First Principles Calculations Of Light Ion Reactions

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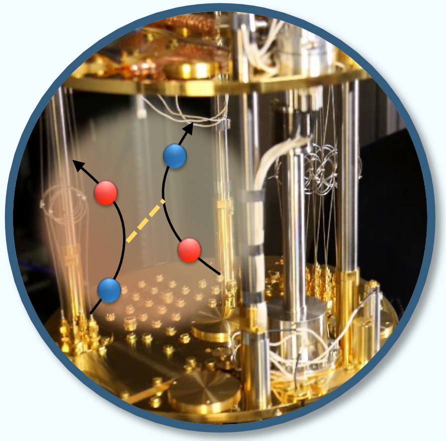
LLNL-PRES-821202

Lawrence Livermore National Laboratory

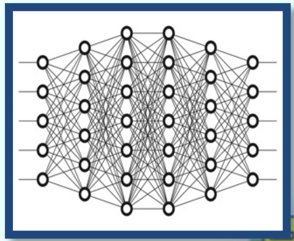
The NDT Group combines state of the art nuclear theory with realistic modeling of nuclear processes to provide accurate data evaluations

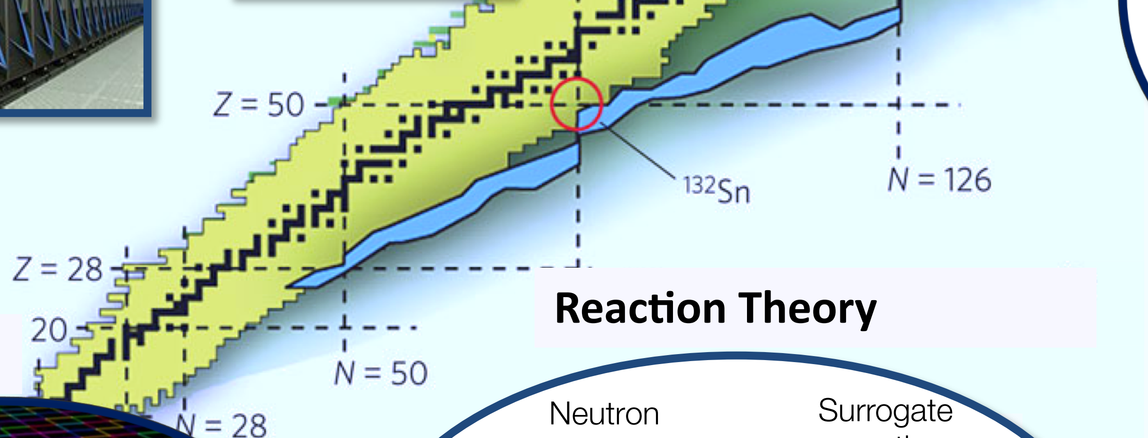
Quantum Computing



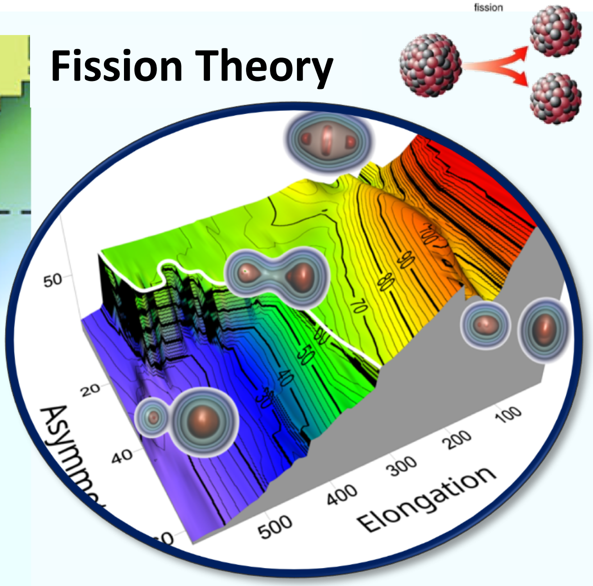
High-Performance Computing

Deep Learning

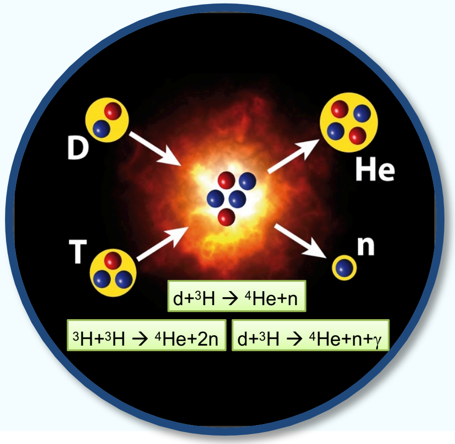




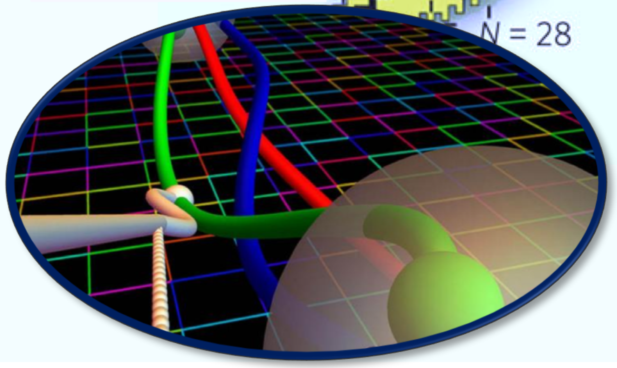
Fission Theory



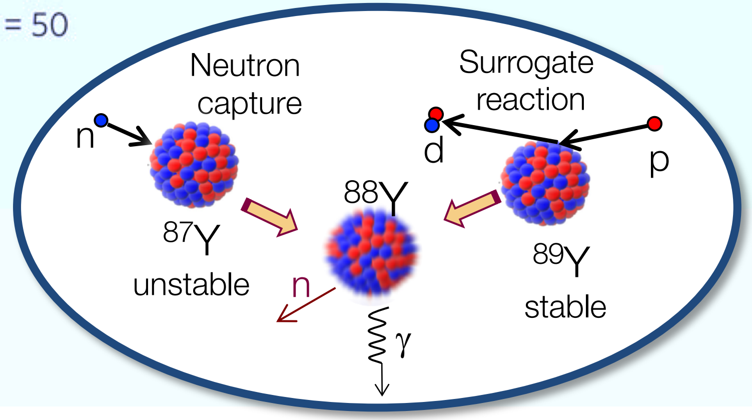
