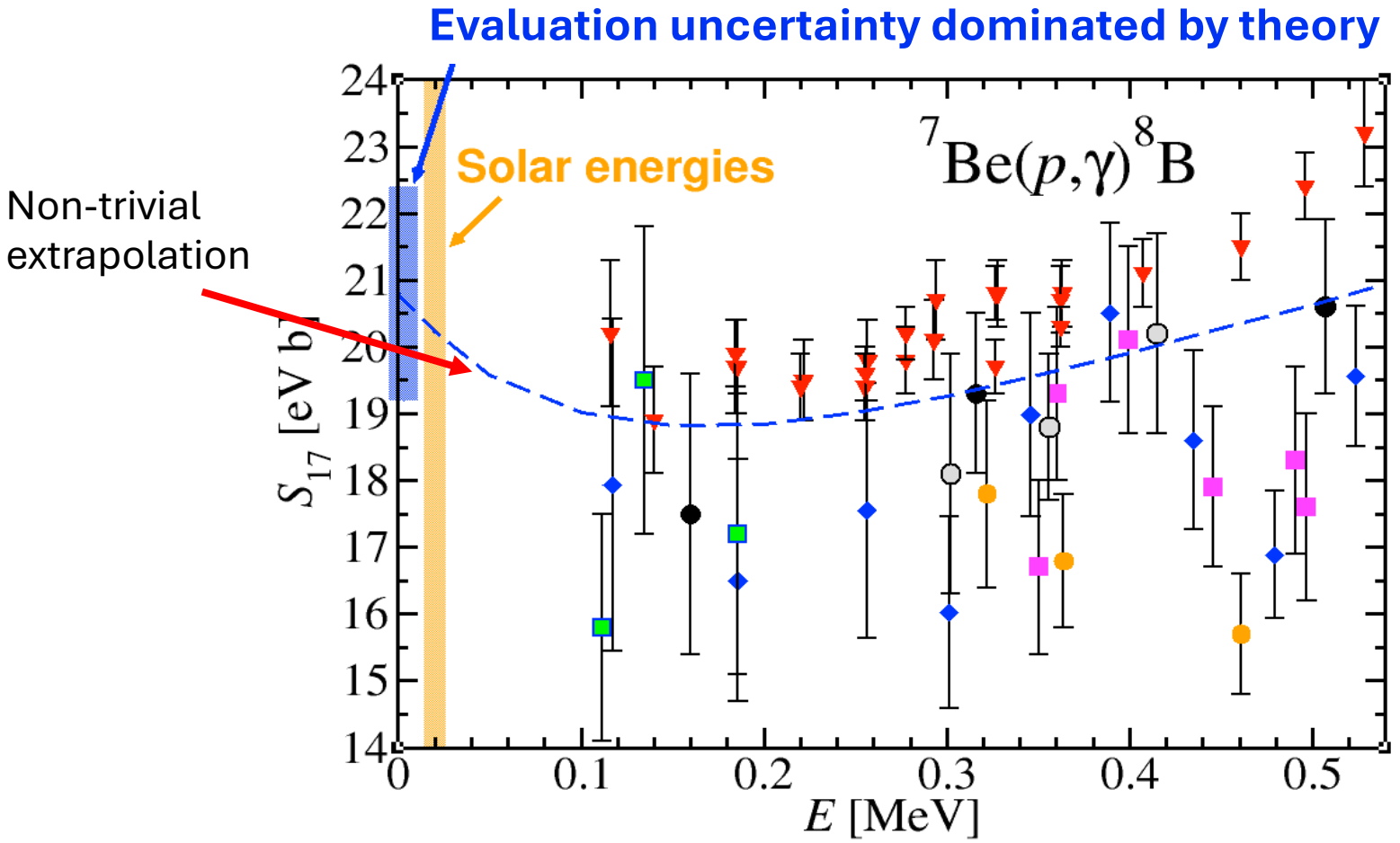
PRC 90, 061601(R)



PRL114, 212502



Since it works, we should go ahead and use it: Predicting solar fusion reaction cross sections



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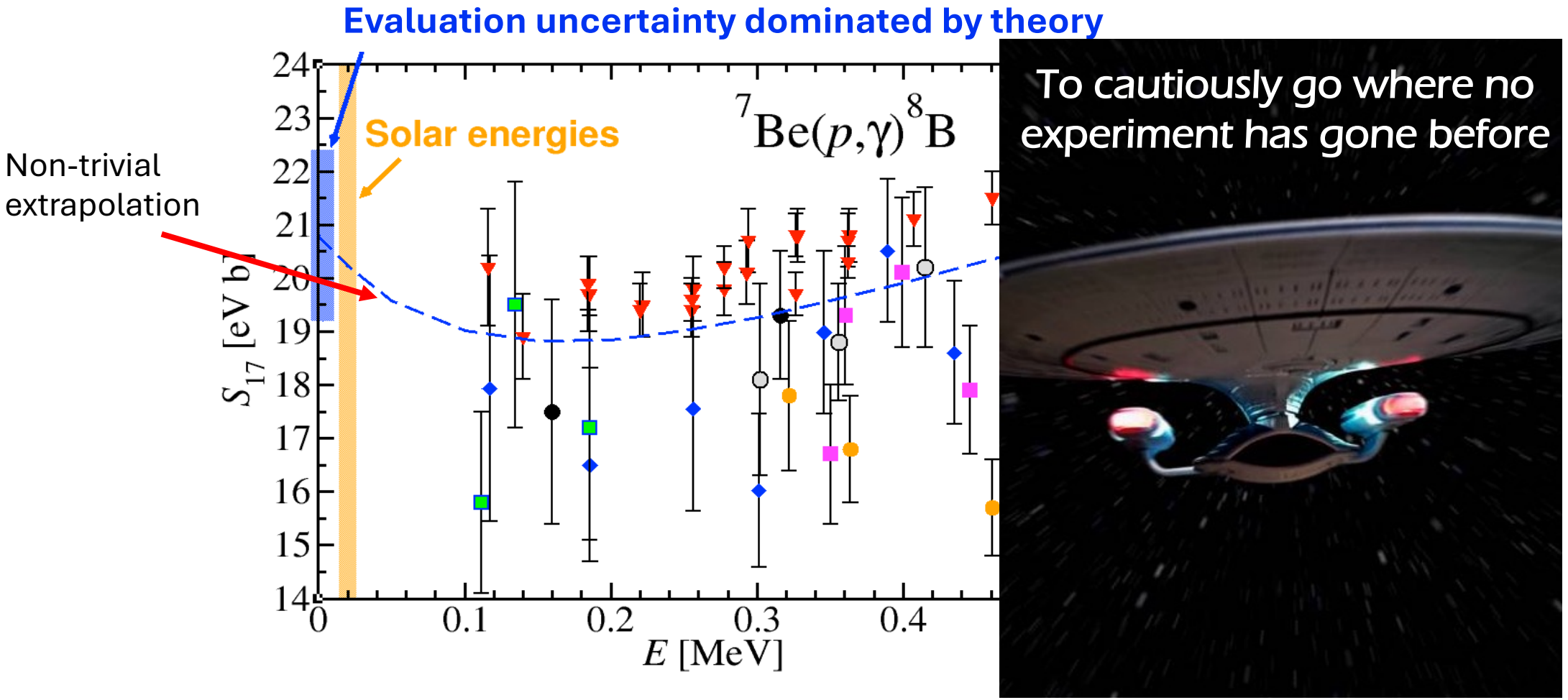
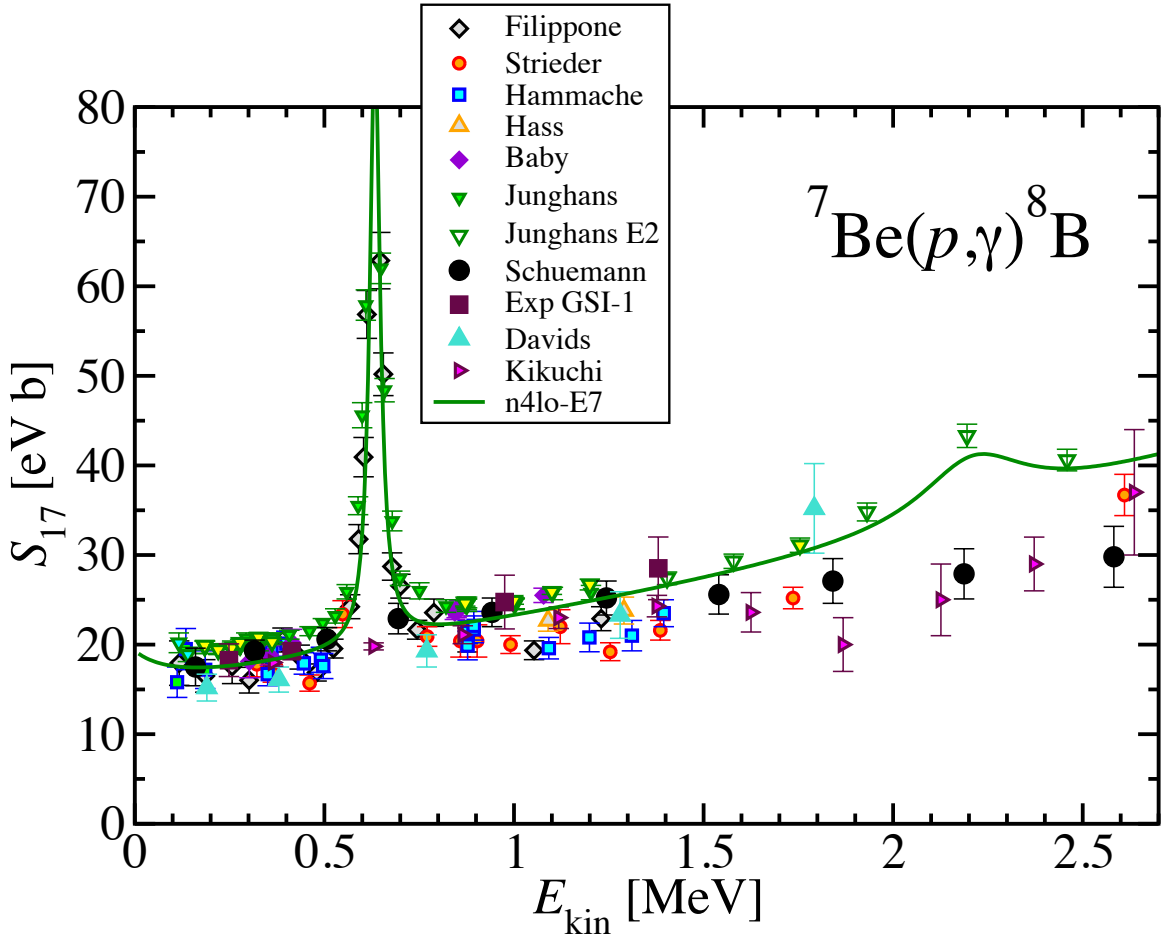


Ab initio theory of nuclear reactions provides a good description of available capture data.



