Ab initio description of nuclear reactions with applications to astrophysics

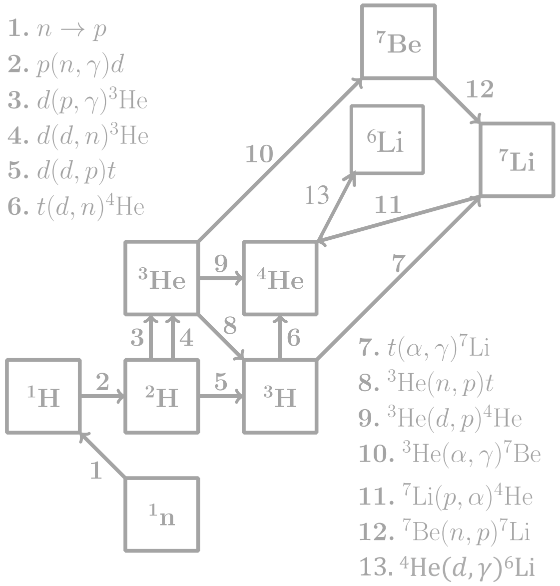
Sofia Quaglioni

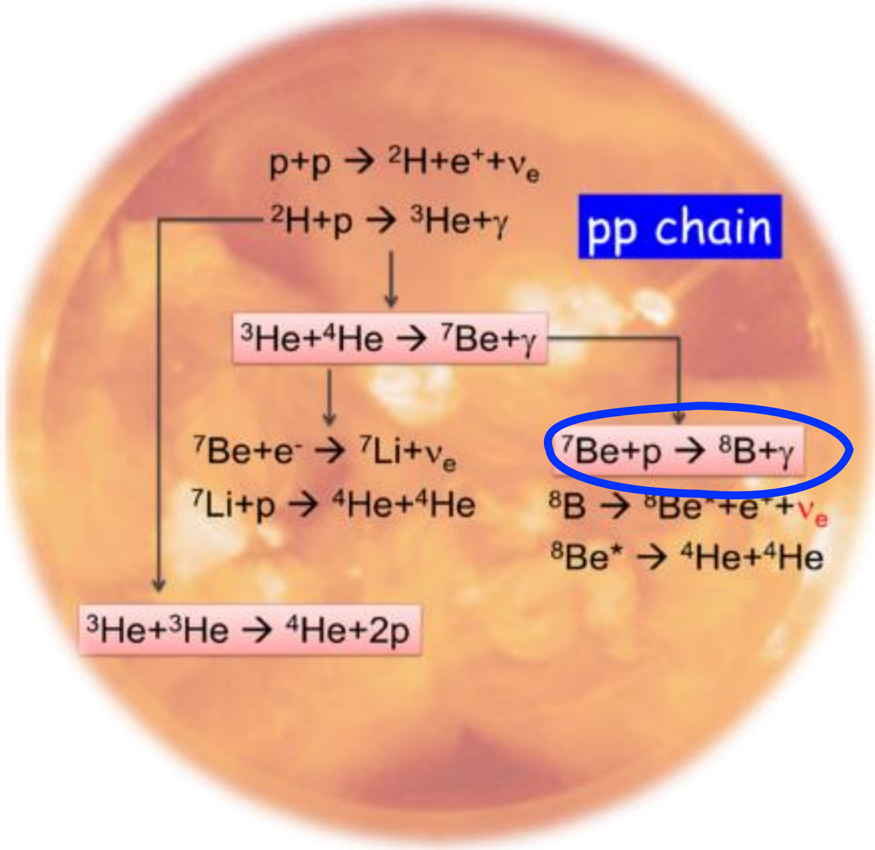
LLNL-PRES-836301
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Reactions 'R' Us

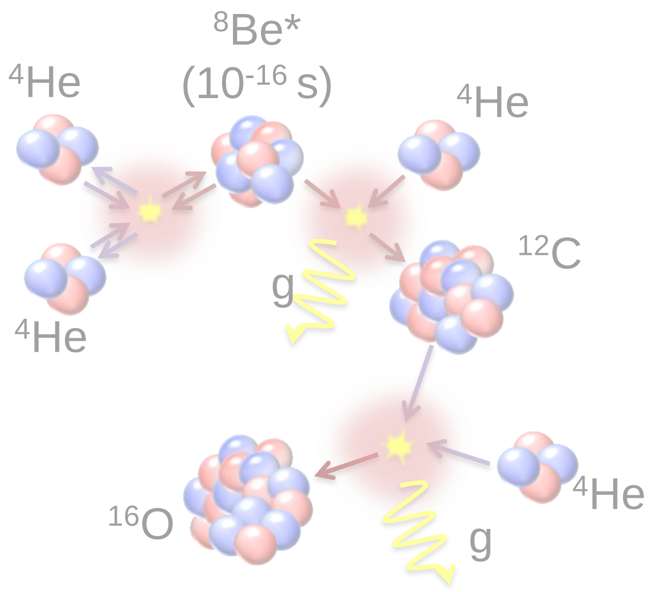
Solar Fusion

Big Bang





Helium Burning



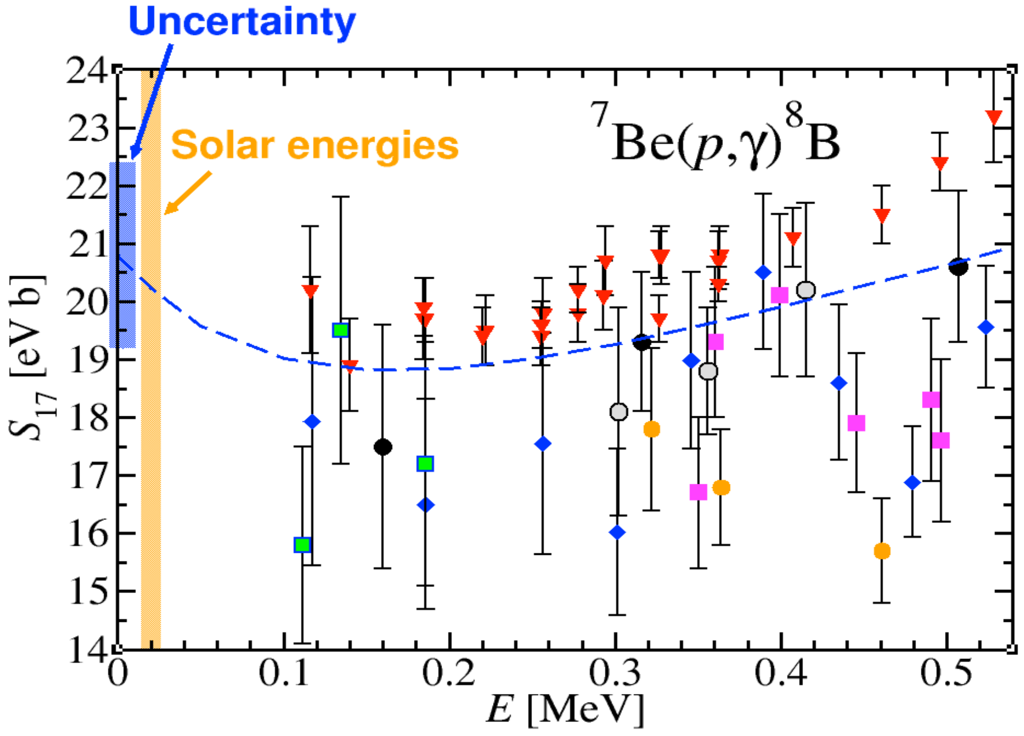
We need reliable theory to accurately evaluate S-factors at stellar energies

$$S_{17}(0) = 20.8 \pm (0.7)_{\text{exp}} \pm (1.4)_{\text{th}} \text{ eV·b}$$

Astrophysical S-factor: nuclear contribution

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar\sqrt{2E/m}}\right)$$

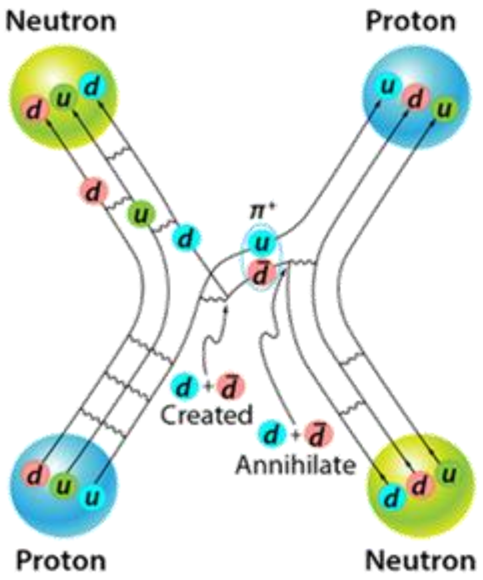
'Coulomb' contribution (tunneling)



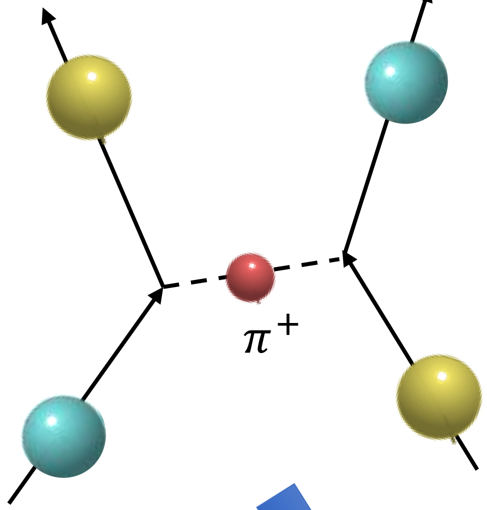
Adelberger EG et al. (2011), Rev. Mod. Phys. 83, 195

We combine nuclear forces derived within chiral effective field theory with ab initio methods