Ab Initio Nuclear Reactions



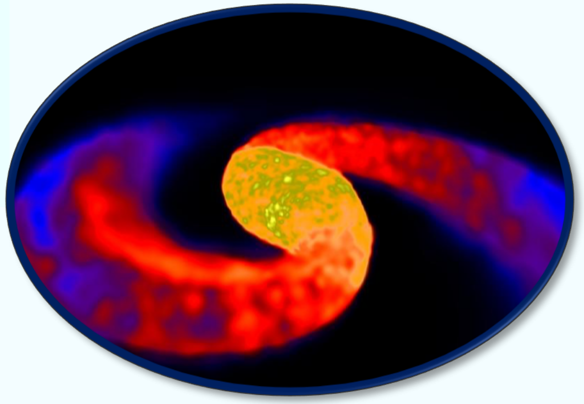
Lattice QCD



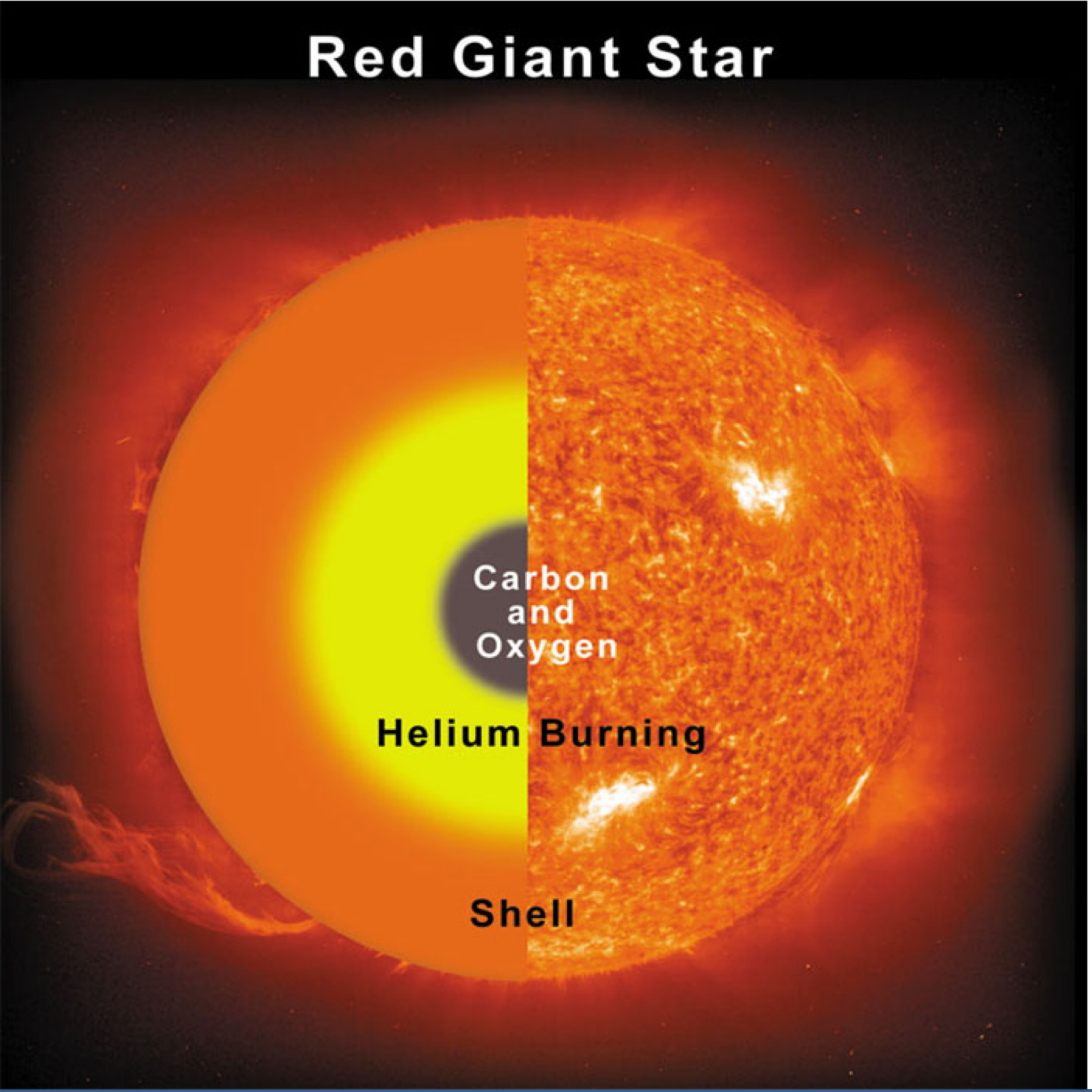
Reaction Theory

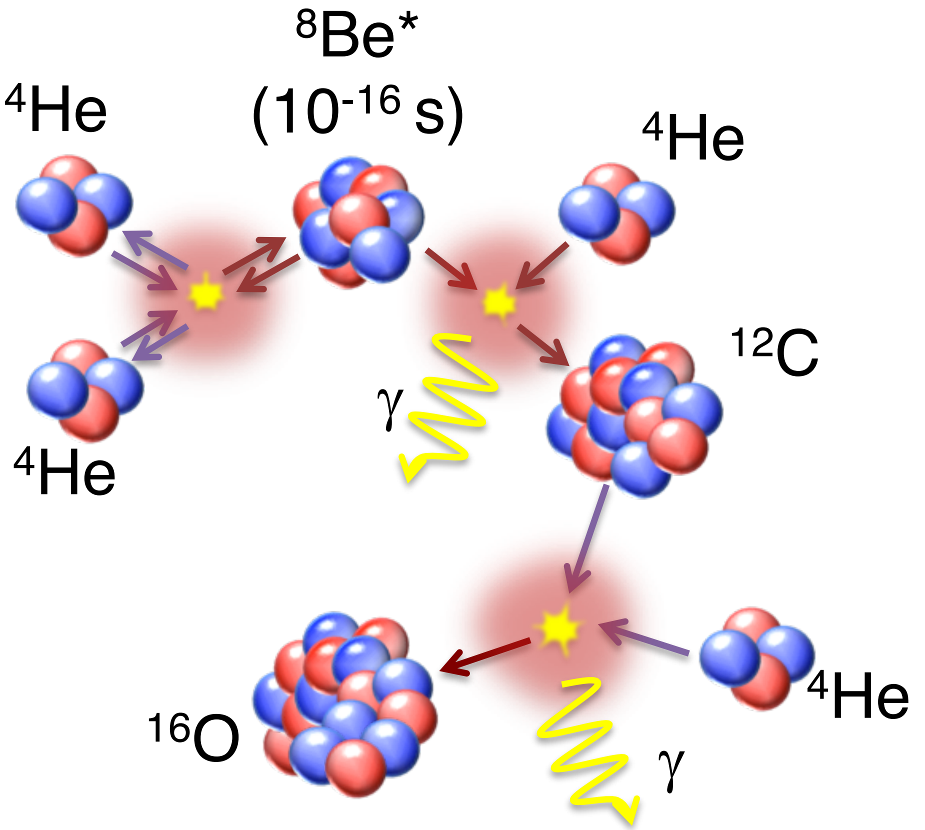


Nuclear data for nucleosynthesis



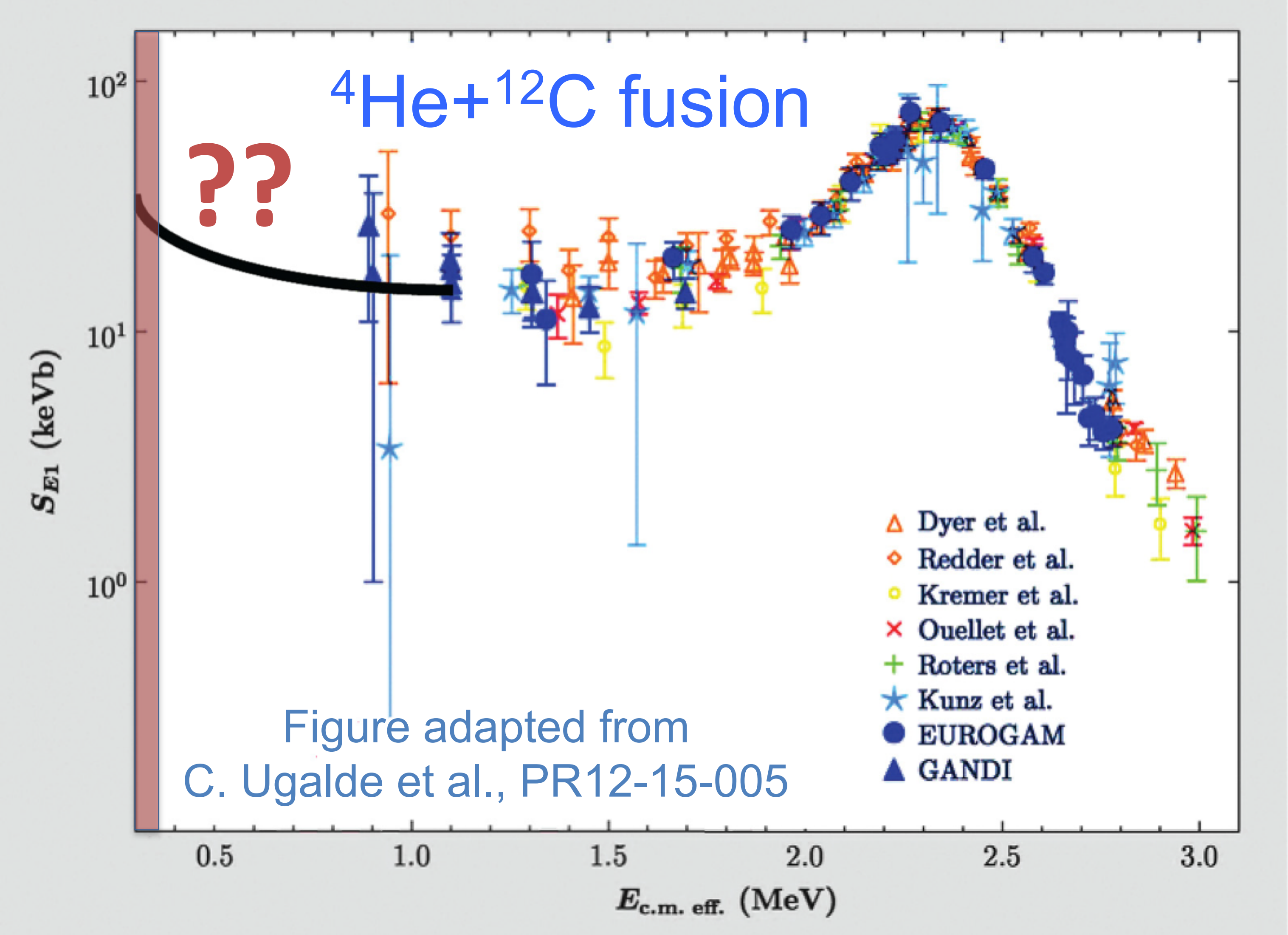
Reaction rates of solar cross sections determine element abundancies in the universe