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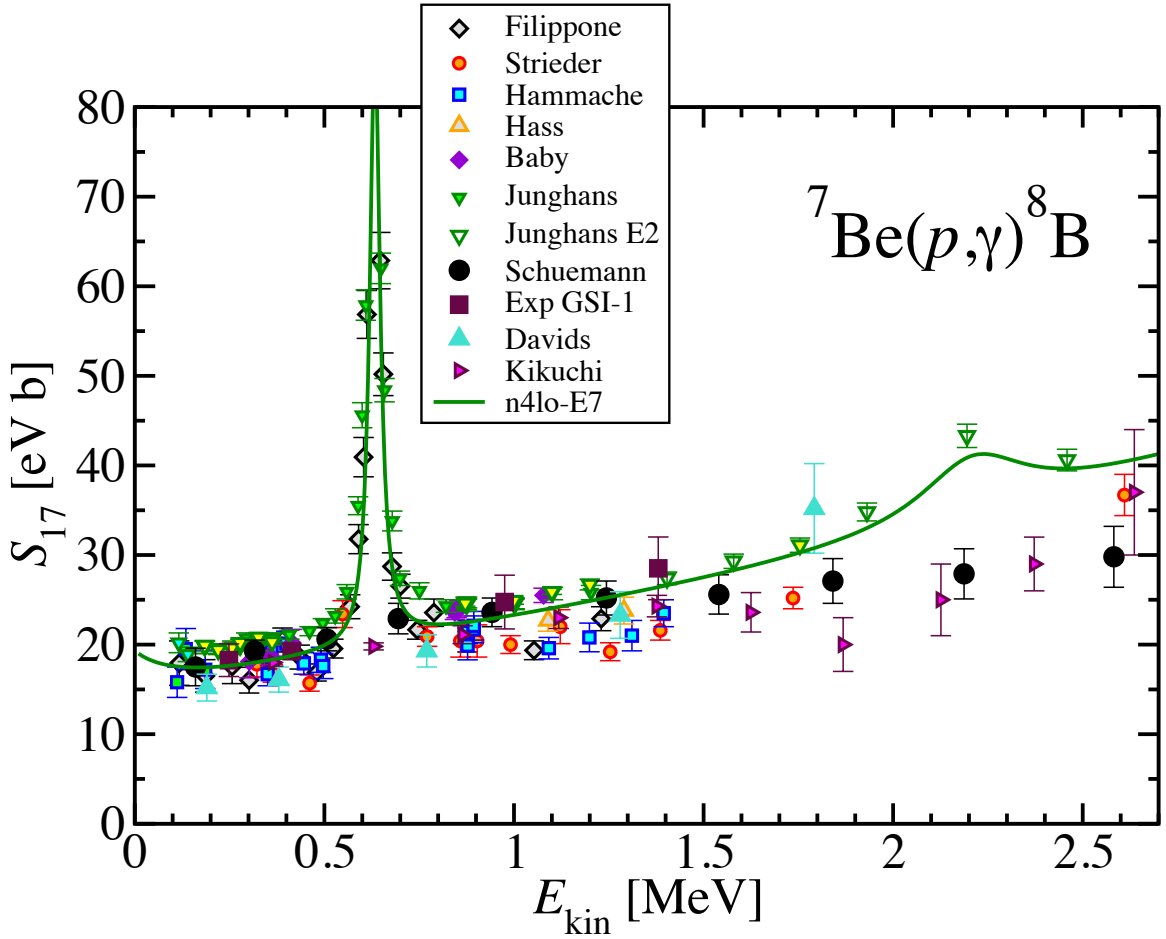
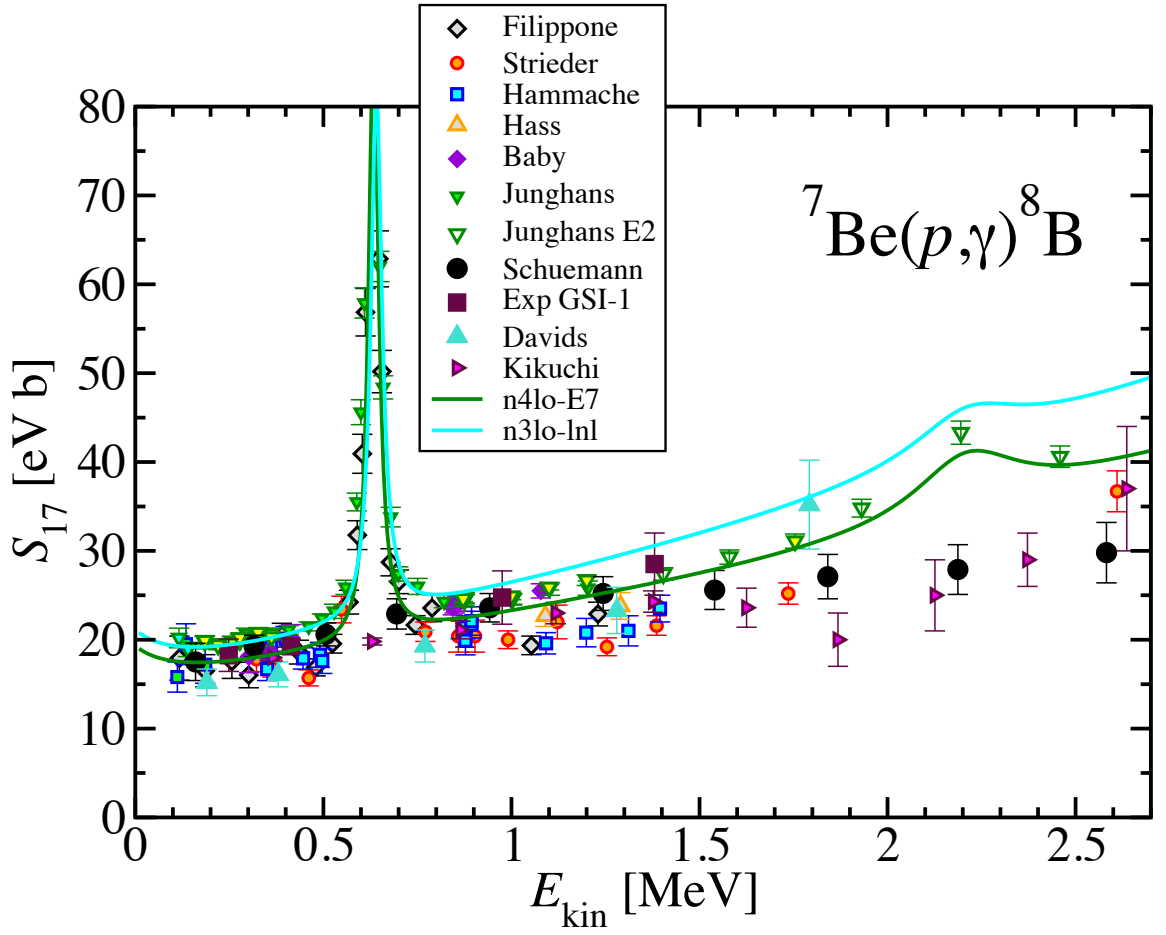
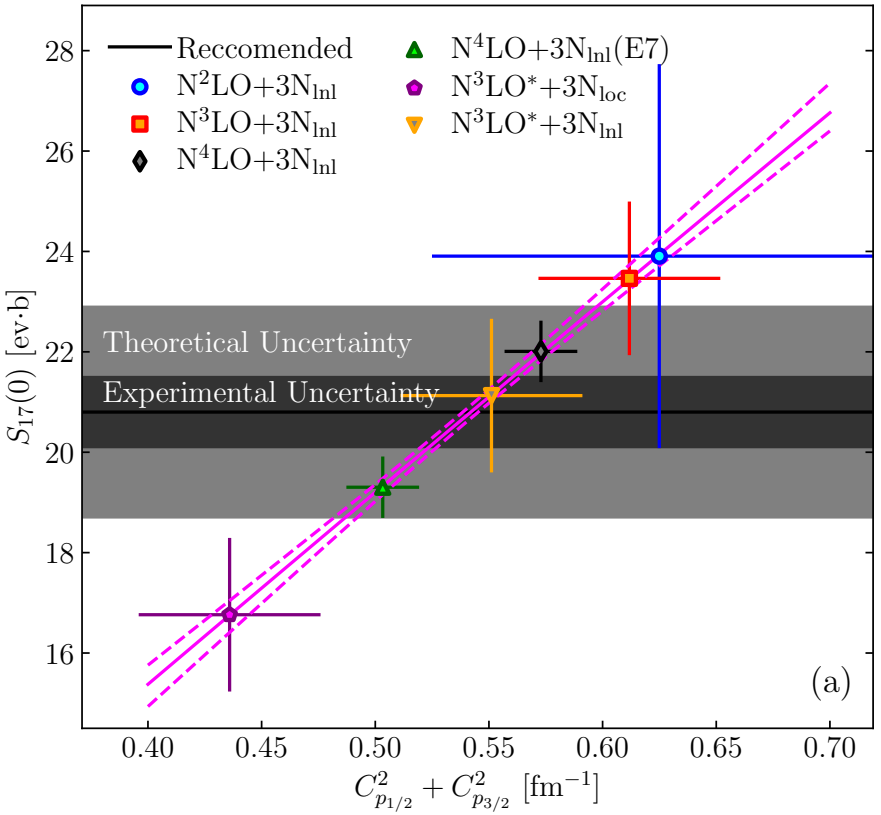




We can extract universal features of the reaction with multiple calculations using different interactions



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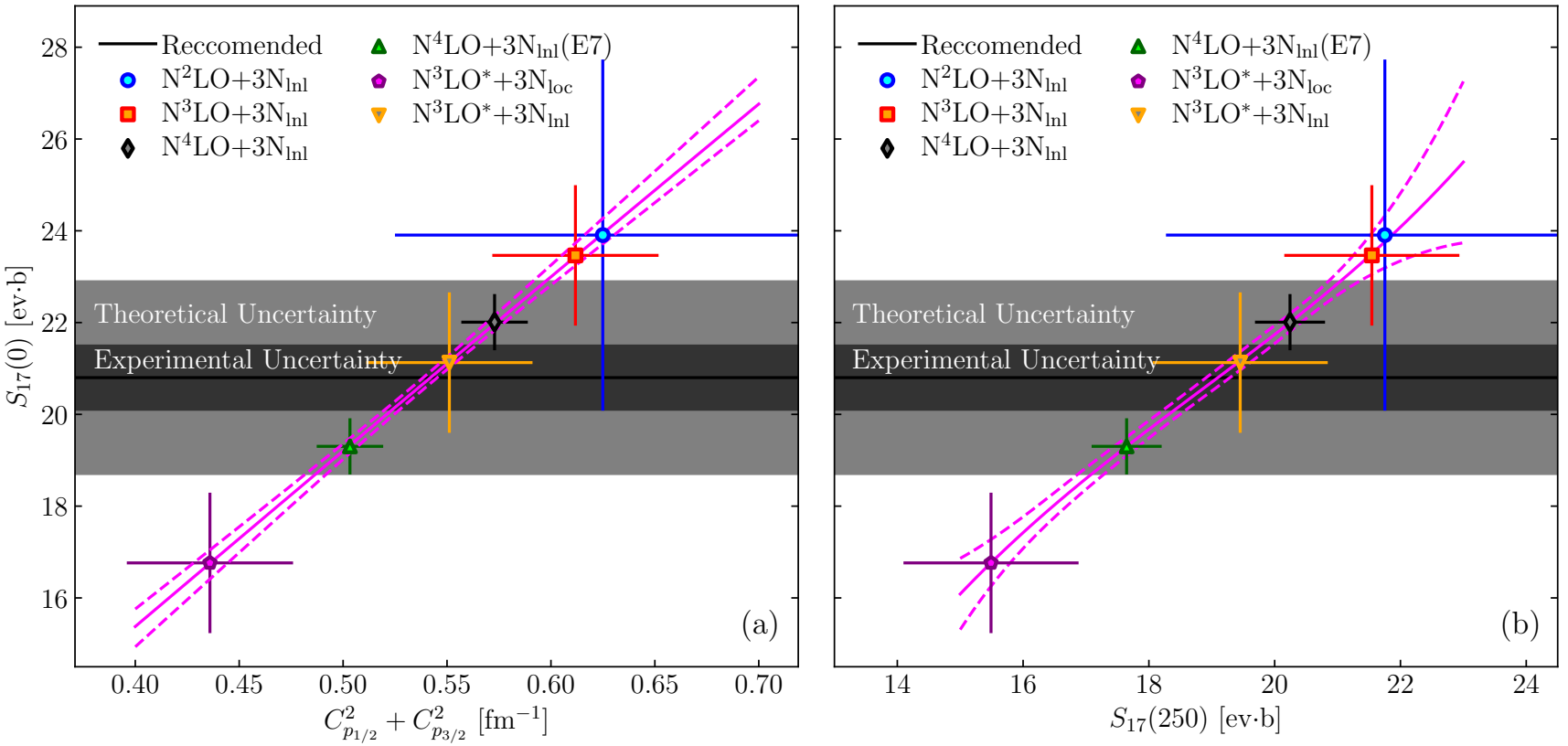