Quantum Chromodynamics

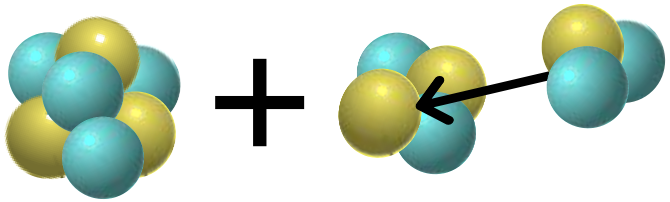


Chiral Effective Field Theory



Chiral NN+3N forces

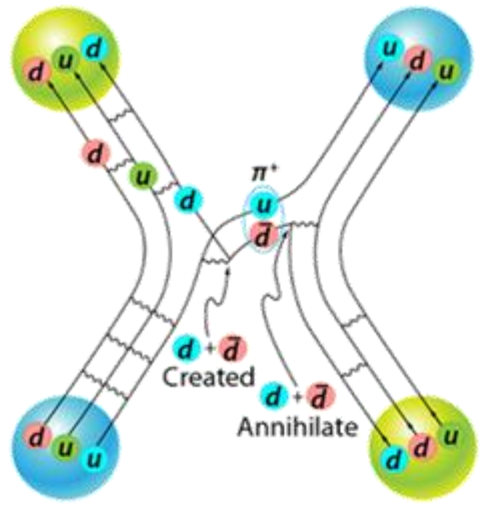
No Core Shell Model with continuum (NCSMC)



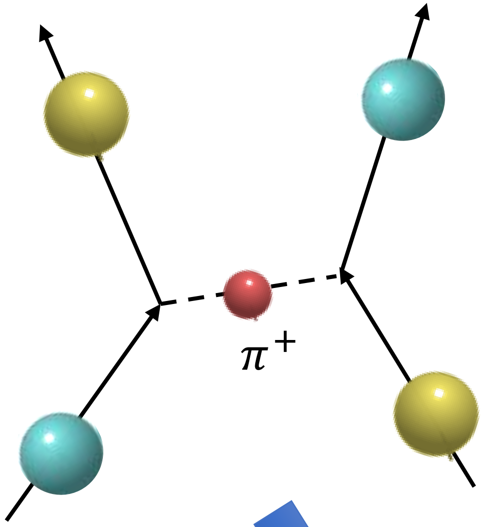
Unified ab initio many-body approach to structure and reactions

We combine nuclear forces derived within chiral effective field theory with ab initio methods

Quantum Chromodynamics

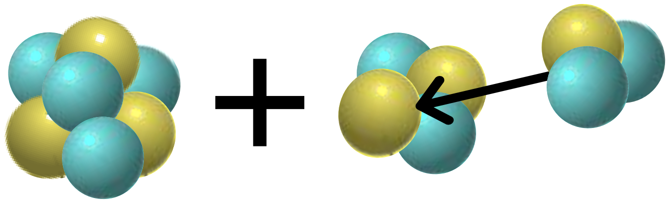


Chiral Effective Field Theory



Chiral NN+3N forces

No Core Shell Model with continuum (NCSMC)



Possibility to adjust some parameters

NCSMC-pheno

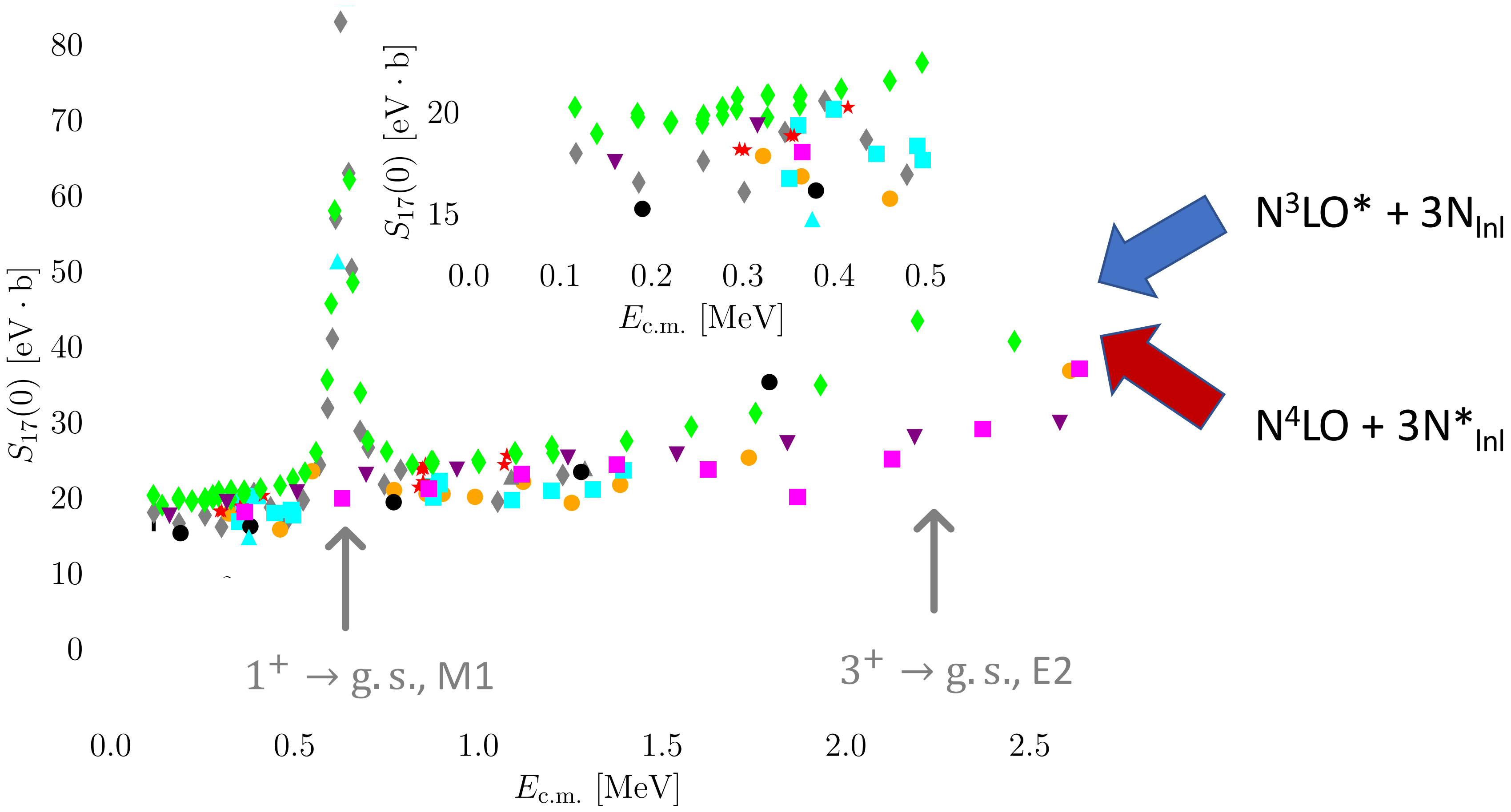
Can use multiple chiral models, truncation errors to quantify uncertainties

	EMN (2017)				EM (2003)	
	$N^2LO + 3N_{lnl}$	$N^3LO + 3N_{lnl}$	$N^4LO + 3N_{lnl}$	$N^4LO + 3N^{*}_{lnl}$	$N^3LO^{*} + 3N_{lnl}$	$N^3LO^{*} + 3N_{loc}$
NN	N^2LO	N^3LO	N^4LO	N^4LO	N^3LO	N^3LO
3N	N^2LO	N^2LO	N^2LO	N^2LO + $O(N^3LO)$	N^2LO	N^2LO (local)

Chiral truncation uncertainty

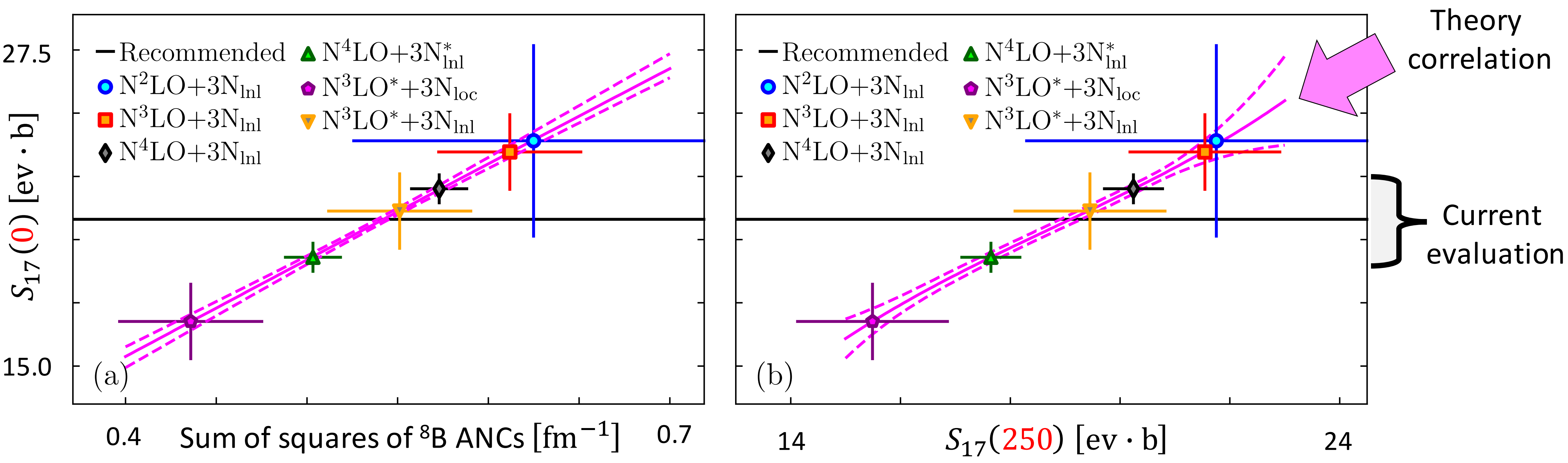
$$\left(\frac{Q}{\Lambda_\chi}\right)^{n+1}$$