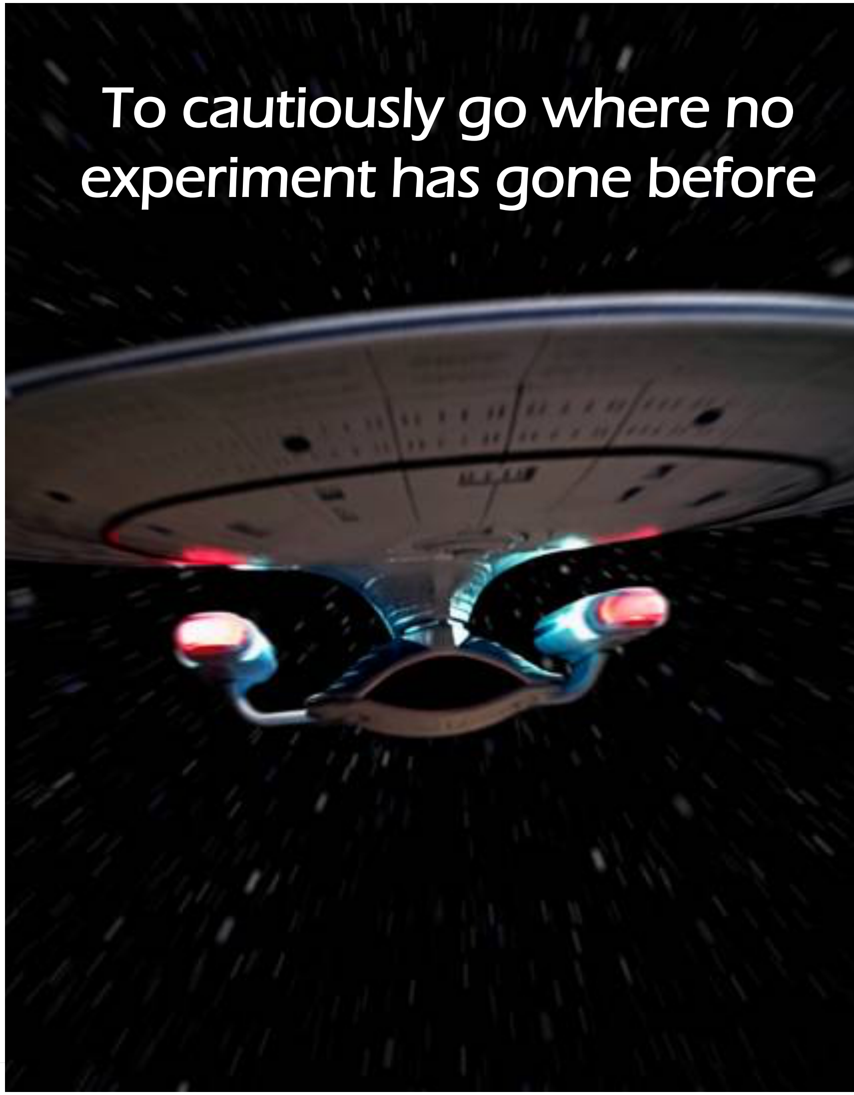




"Not only important for the development of the chemical building blocks of life but also for the entire scheme and sequence of nucleosynthesis events as we imagine them now." (2015 LRP)

We need reliable theory to estimate the S-factor at stellar energies





Nuclear Clustering is found throughout the mass chart and is intimately linked with above-threshold behavior of nuclear spectra.