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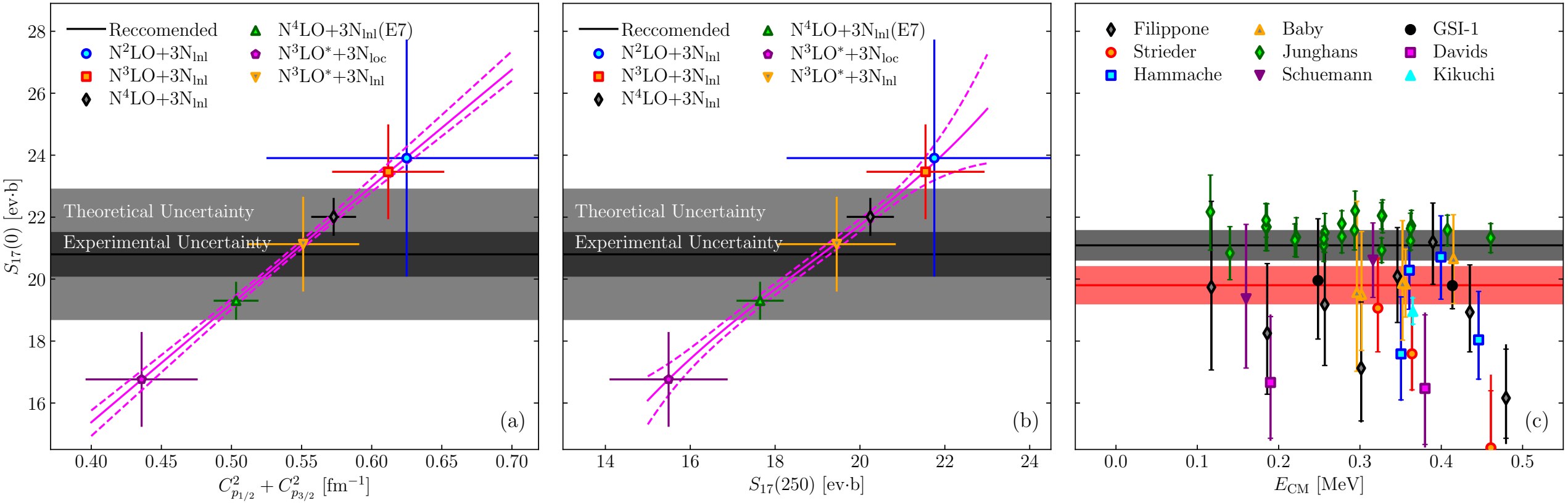

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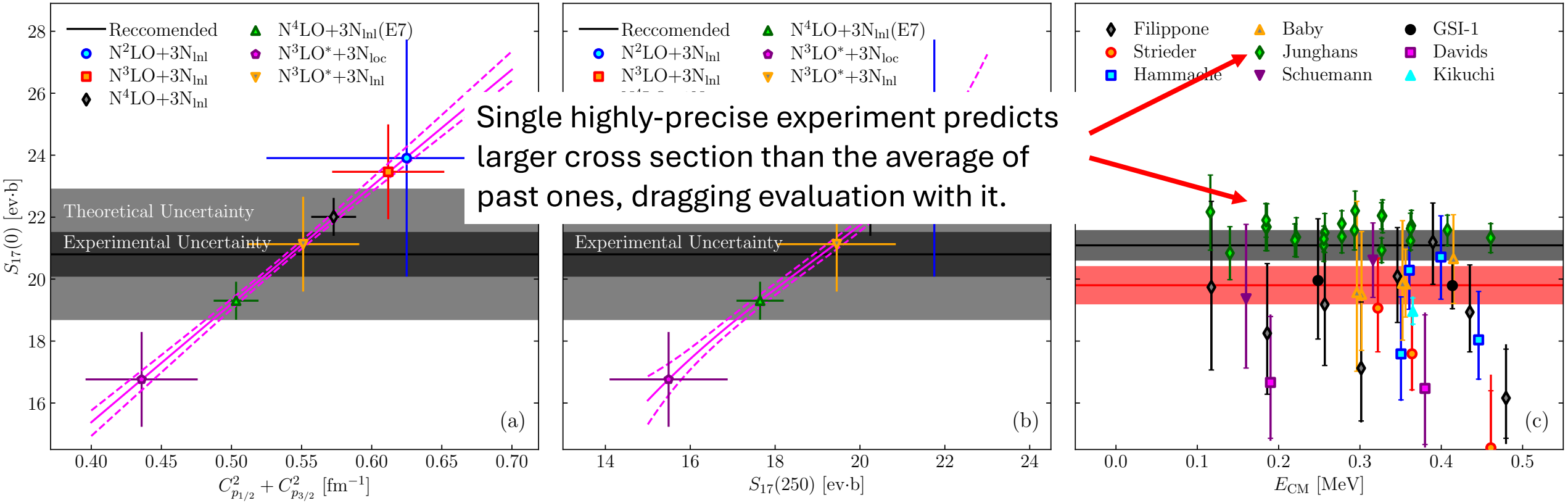
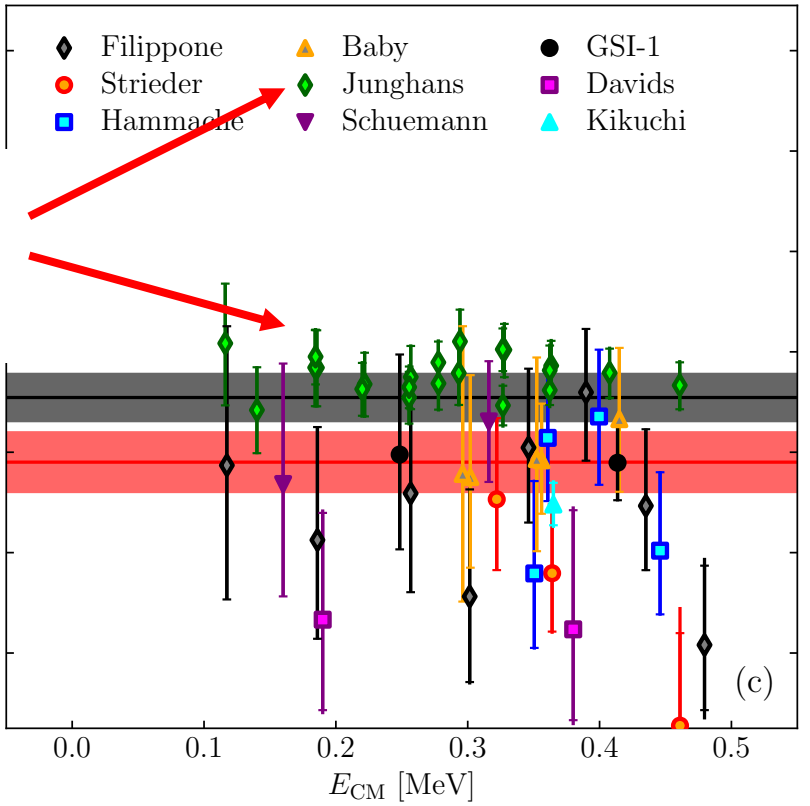


Single highly-precise experiment predicts larger cross section than the average of past ones, dragging evaluation with it.

We can extract universal features of the reaction with interactions



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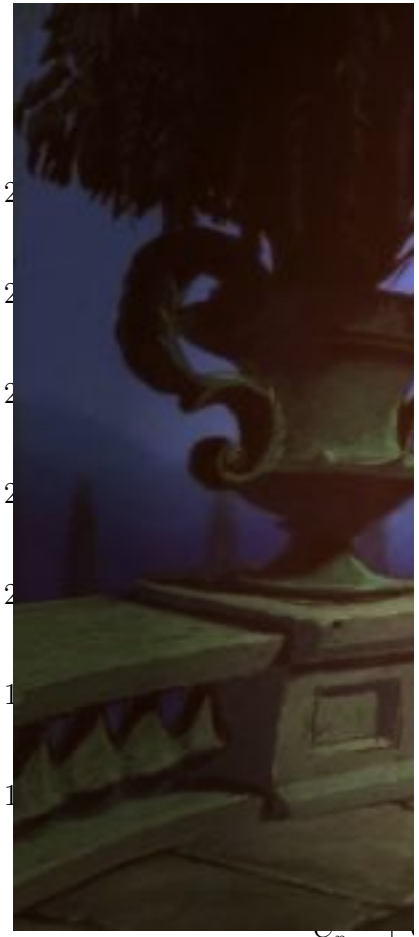
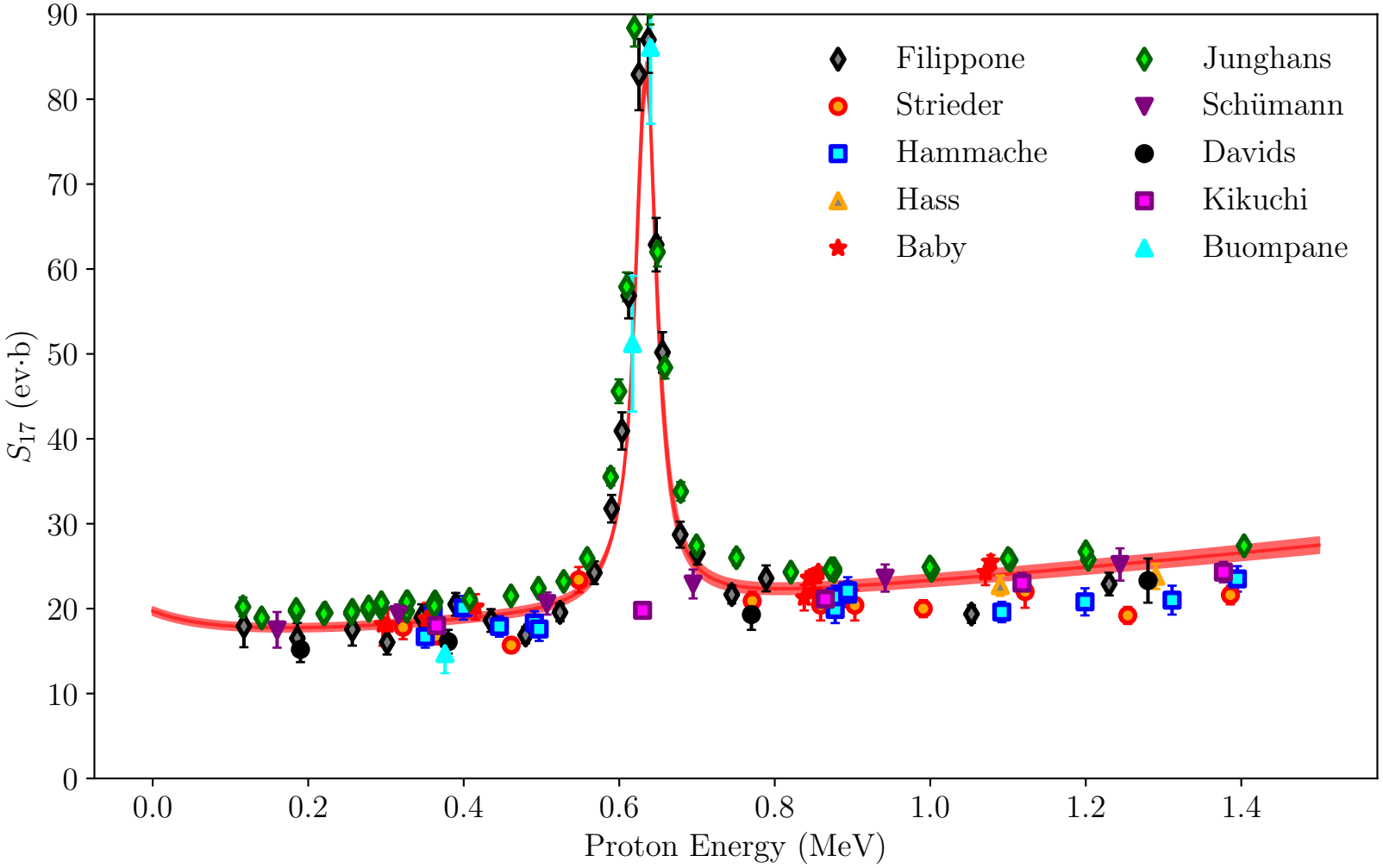
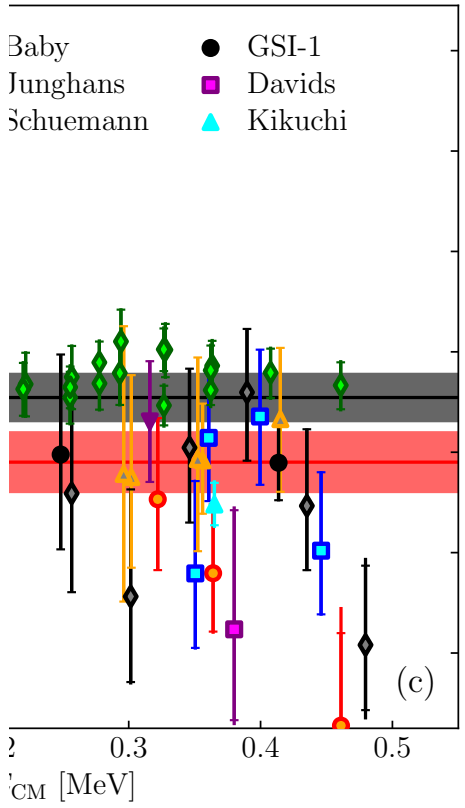
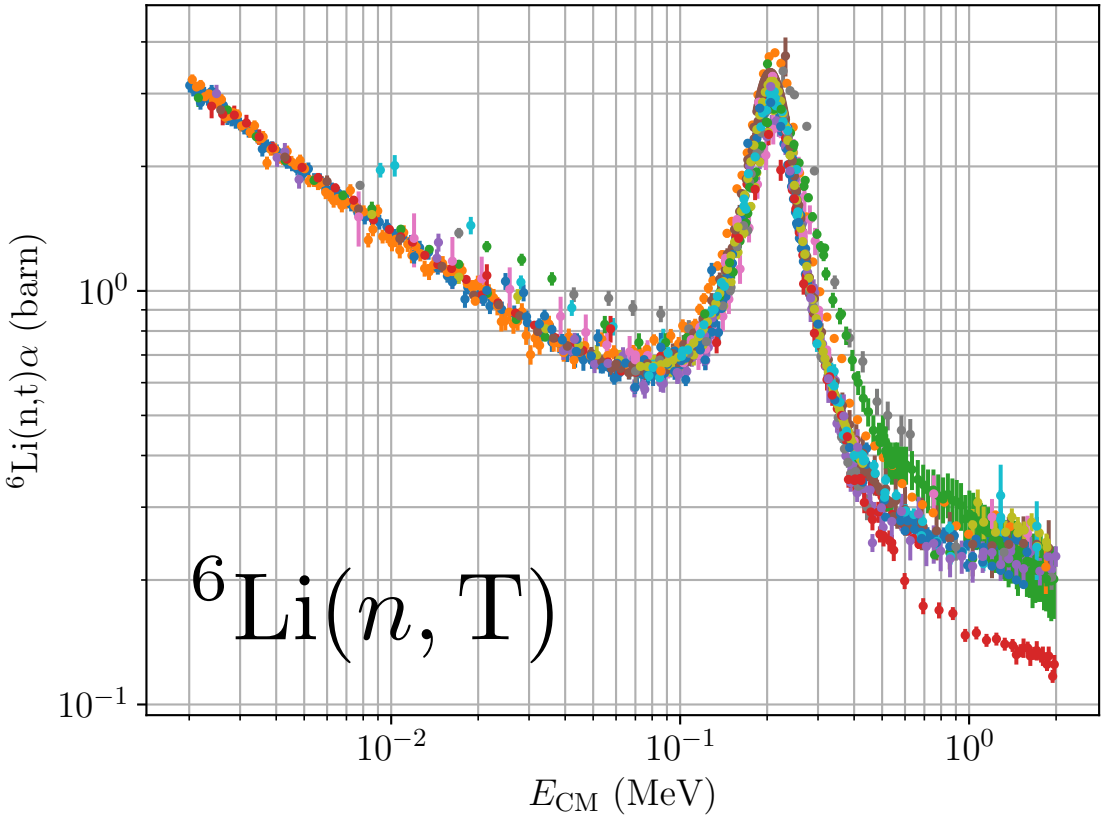