Chiral NN+3N forces describe expt. ^{7}Be(p,γ)^{8}B S-factor with varying success for energies up to 2.5 MeV



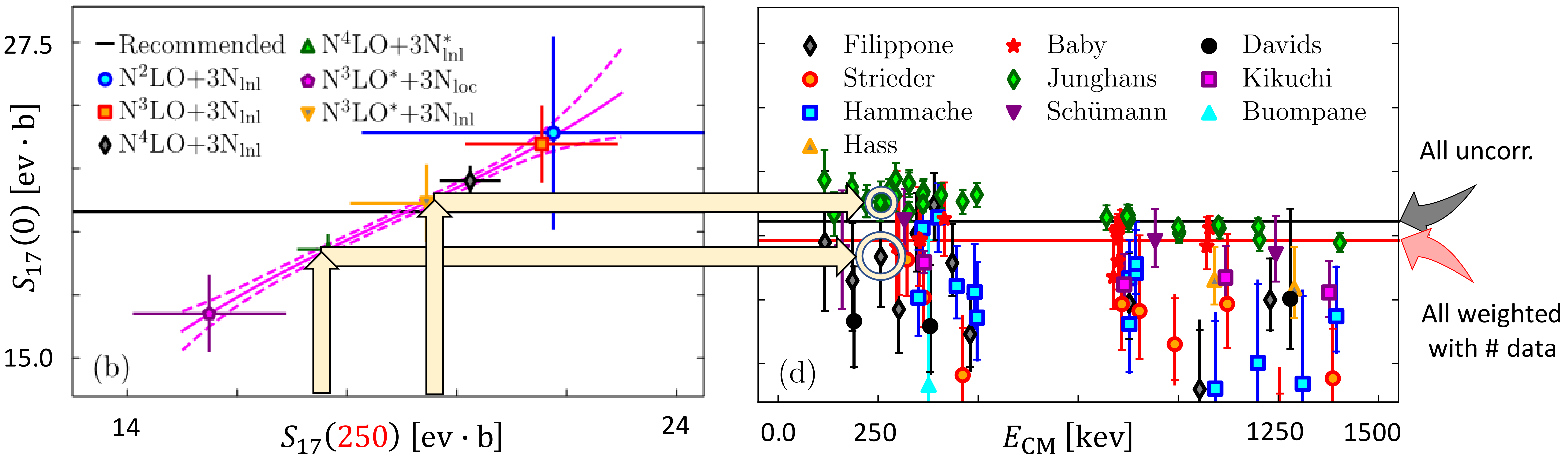
Kravvaris K et al. (2022), arXiv:2202.11759

Can extract universal correlation functions leveraging calculations with different interactions …



… combine them with experimental data to arrive at an improved evaluation of $S_{17}(0)$

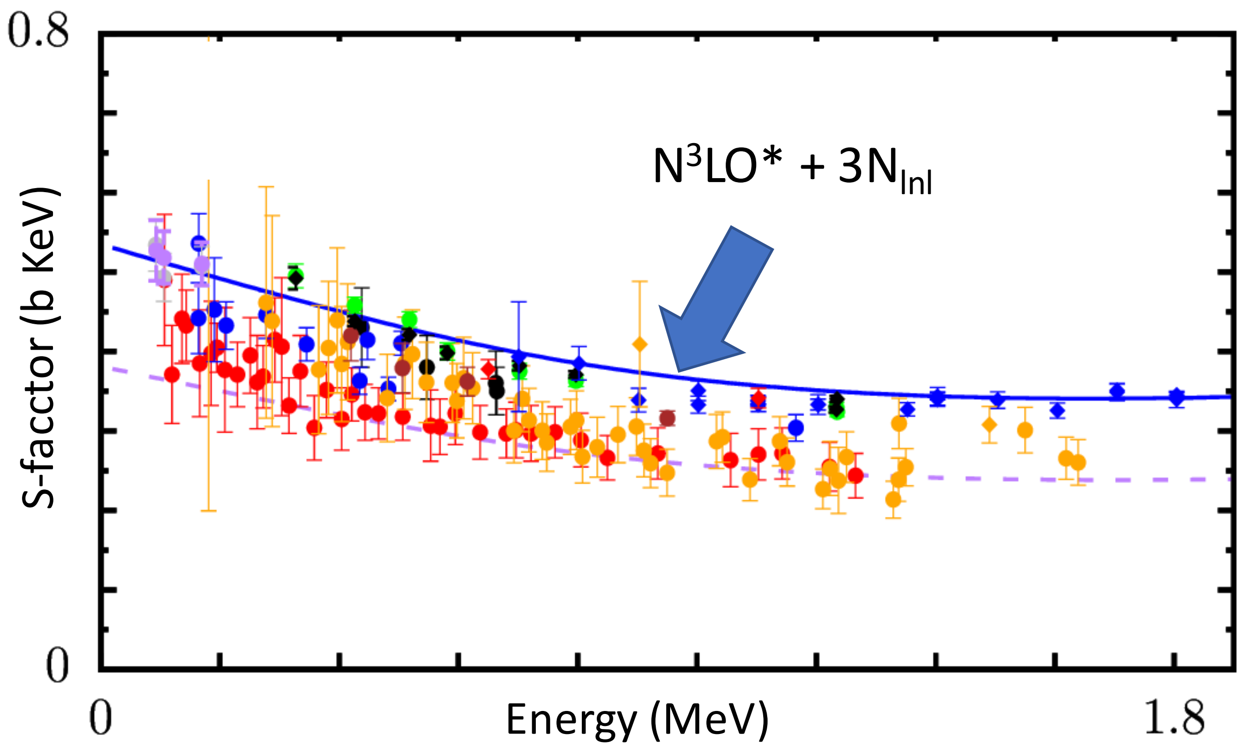
$S_{17}(0) = 19.8 \pm\ 0.3$ eV·b

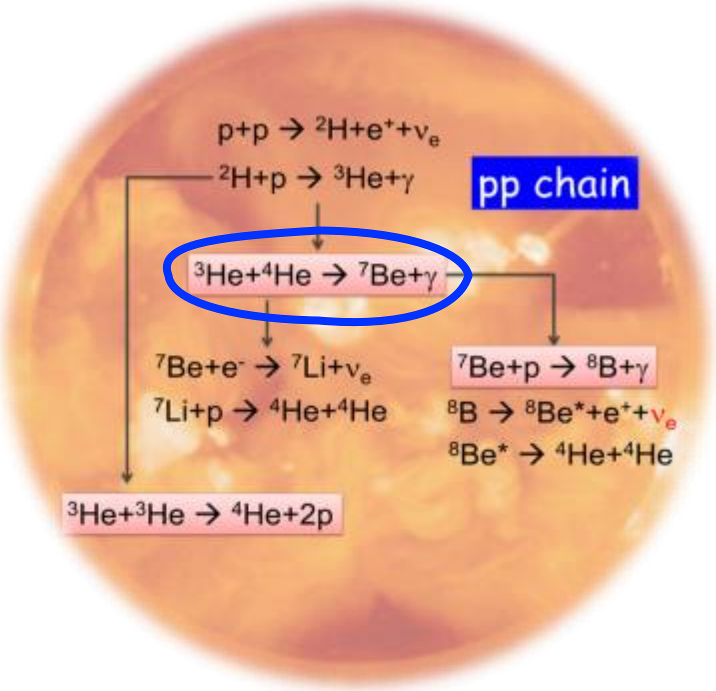


Repeat with computed correlations for energies up to 1.5 MeV

Kravvaris K et al. (2022), arXiv:2202.11759

Now employing NN+3N forces to compute $^3He(\alpha,\gamma)^7Be$, perform analogous ab initio informed evaluation