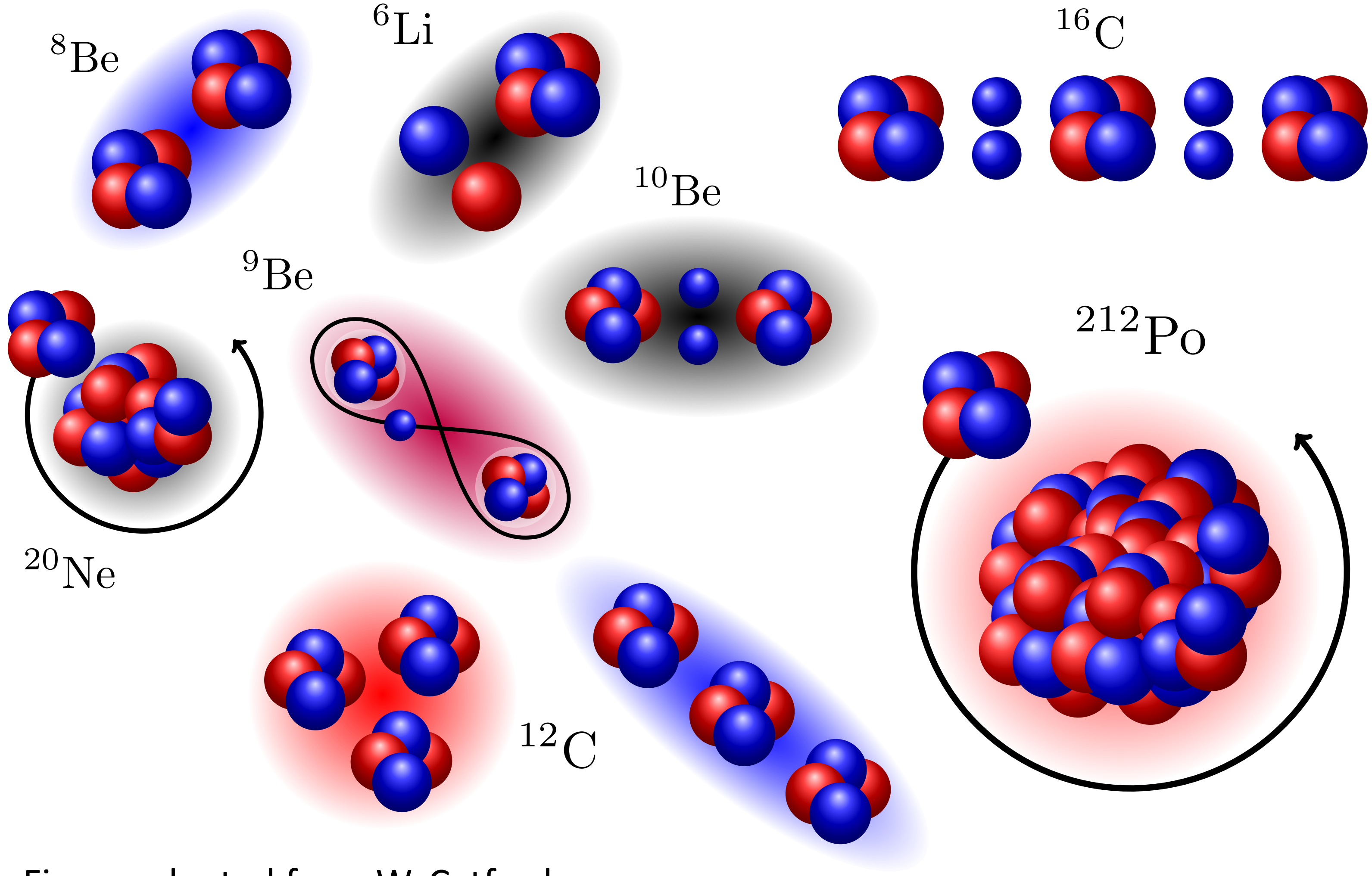
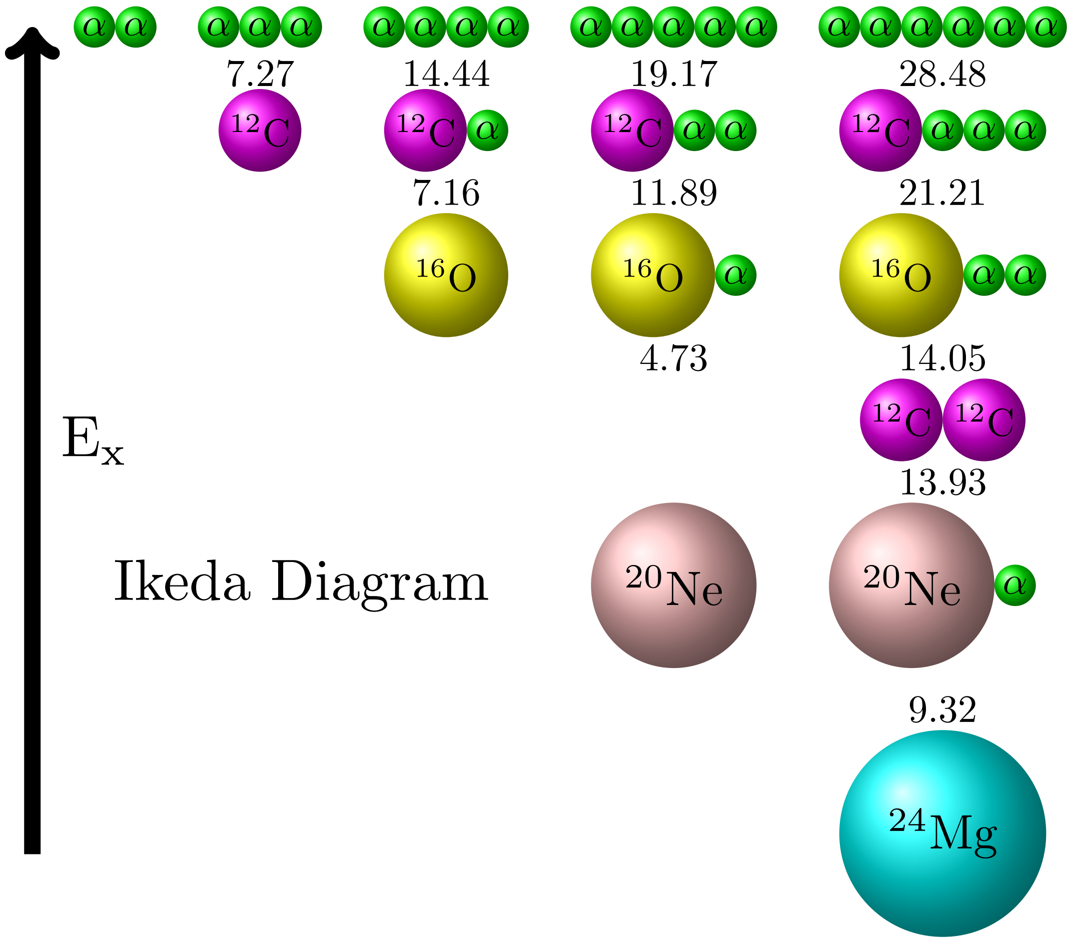
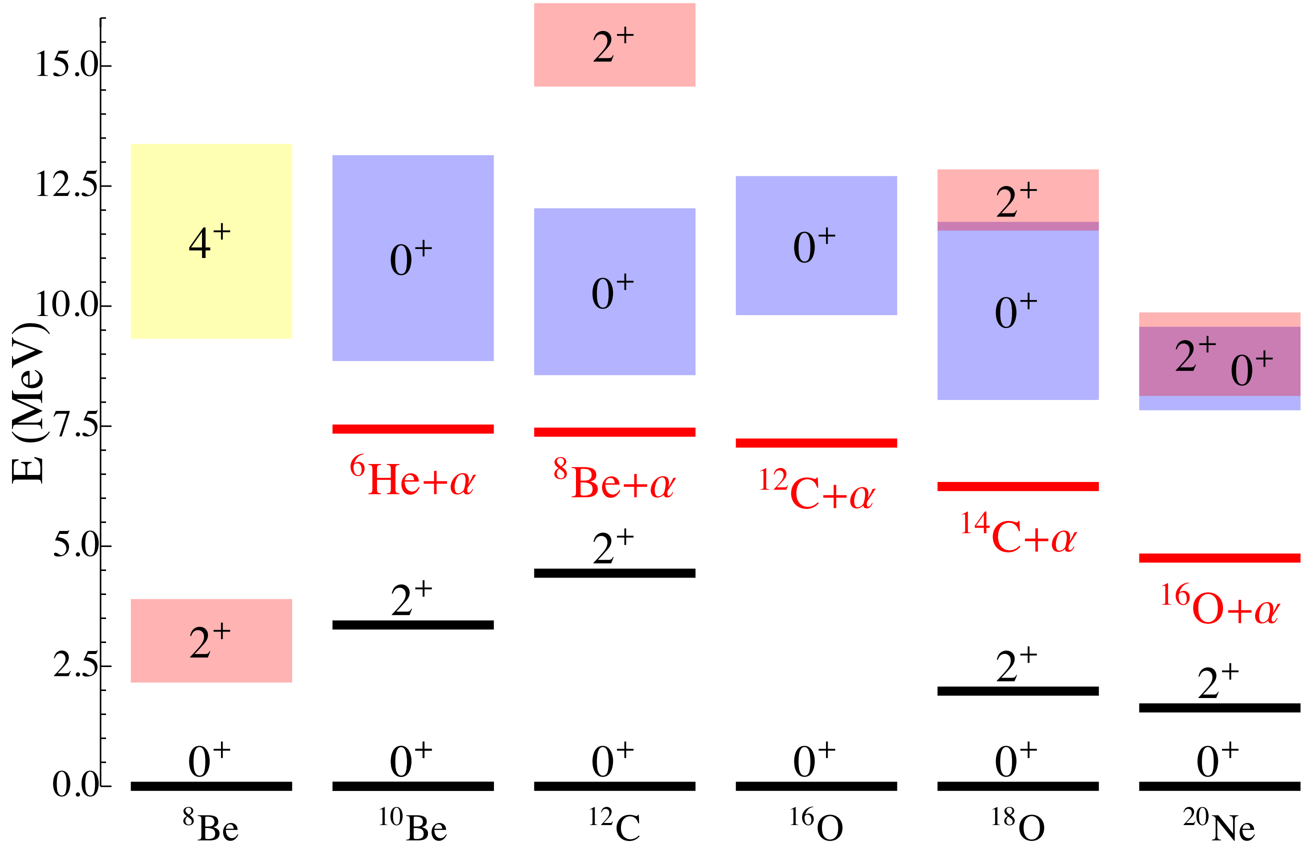