Ab initio nuclear reaction theory can provide an independent method for predicting standards cross sections



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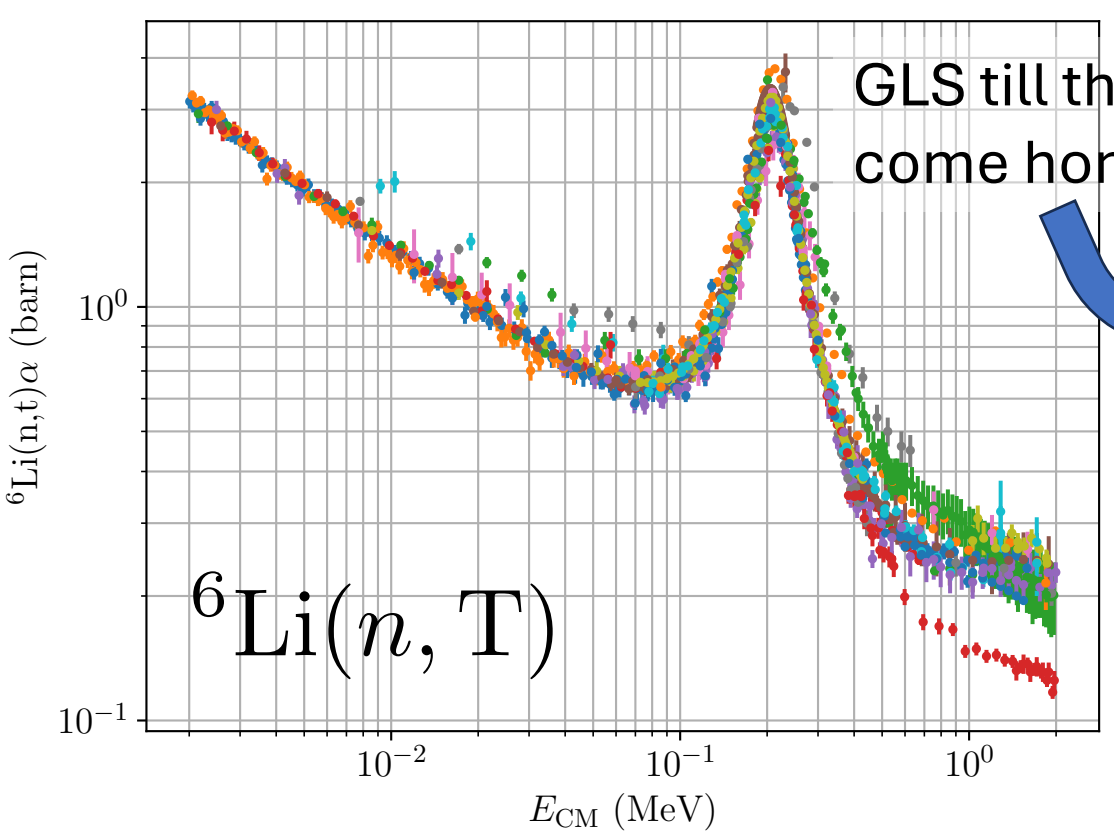
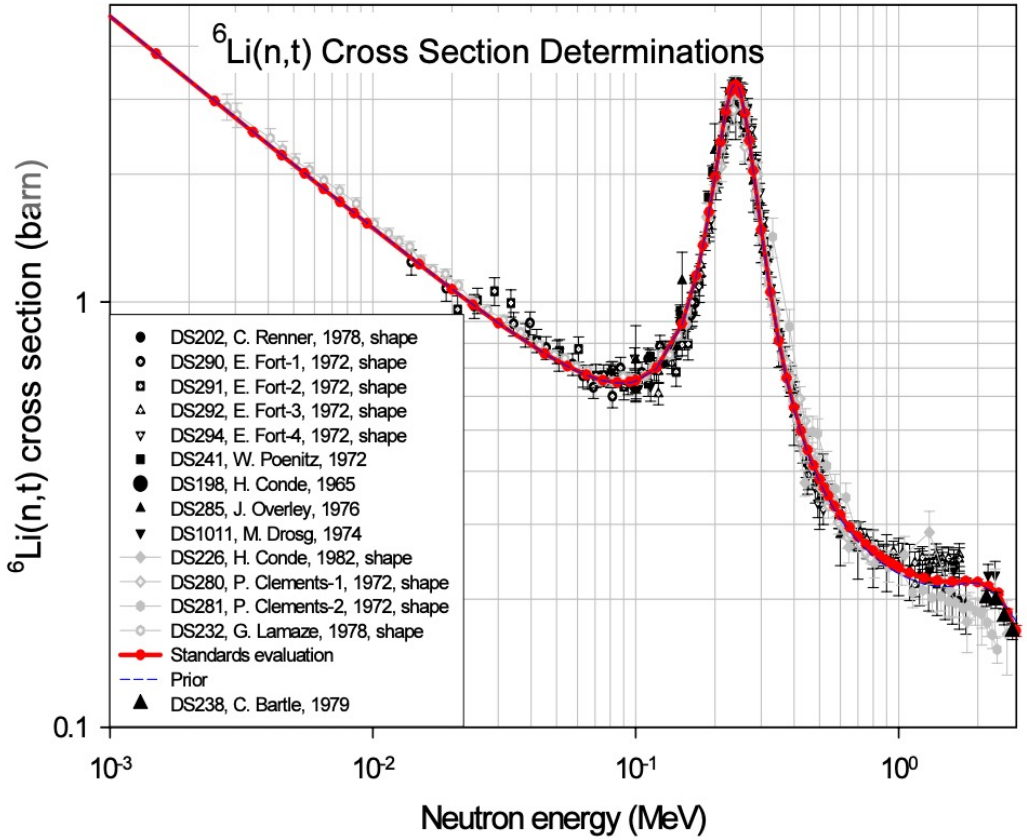


GLS till the cows come home



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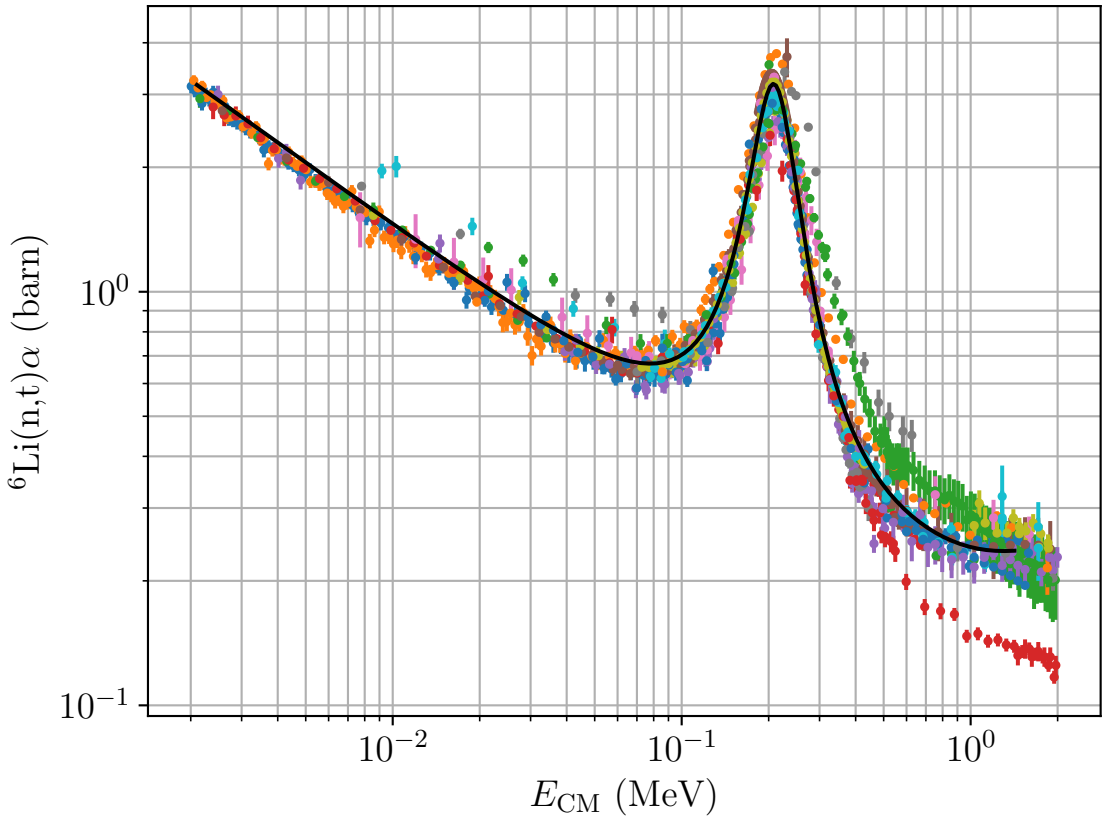
NCSMC parameters tuned to reproduce reaction cross section