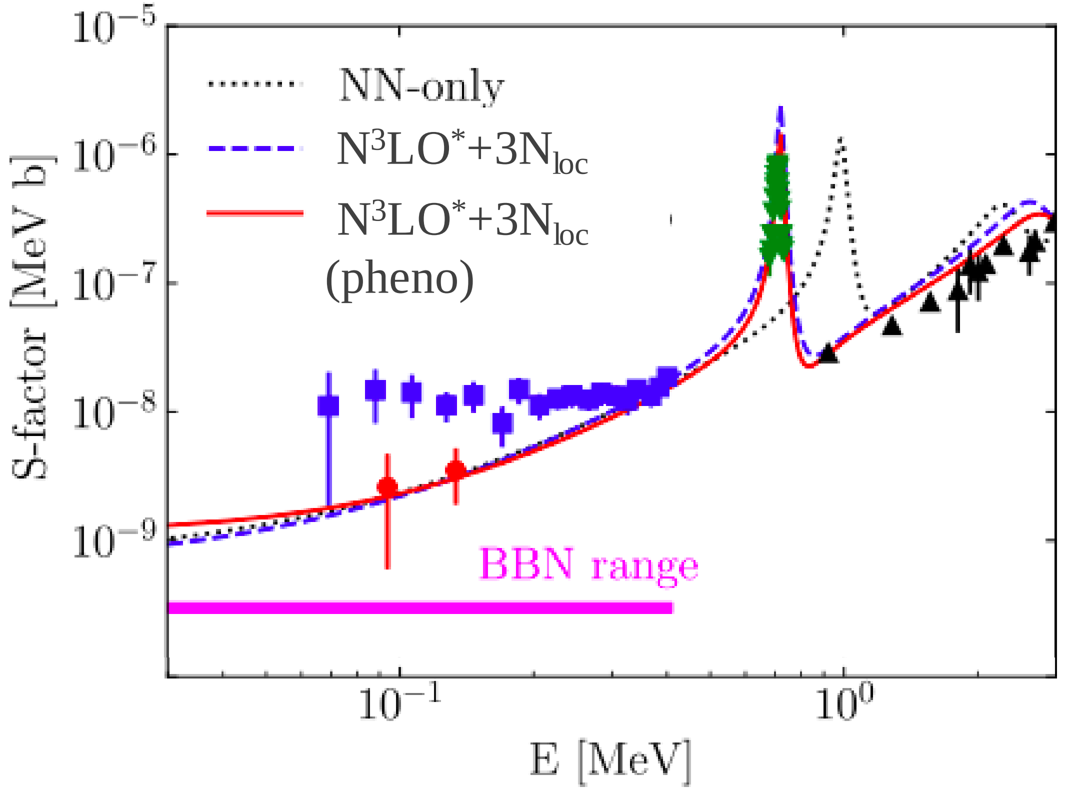




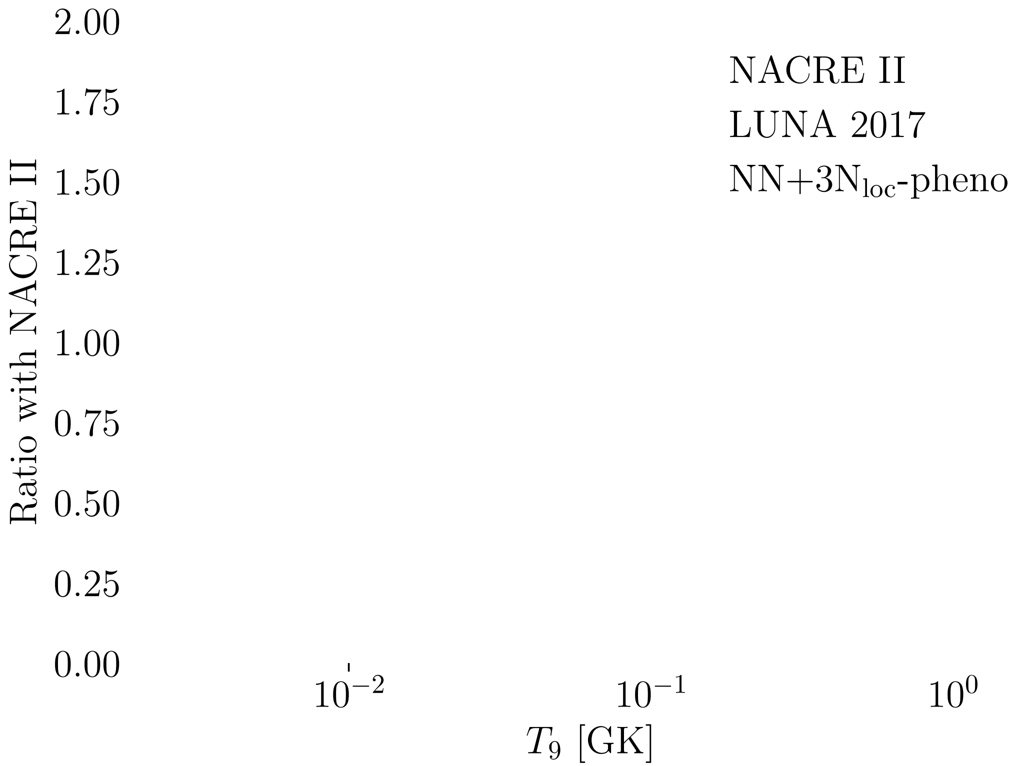
Atkinson MC et al., in preparation

The NCSMC also successfully applied to BBN reactions (yielding again significantly reduced uncertainties)

$^4He(d,\gamma)^6He$ S-factor (Big Bang)

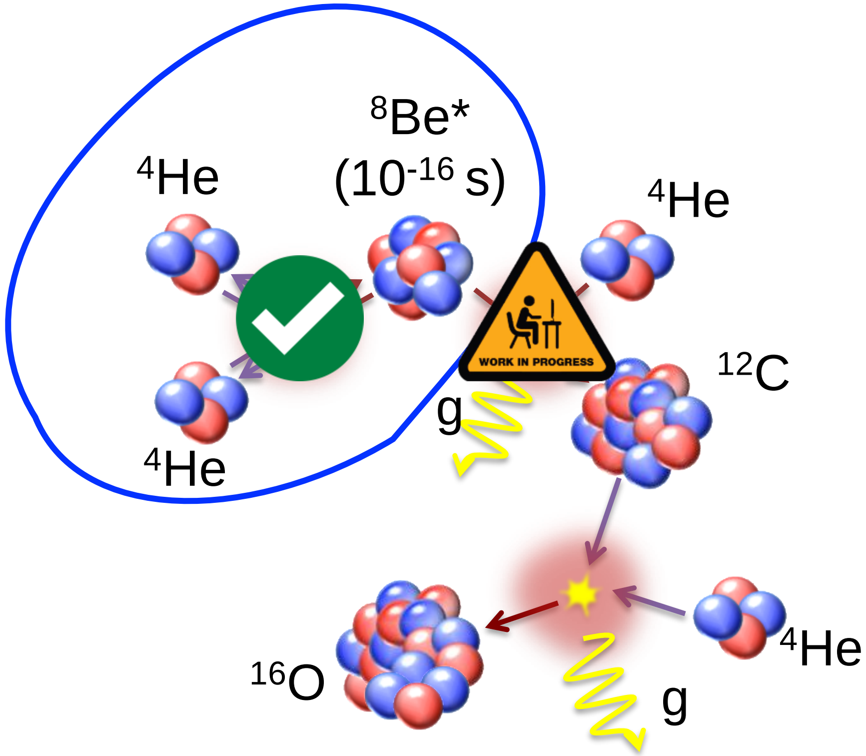


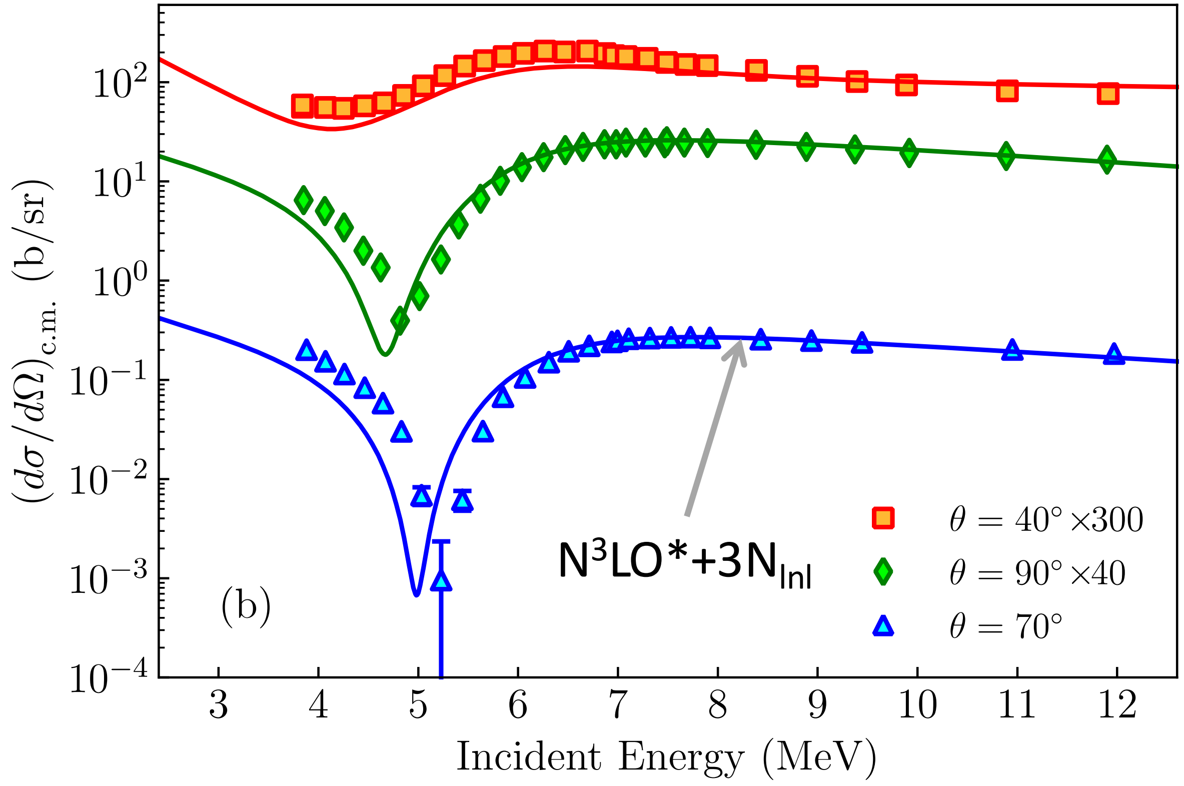
BBN thermonuclear reaction rate



Hebborn C et al. (2022), arXiv:2203.15914

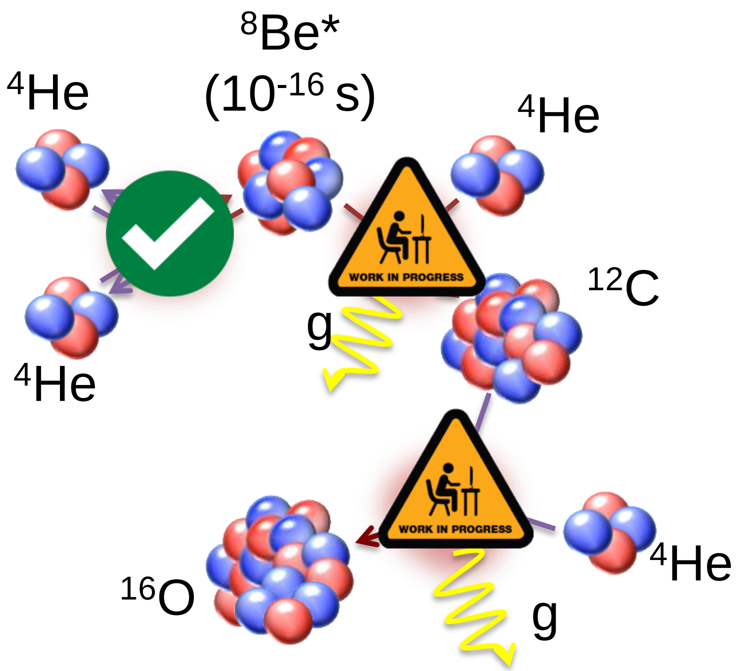
Smart formalism, GPUs also enabled description of ^{4}He + ^{4}He scattering, first stage of helium burning