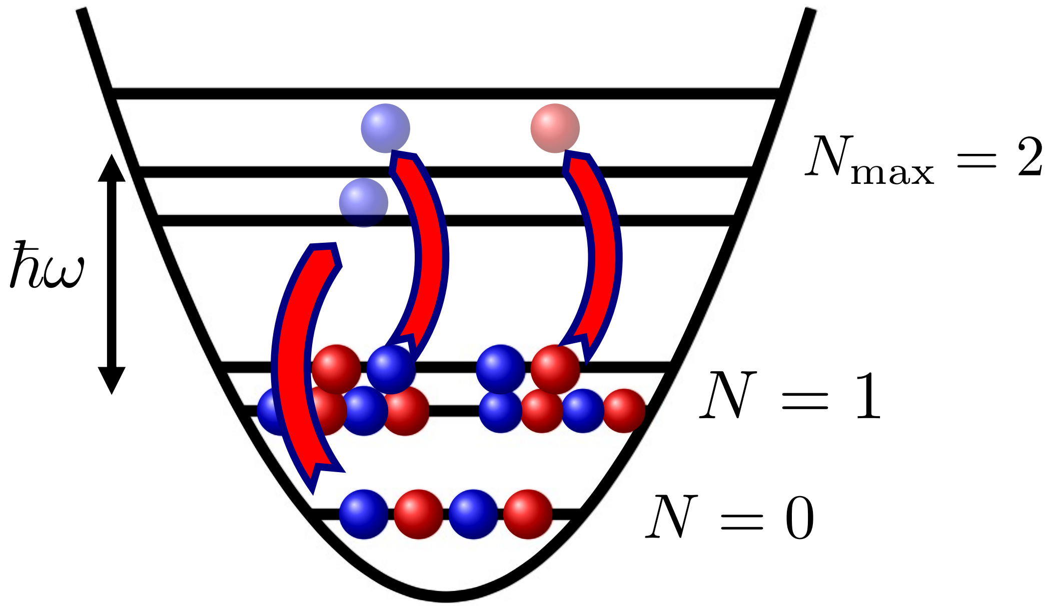
Figure adapted from W. Catford.