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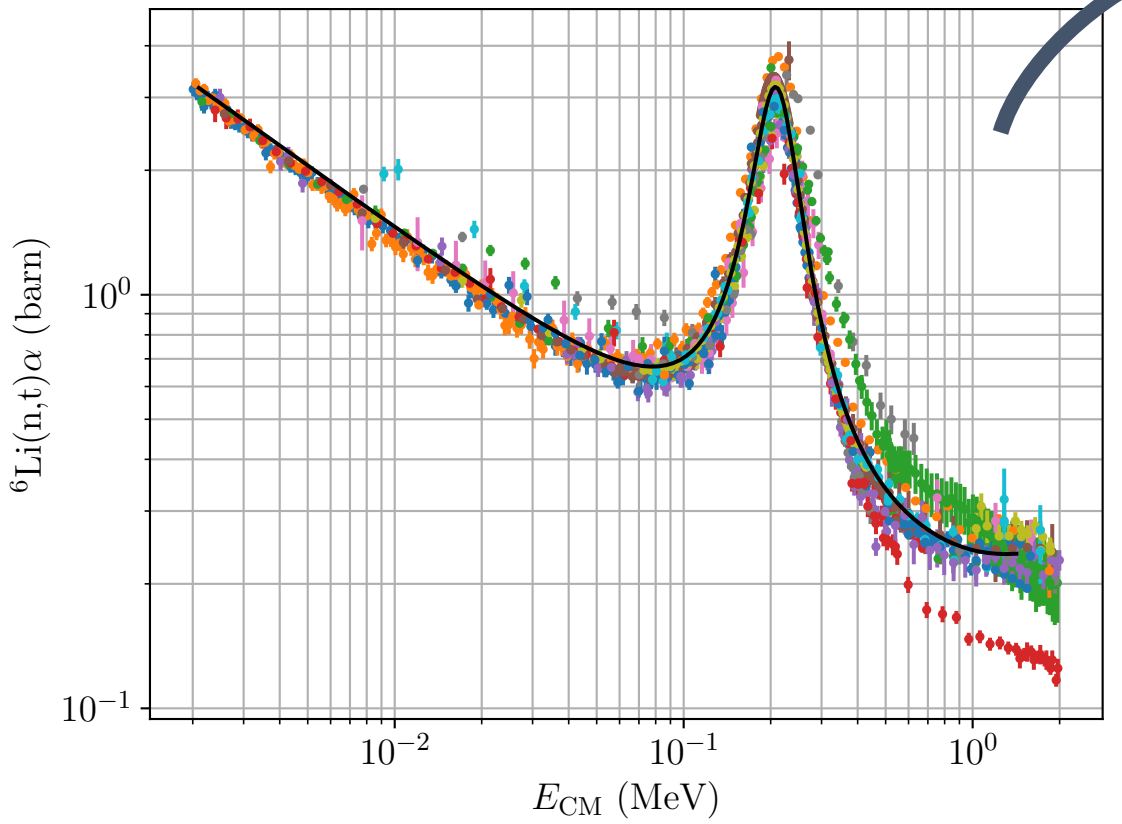
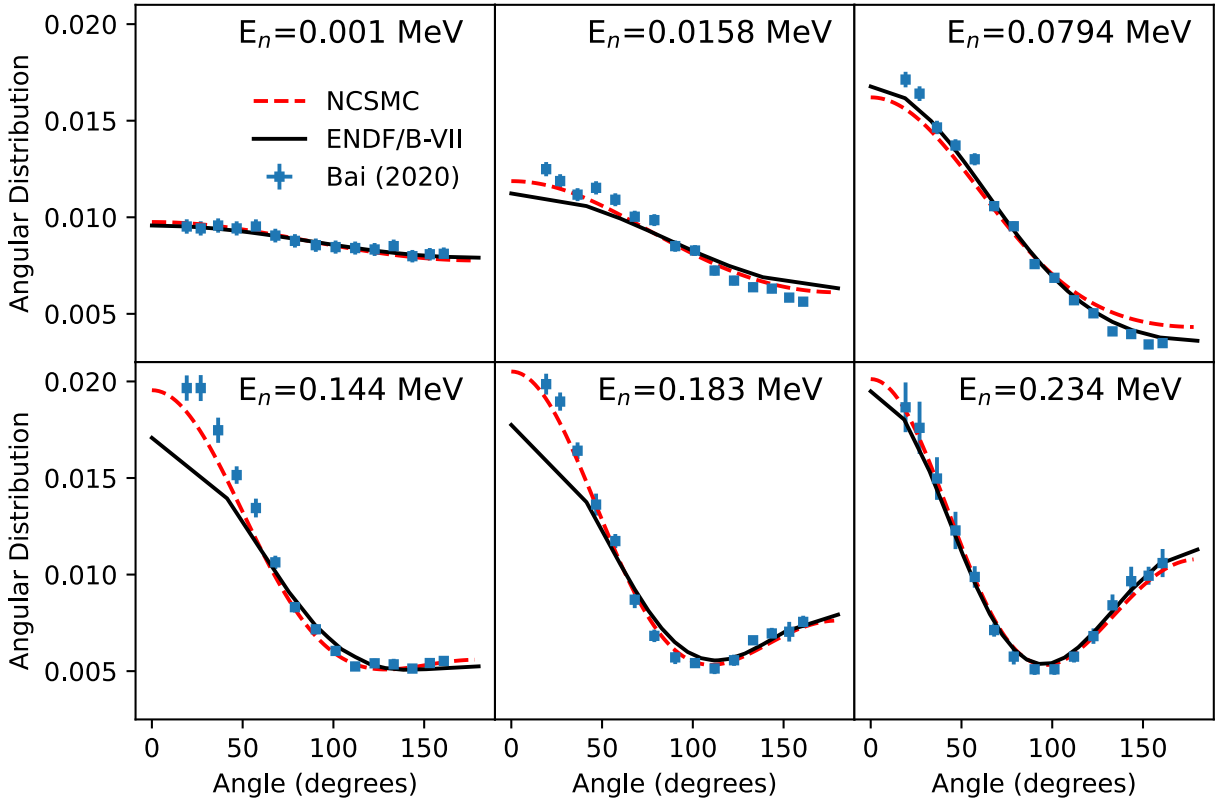


Angular distributions are predicted with no further experimental input



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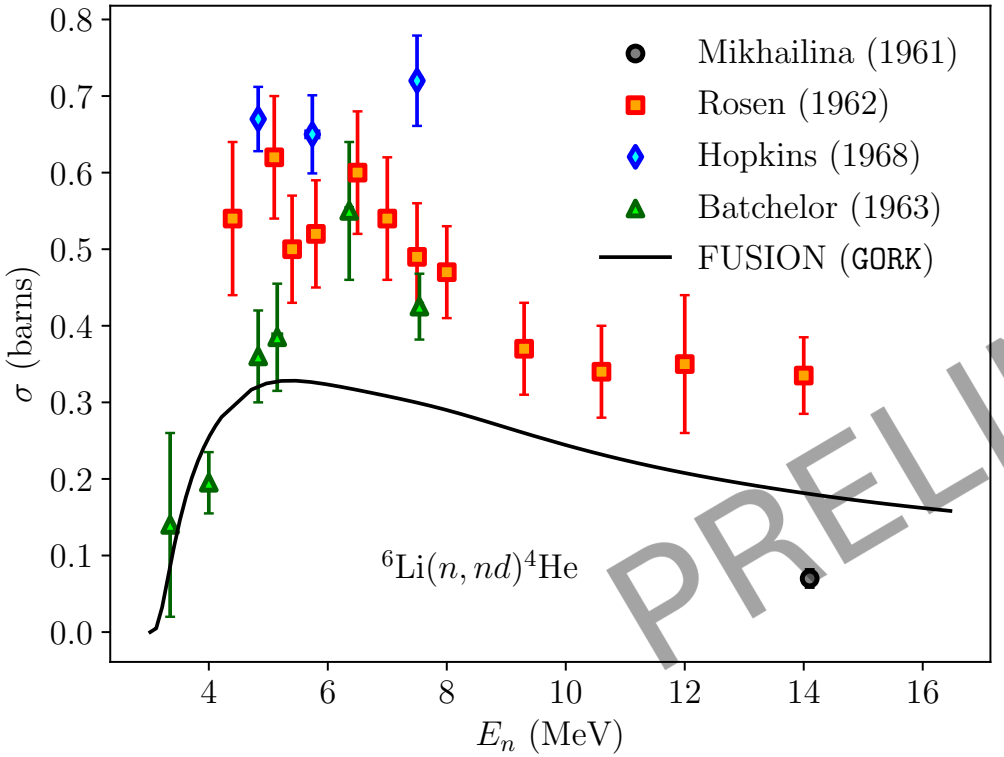
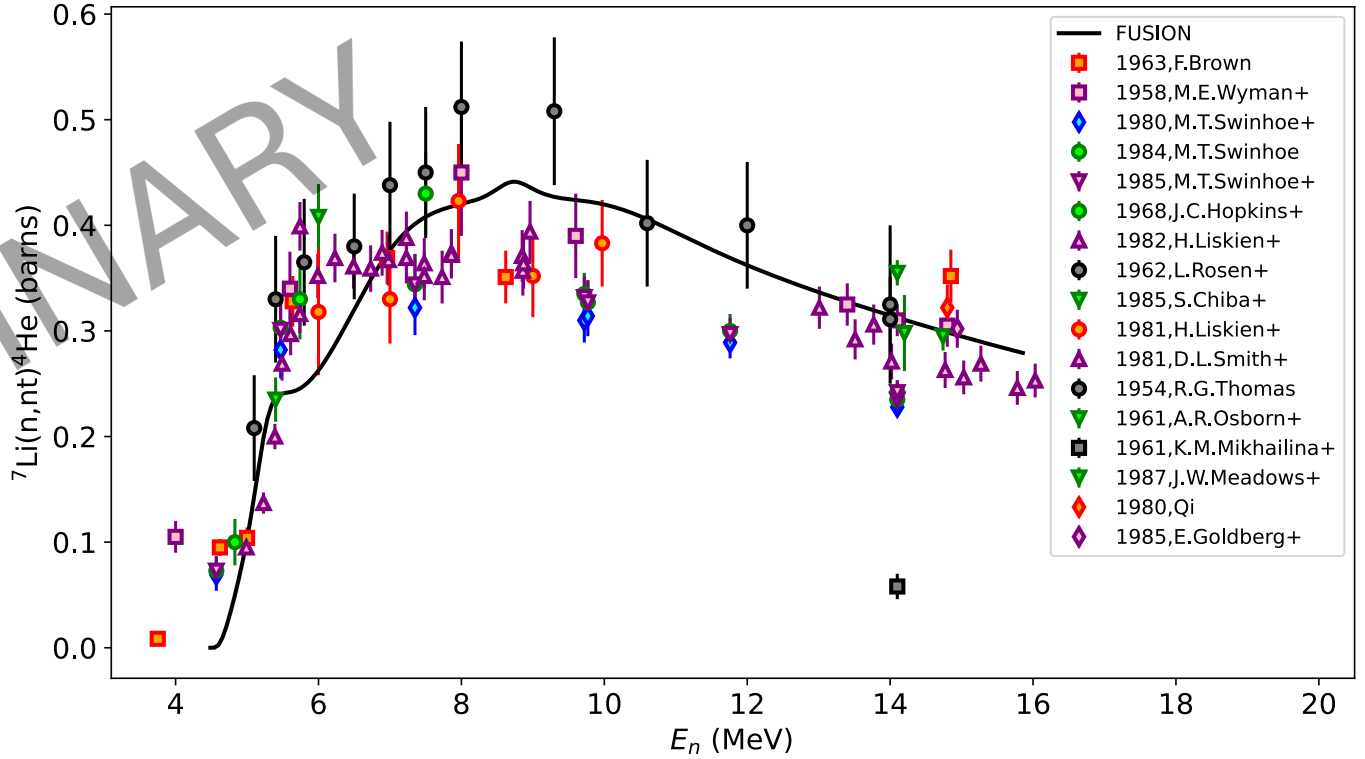
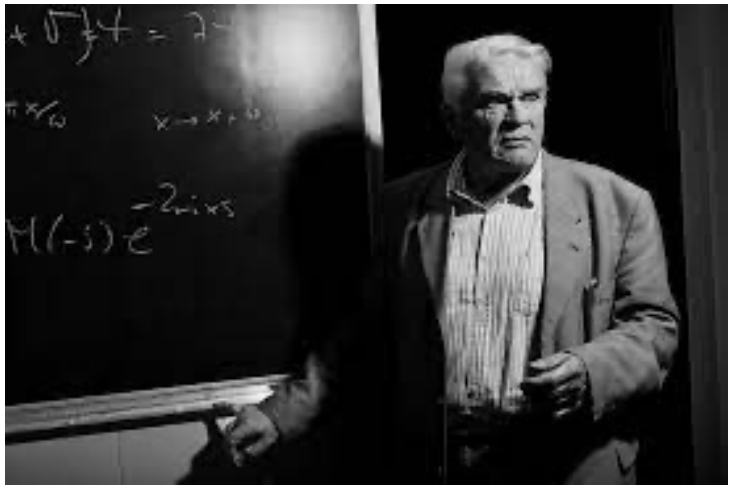