Kravvaris K et al. (2020), arXiv:2012.00228

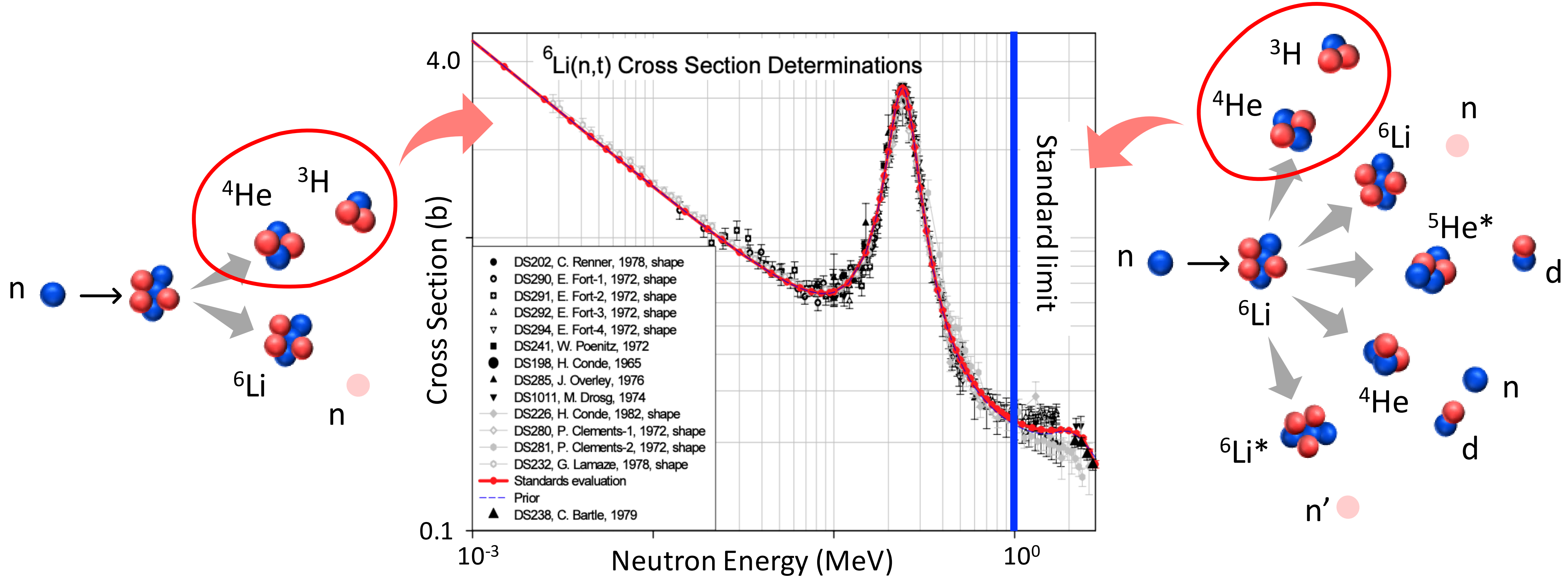
Smart formalism, GPUs also enabled description of ^{4}He + ^{4}He scattering, first stage of helium burning



Kravvaris K et al. (2020), arXiv:2012.00228

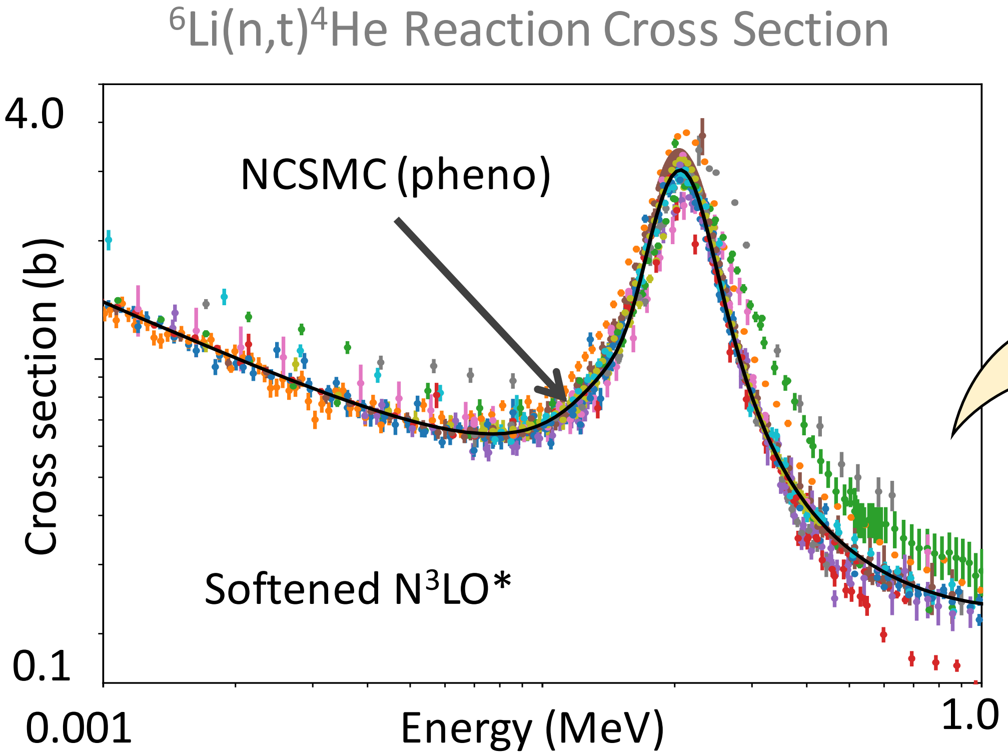
* NN = N^{3}LO (EM 2003)

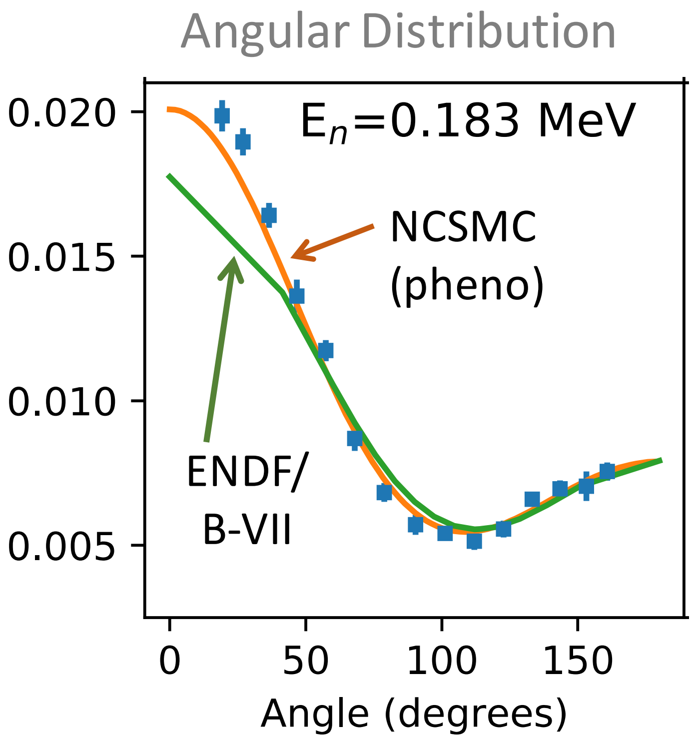
Ab initio reaction theory can also aid in improving evaluation of neutron standard cross sections



Carlson et al. (2009) Nuclear Data Sheets 110, 3215

Calculation adjusted to reproduce reaction cross section yields improved predictions for angular distributions