Cluster states in light ions exist across the energy spectrum





For a complete ab initio description we need both structure…

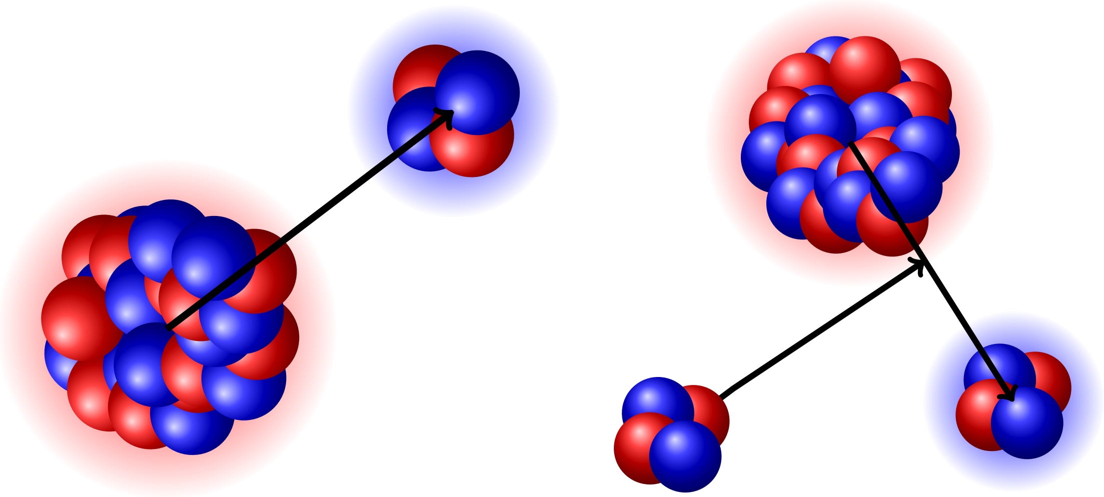


Configuration Interaction
No Core Shell Model (NCSM)

- This picture works fine for well-bound states.
- An increase in the number of allowed excitations encompasses more many-body correlations (lower variational energy).
- Each increase comes with an order-of-magnitude increase in computational effort.
- No coupling to decaying states is considered. (Though check out Phys. Rev. C **98**, 044624)

… and dynamical clustered descriptions

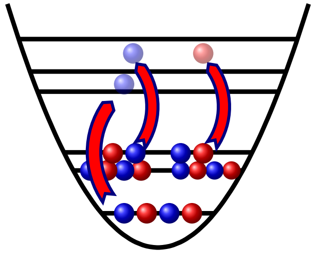
- The CI picture is no longer sufficient to describe the many-body system.
- We need to expand the basis with collective excitations targeting the cluster effects.