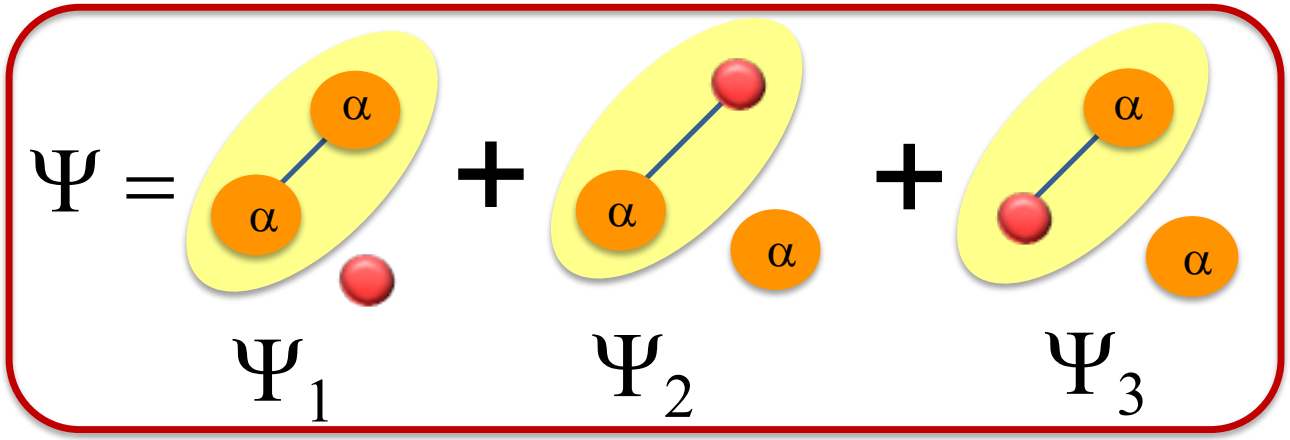
DISCLAIMER: Pseudostates used to model 3-body continuum

Coulomb generalized Faddeev (CGF) theory provides an exact description of ternary reactions

Work by Linda Hlophe



- Only exact method for three-body dynamics
- Phenomenological interactions between particle pairs



There ain’t nothing in this world for free: Revisiting irreducible 3-body forces.

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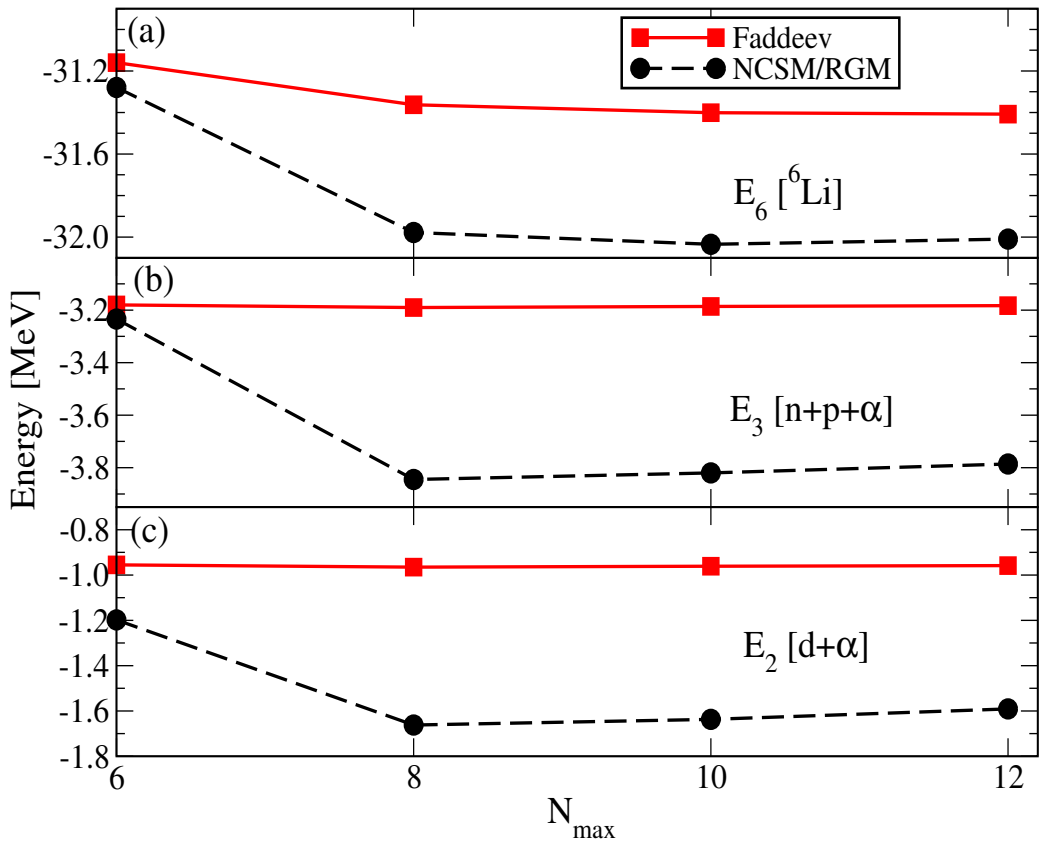
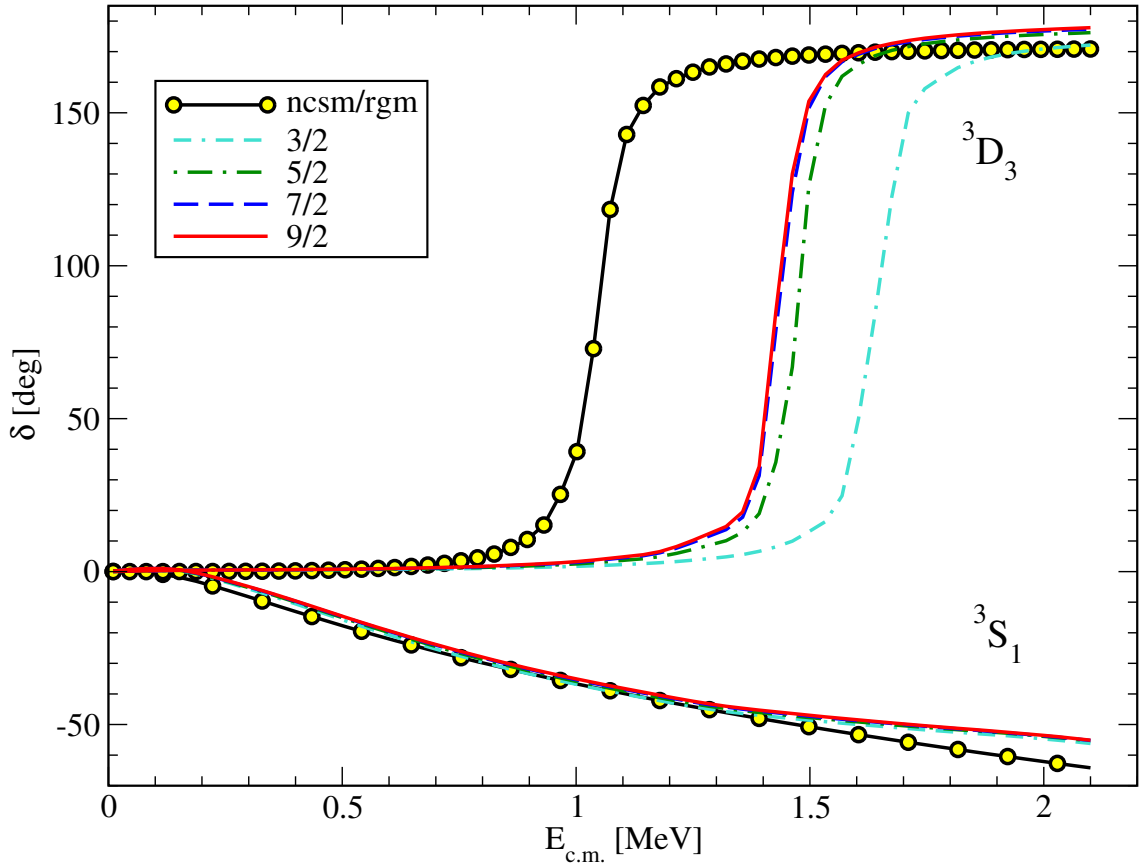
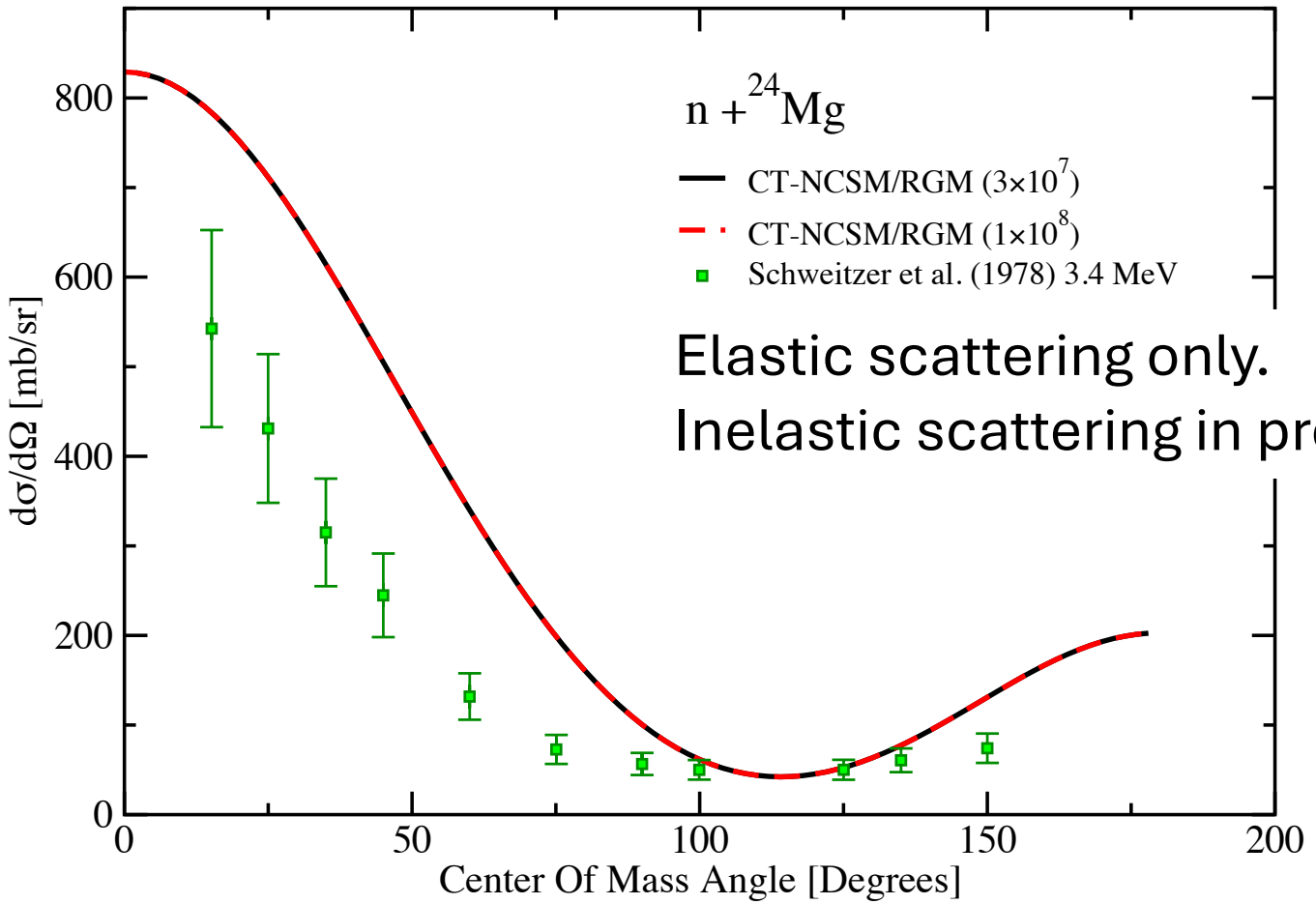




L. Hlophe, KK, and S. Quaglioni, Phys. Rev. C **107**, 014315

Approaching usefulness: first steps towards inelastic scattering descriptions in higher-mass nuclei

Physical Review C 109 (5), 054603



Elastic scattering only.