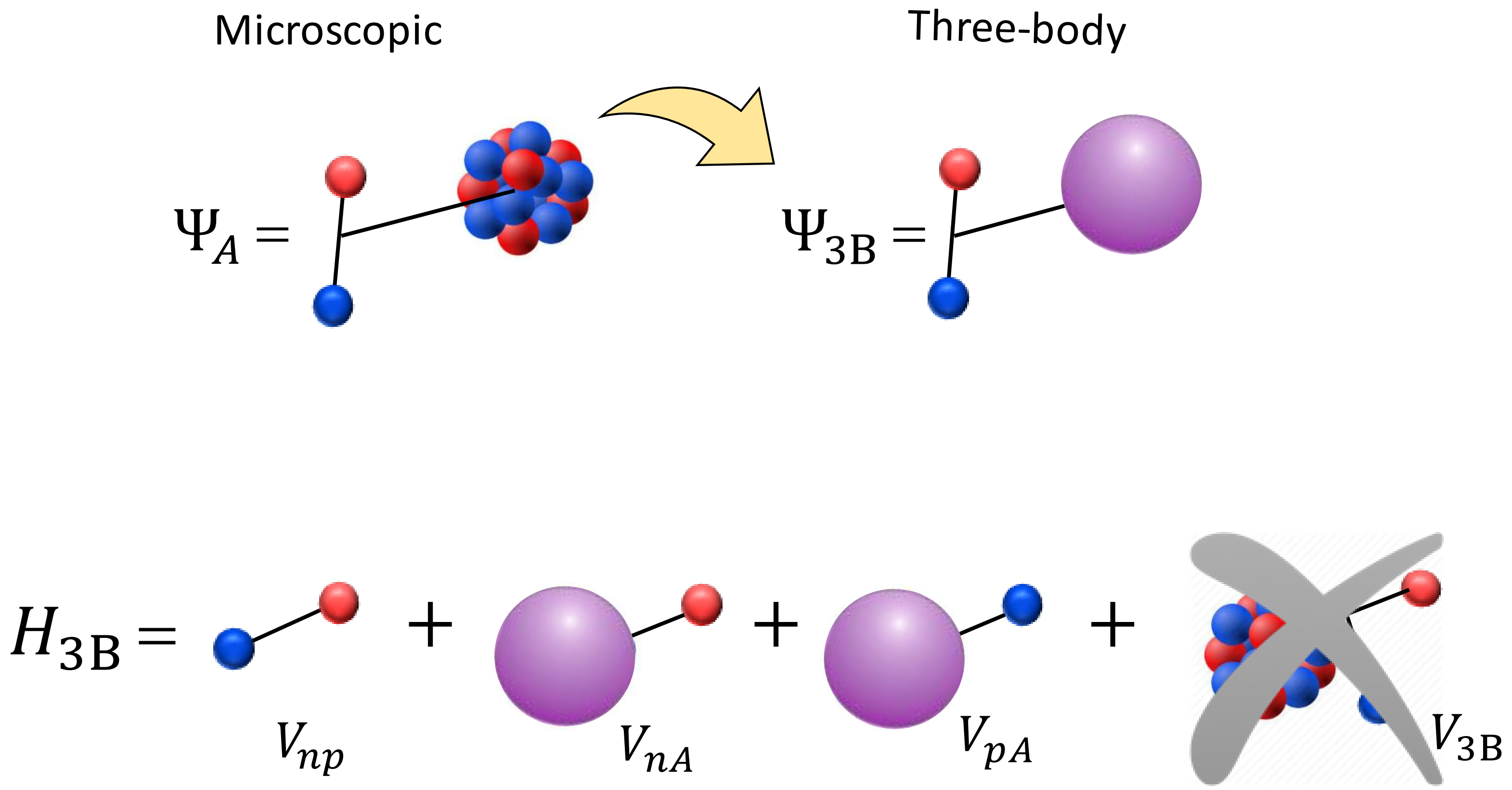




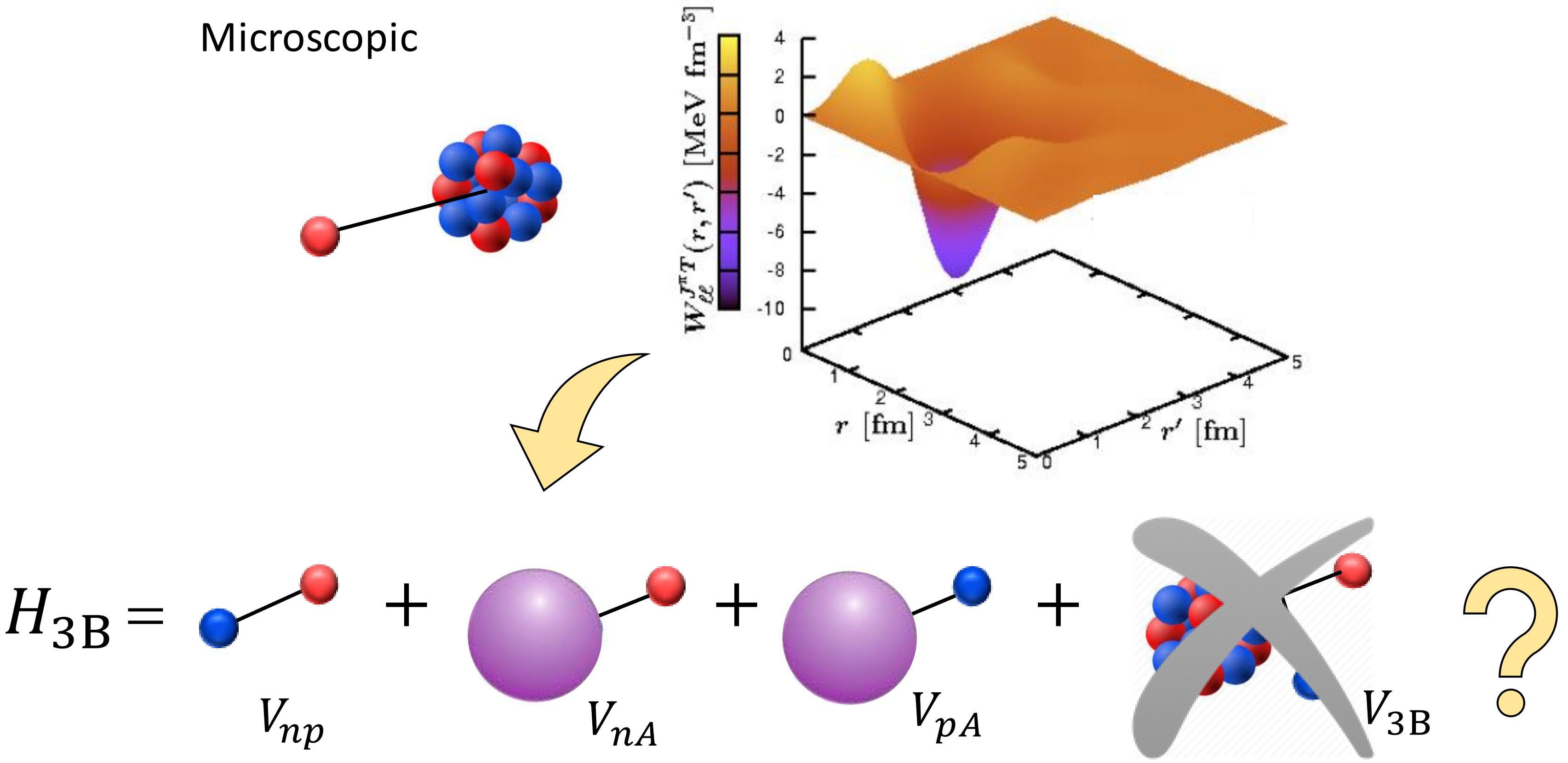
Stay tuned for NCSMC predictions with chiral NN+3N forces

Kravvaris K et al., in preparation

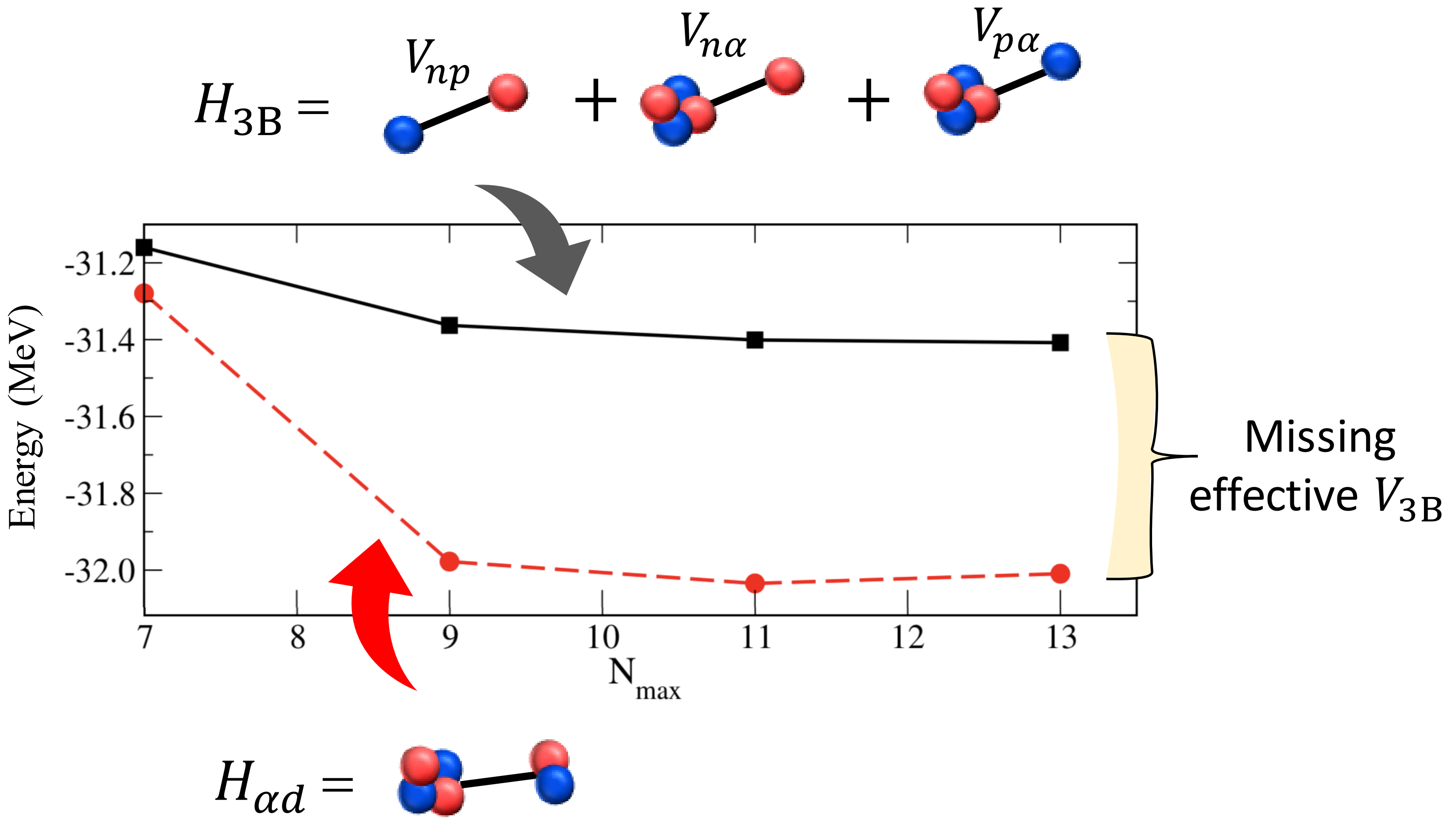
For heavier systems,
few-body reaction models are more effective



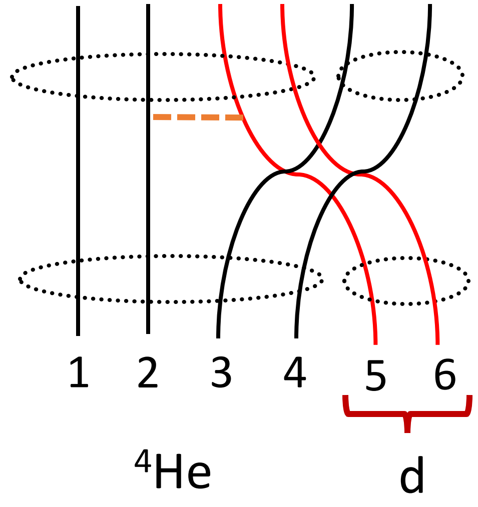
Can we bridge the gap between ab initio calculations and few-body models of nuclear reactions?



In test ground ^{4}He(g.s)+d system, omission of 3-body force causes ~600 keV underbinding for the ^{6}Li ground state …

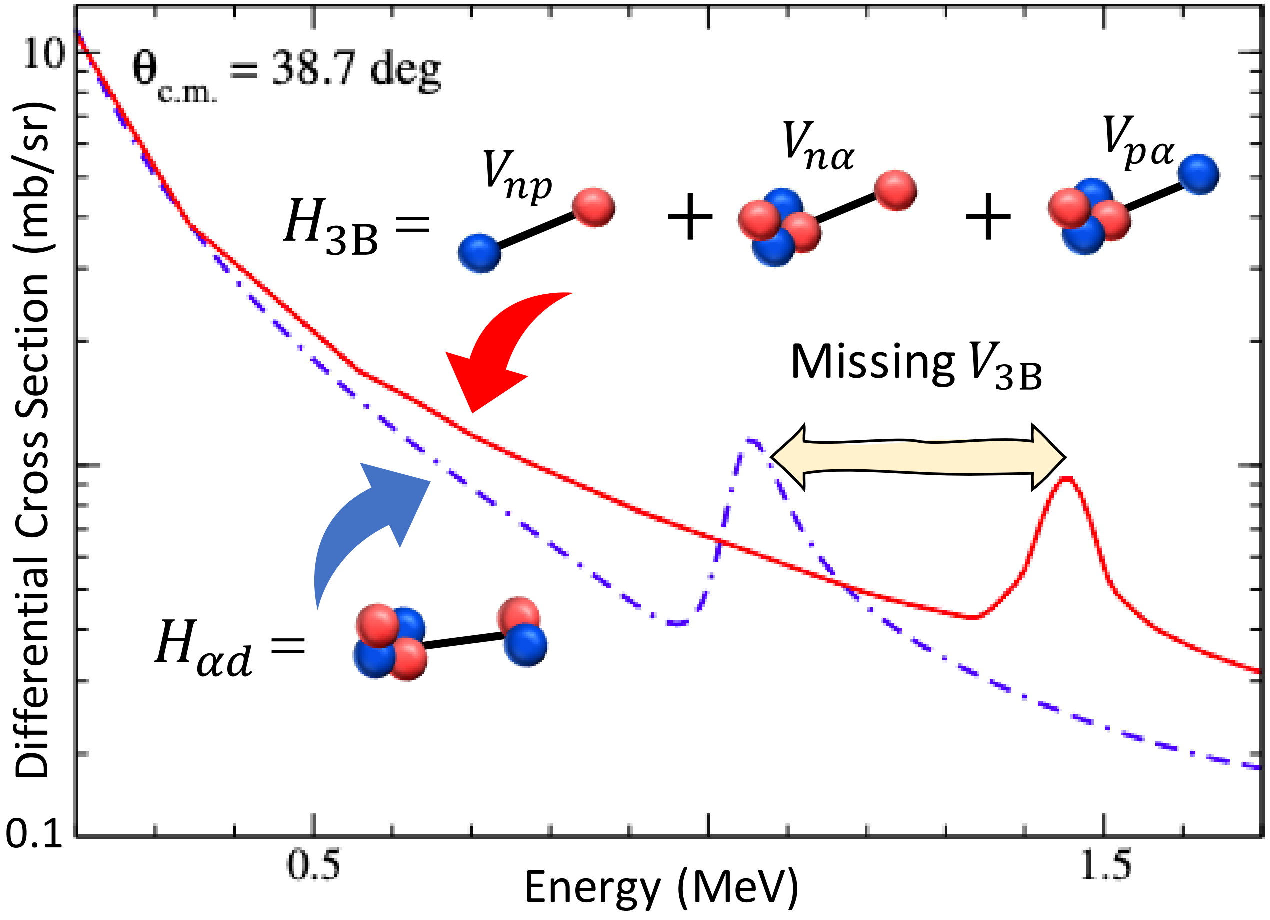


Simultaneous interaction & two-nucleon exchange

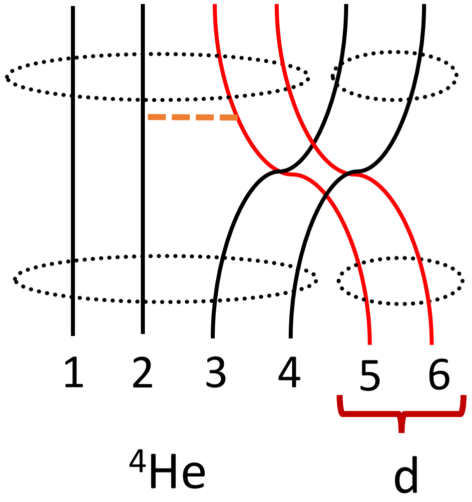


Hlophe LD et al., in preparation

… ~400 keV shift to higher energy of 3^+ ^{4}He-d resonance



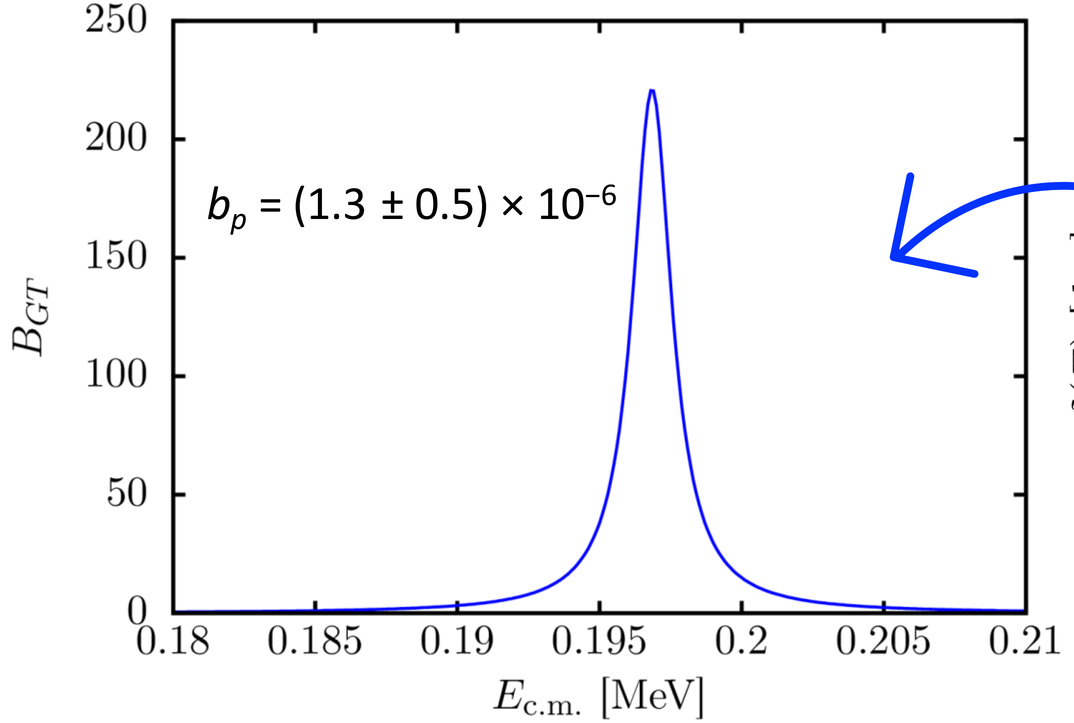
Simultaneous interaction
& two-nucleon exchange



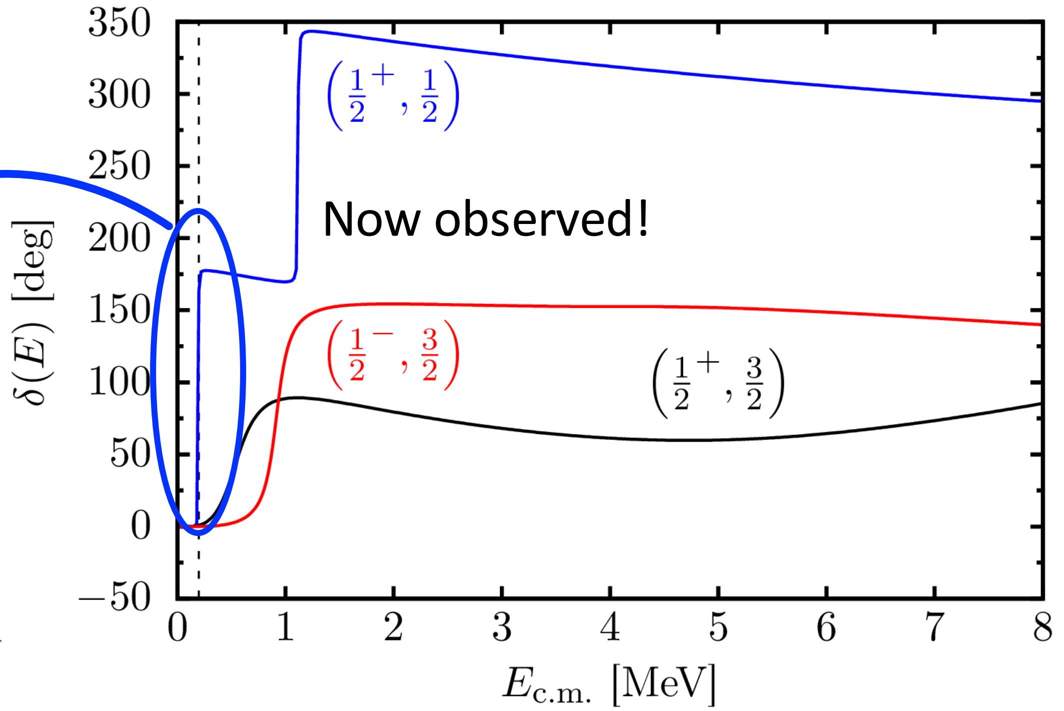
Hlophe LD et al., in preparation

NCSMC extended to describe exotic ^{11}Be βp emission, supports large branching ratio due to narrow ½⁺ resonance