Inelastic scattering in progress.

My personal next-decade laundry list.

1. First evaluation of a light system with all (binary) competing channels.
   - Probably 4He aggregate.
   - GNDS files for realizations
   - Model mixing for calculations with different priors, using all available data.
2. Covariance between cross sections across different nuclei.
3. Three-body channels & effects in microscopic light-ion reactions: 9Be(n,2n), 6Li(n,nd)a, 7Li(n,nt)a
4. Robust method for describing Inelastic scattering in not-super-light nuclei
5. Covariances and connections between different channels: (d,p)/(n,g), (6Li,d)/(a,g), (t,p)/(2n,g).
6. Microscopic cluster optical potentials from folding + corrections
7. I ran out of space (and probably years).

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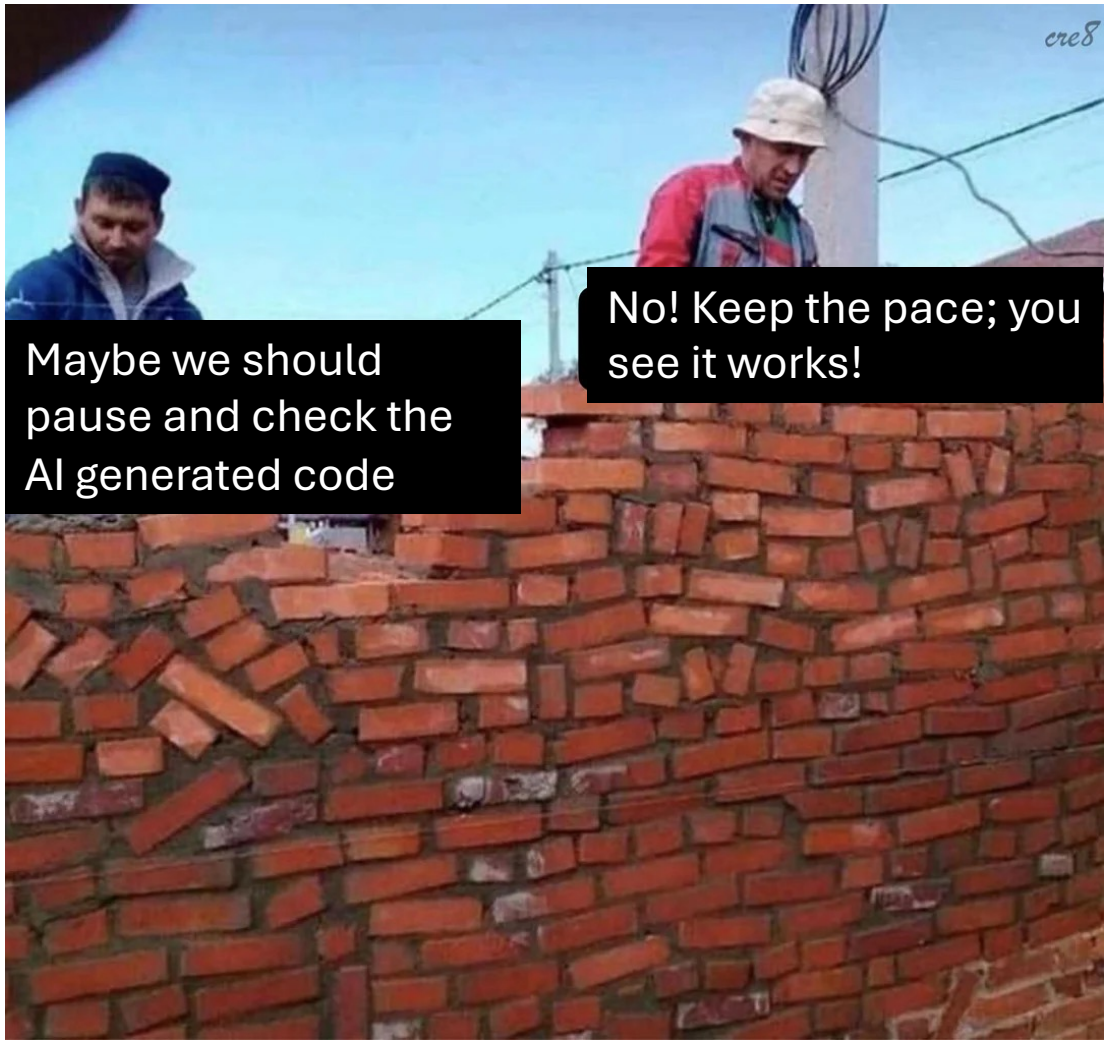
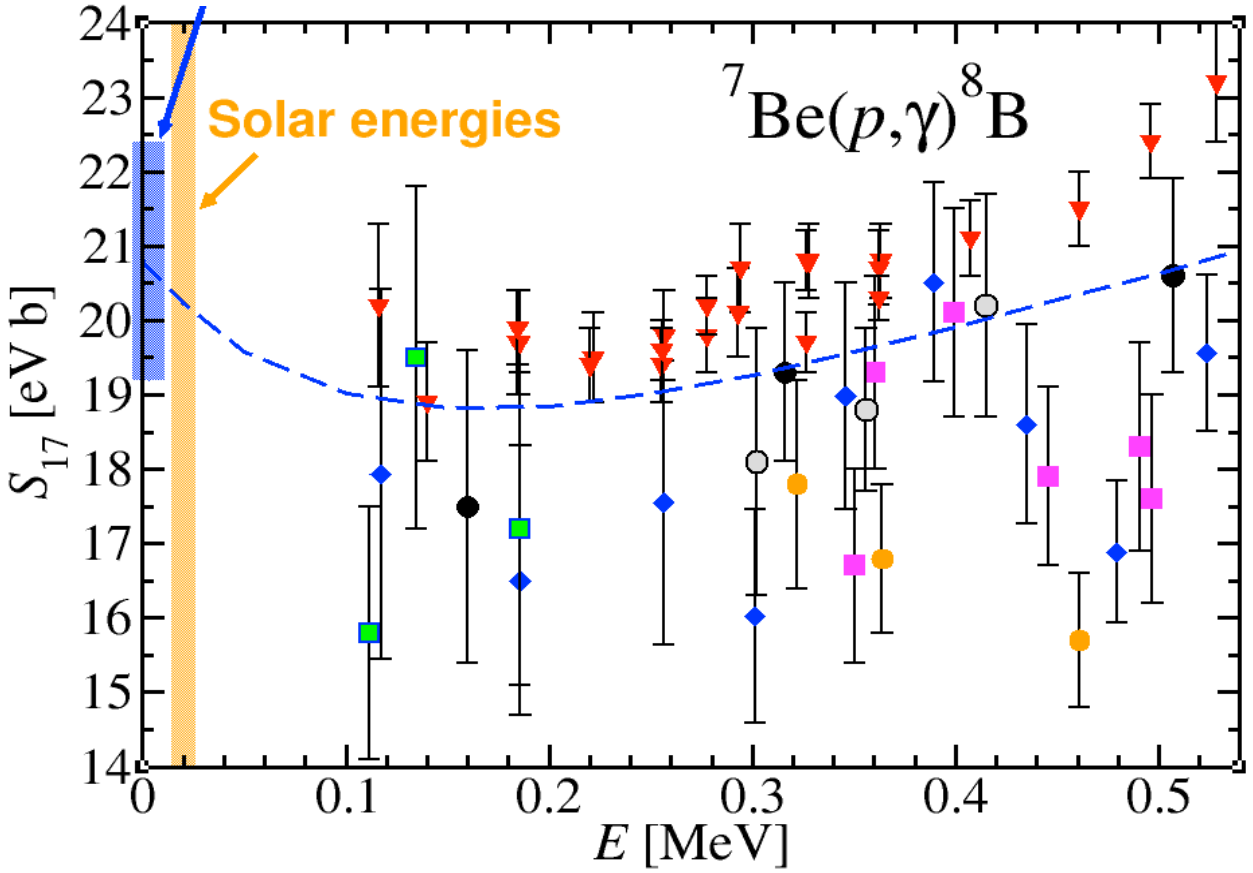
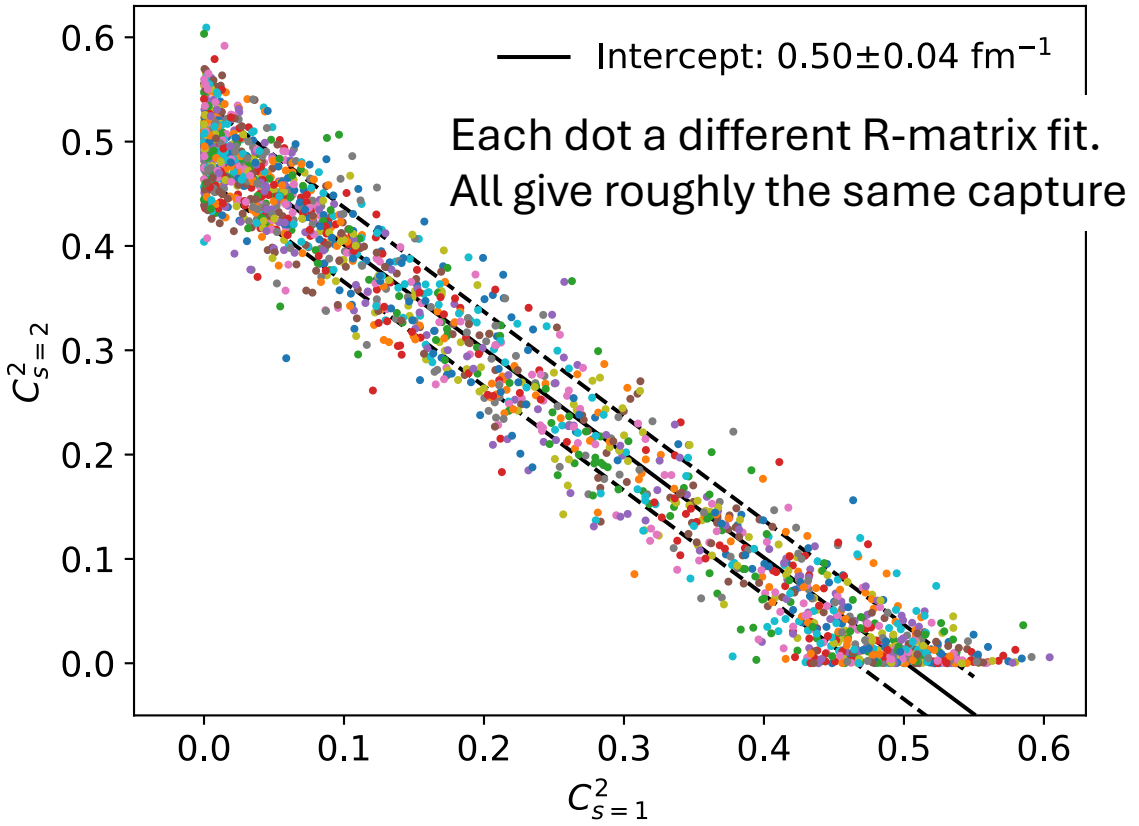


Thank you!

Low-energy direct capture cross section magnitude is determined by the asymptotic normalization coefficient(s)

Evaluation uncertainty dominated by theory

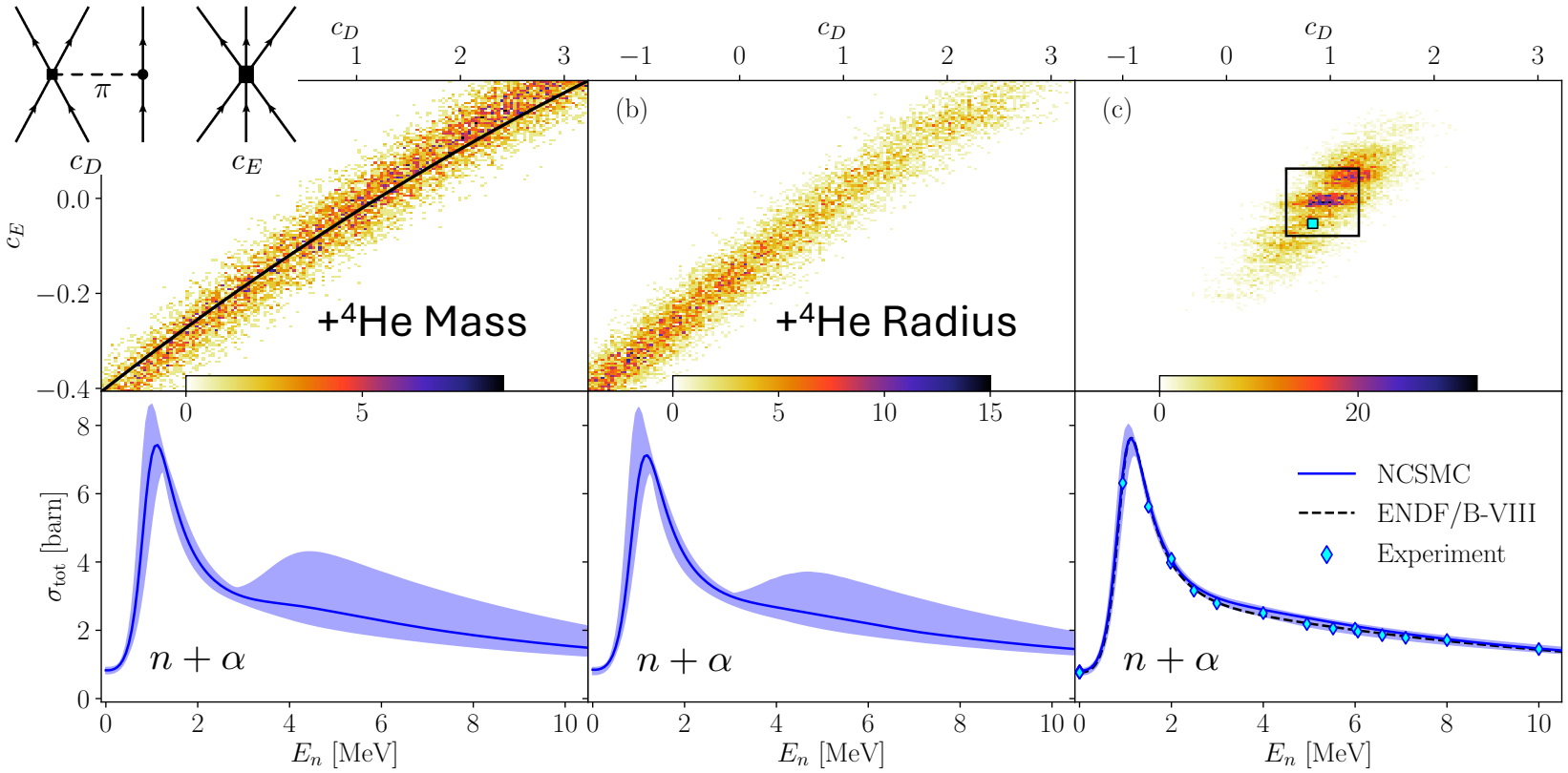




Rev. Mod. Phys. **97**, 035002 (2025)

The use of nuclear interactions that originate in chiral EFT have significant implications for evaluations

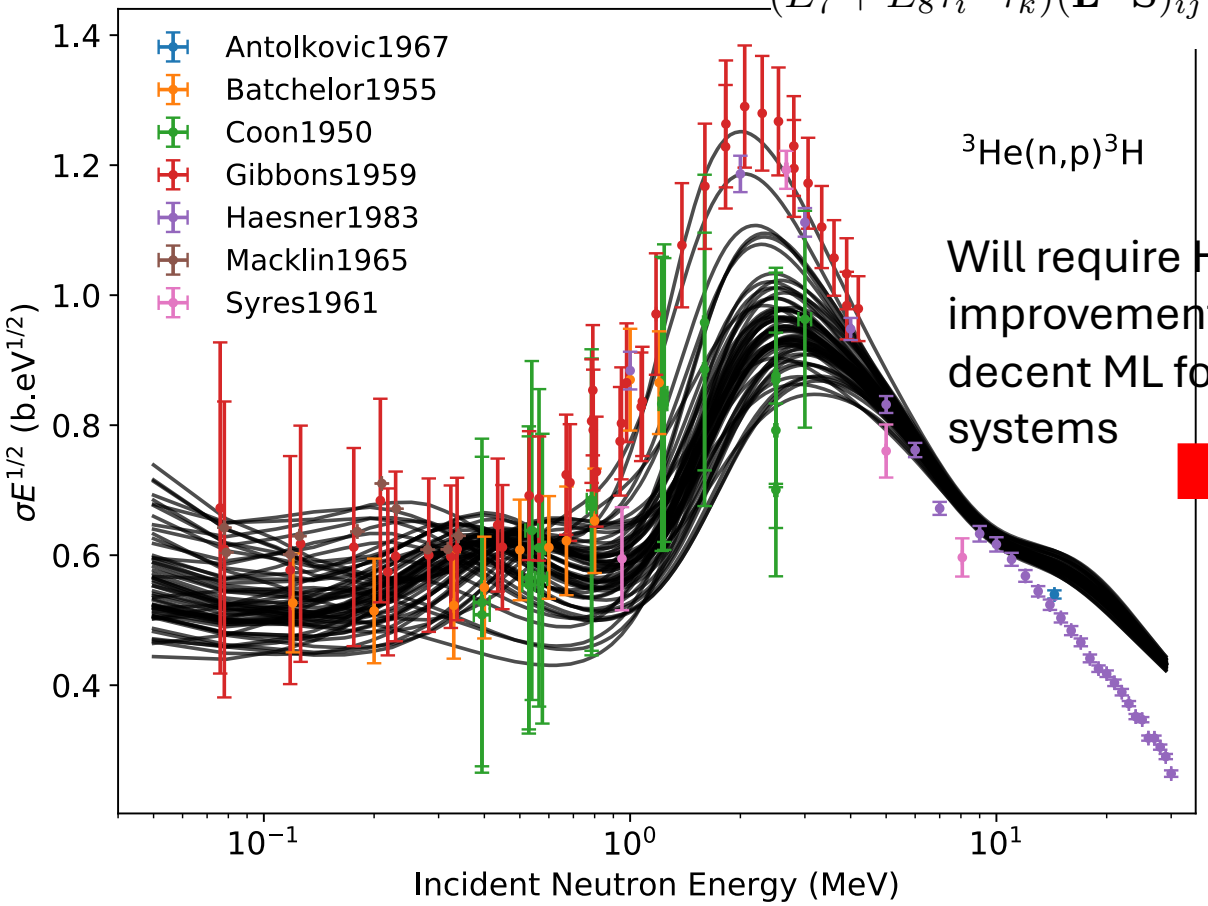
- Single set of inputs for all predictions—covariances to a new level
- Covariances between ENSDF quantities and cross sections can be calculated
- Cross-material covariances can be recursively calculated.



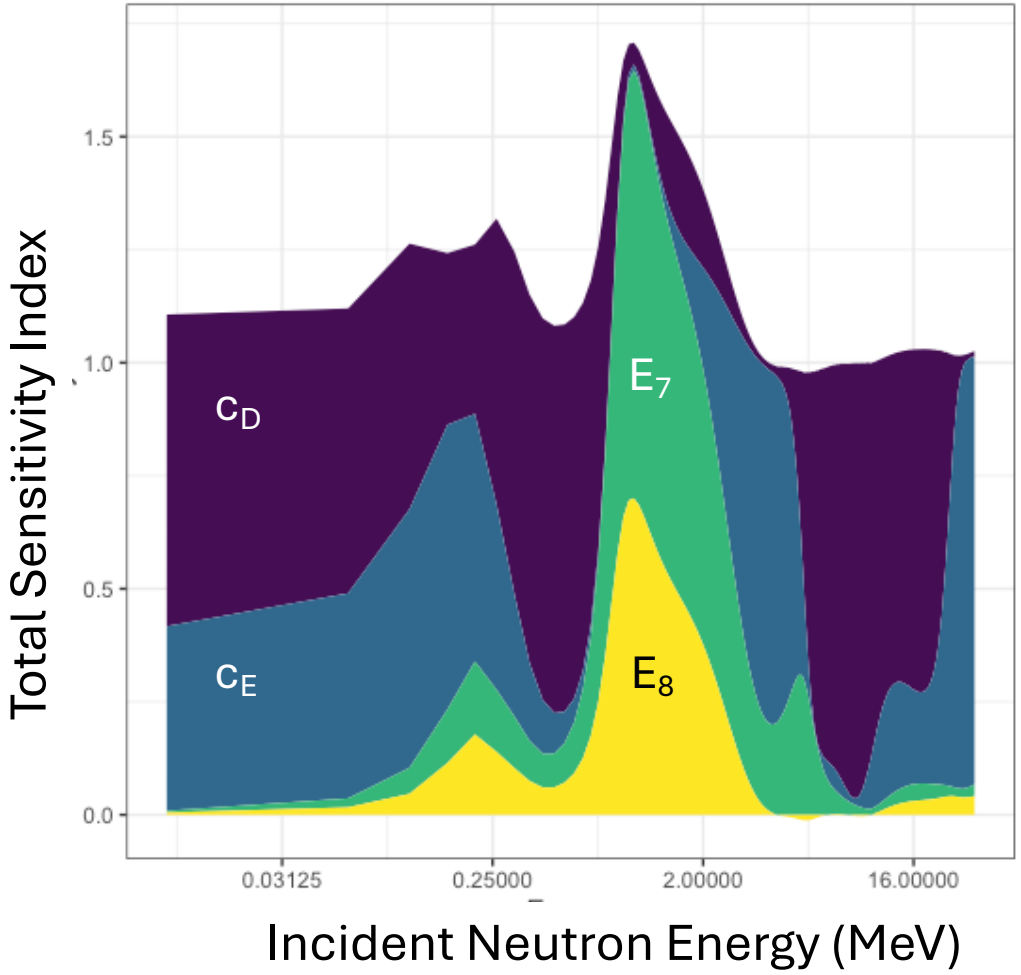
Phys. Rev. C **102**, 024616 (2020)

Sensitivity index for cross sections will help identify correlated parameters of the nuclear force

$$(E_7 + E_8 \tau_i \cdot \tau_k)(\mathbf{L} \cdot \mathbf{S})_{ij} \frac{Z_0'(r_{ij})}{r_{ij}} Z_0(r_{ik})$$



Will require HPC improvements and some decent ML for heavier systems



ID	Type	Target	Reaction	Quantity	Energy		Accuracy (%)	Status	Last update
					Min	Max		Work in progress	
114	H	83-Bi-209	(n,g)Bi-210g,m	BR	500 eV	300 keV	10	Work in progress	2018-Nov-09
8	H	1-H-2	(n,el)	DA/DE	0.1 MeV	1 MeV	5	Work in progress	2007-Apr-16
121	S	8-O-16	(n,xα)	DE	20 MeV	200 MeV	10	Work in progress	2023-May-20
81	S DOS	26-Fe-0	(n,x)Mn-54	SIG	15 MeV	100 MeV	5-10	Work in progress	2017-Oct-06
43	S STD	1-H-1	(n,el)	SIG DA	10 MeV	20 MeV	1-2	Work in progress	2011-May-13
7	G	26-Fe-56	(n,xn)	SIG DA/DE	7 MeV	20 MeV	30	Archived	2007-Apr-16
118	H	68-Er-167	(n,g)	SIG RP	0.01 eV	100 eV	2	Work in progress	2021-Aug-30
117	H	3-Li-0	(d,x)H-3	SIG TTY	5 MeV	40 MeV	10	Work in progress	2021-May-31
70	S DOS	13-Al-27	(n,2n)	SIG/SPA	252Cf(sf)	235U(n,f)	2-5	Work in progress	2017-Oct-06
38	H	94-Pu-240	(n,f)	nubar	200 keV	2 MeV	1-3	Work in progress	2008-Sep-15
9	G	92-U-233	(n,g)	nubar SIG	Thermal	10 keV	.5	Work in progress	2007-Apr-19
4	H	92-U-235	(n,f)	prompt g	Thermal	Fast	7.5	Archived	2006-May-12
17	G	96-Cm-244	(n,f)	prompt n	Eth	10 MeV	10	Work in progress	2008-Sep-10