^{11}Be → (^{10}Be+p) + β^- + $\bar{\nu}_e$ GT transition



p+^{10}Be Scattering Phase Shifts



Atkinson MC et al. (2022), Phys. Rev. C 105, 054316

The ab initio structure and reactions team

Sofia Quaglioni

Kostas Kravvaris

Linda Hlophe

Chloë Hebborn

Mack Atkinson

Guillaume Hupin

IN2P3

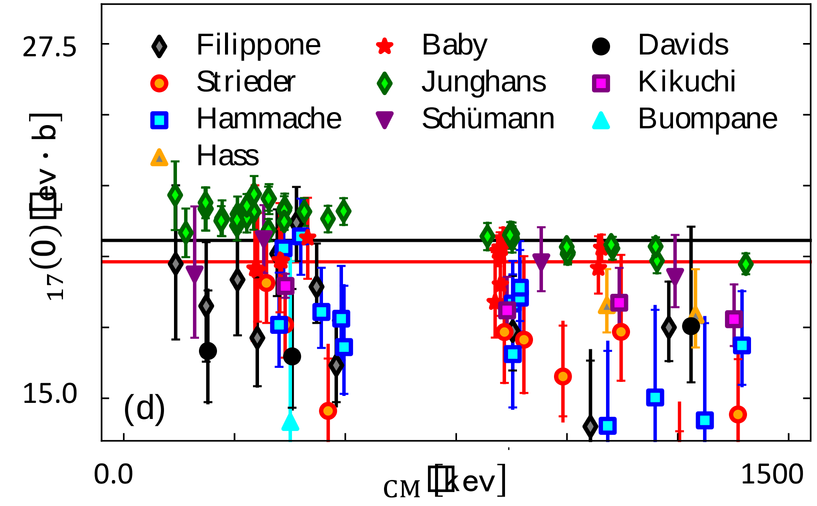
Petr Navratil

TRIUMF

Predictive ab initio calculations are enabling substantially reduced uncertainties for astrophysical rates

New evaluation protocol combines:

- Ab initio calculations with chiral NN+3N forces
- Expt. data both at low and higher energies

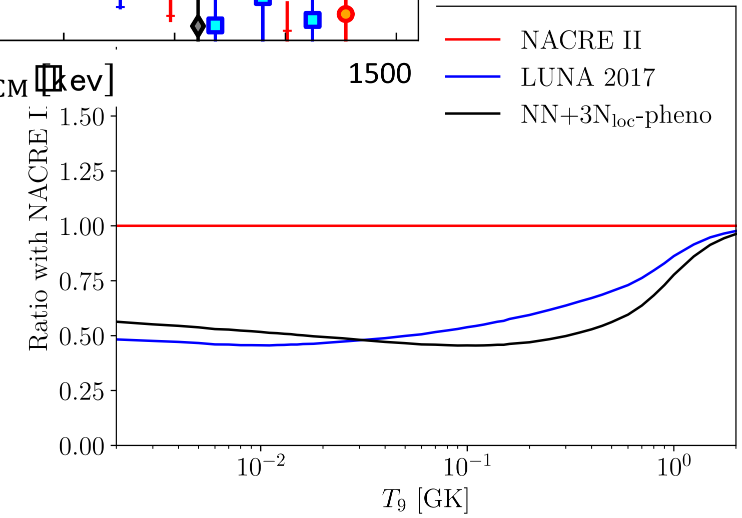


Solar fusion cross sections

Progress also on other fronts:

- Predictions of neutron standard cross sections
- Ab initio informed few-body reaction models
- Predictions of beta-delayed particle emission

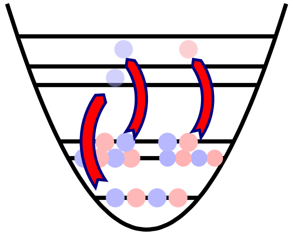
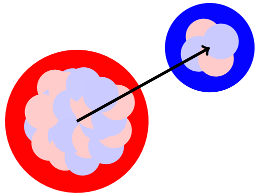
BBN rates



Lawrence Livermore National Laboratory

LLNL-PRES-836301

Structure, scattering and reactions obtained with unified treatment of bound and unbound states

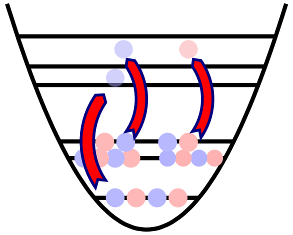
$\Psi = \sum_{\lambda} c_{\lambda} |$  $\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) |$  $\rangle$

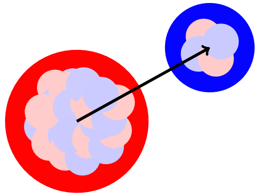
No Core Shell Model with continuum
(NCSMC)

Navratil P et. al (2016), Physica Scripta 91, 053002

Structure, scattering and reactions obtained with unified treatment of bound and unbound states

$$\Psi = \underbrace{\sum_{\lambda} c_{\lambda} | \qquad \rangle}_{} + \sum_{\nu} \int dr u_{\nu}(r) | \qquad \rangle$$

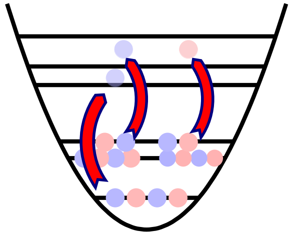
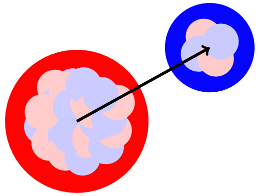




Static solutions for aggregate system,
describe all nucleons close together

Navratil P et. al (2016), Physica Scripta 91, 053002

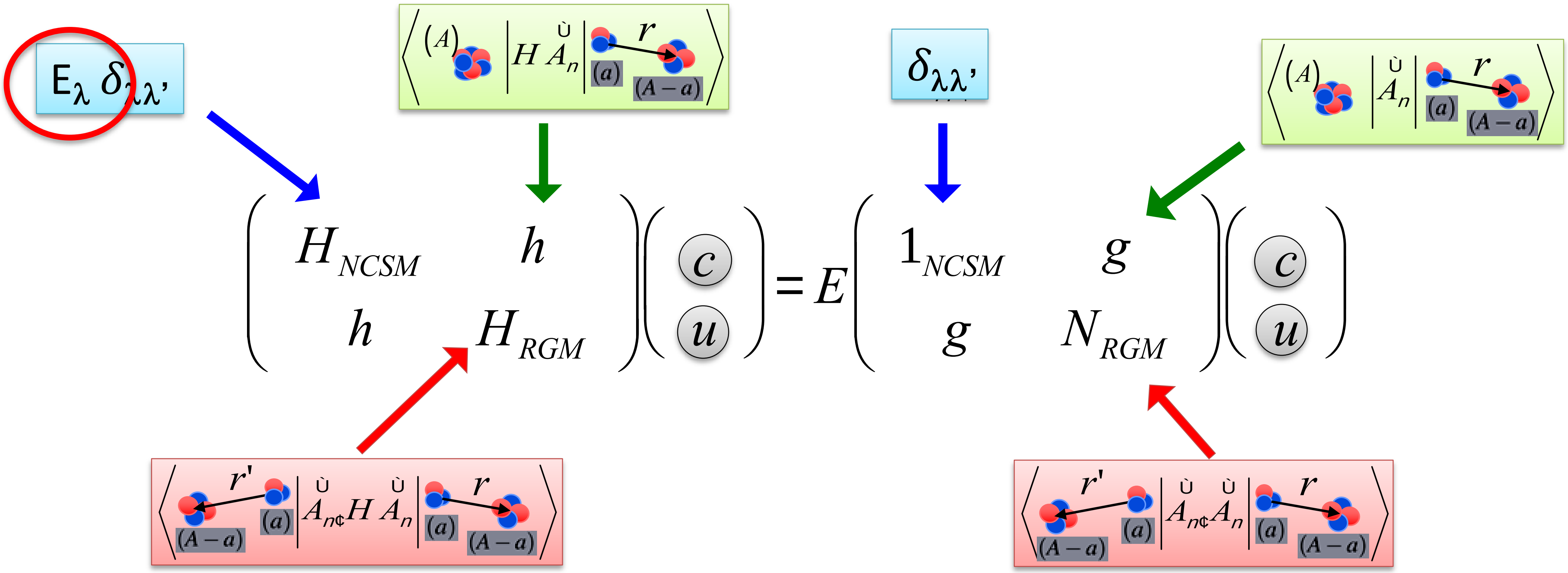
Structure, scattering and reactions obtained with unified treatment of bound and unbound states

$$\Psi = \sum_{\lambda} c_{\lambda} \Big|$$

$$\Big\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) \Big|$$

$$\Big\rangle$$

Continuous microscopic cluster states,
describe separated projectiles & targets

Navratil P et. al (2016), Physica Scripta 91, 053002

Phenomenological correction obtained by treating NCSM eigenenergy as an adjustable parameter



$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ u \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ u \end{pmatrix}$$

All other characteristics of the S-matrix still predicted from ab initio theory.