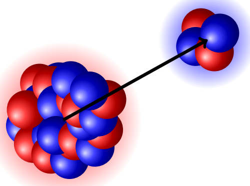
Discrete structure information input

Continuous dynamical input (clustering/reactions)

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

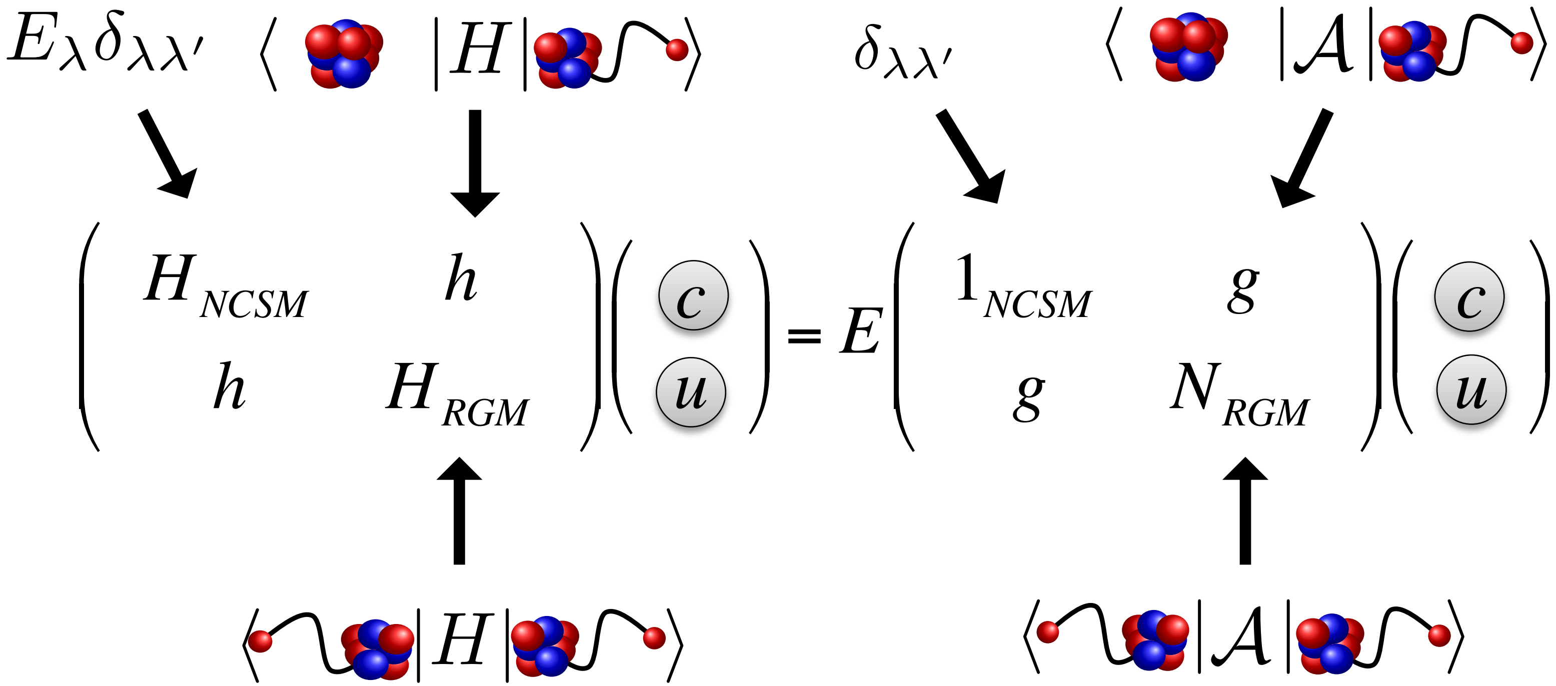


$$\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) \,|$$



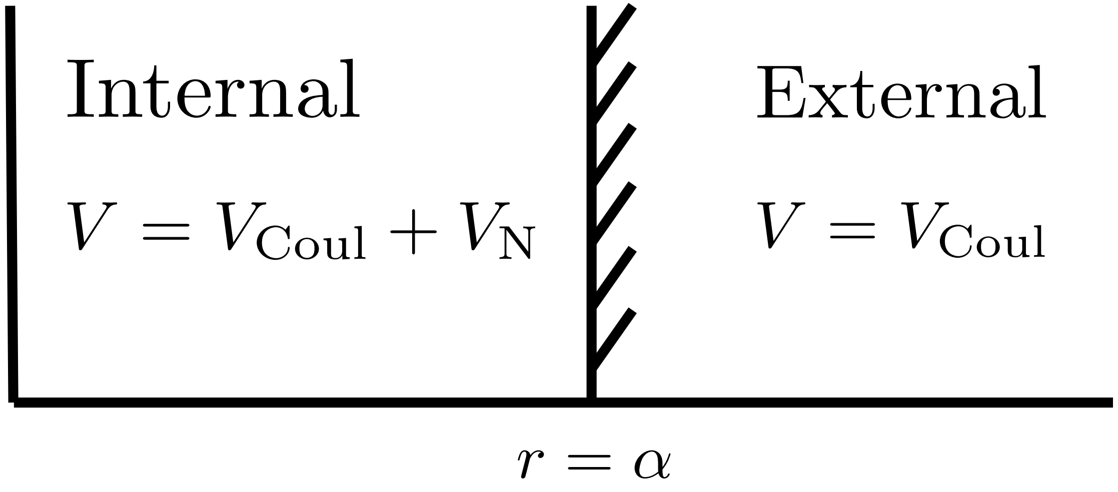
$$\rangle$$

Generalized problem for No Core Shell Model With Continuum



Solving for the unknowns with the R-Matrix.

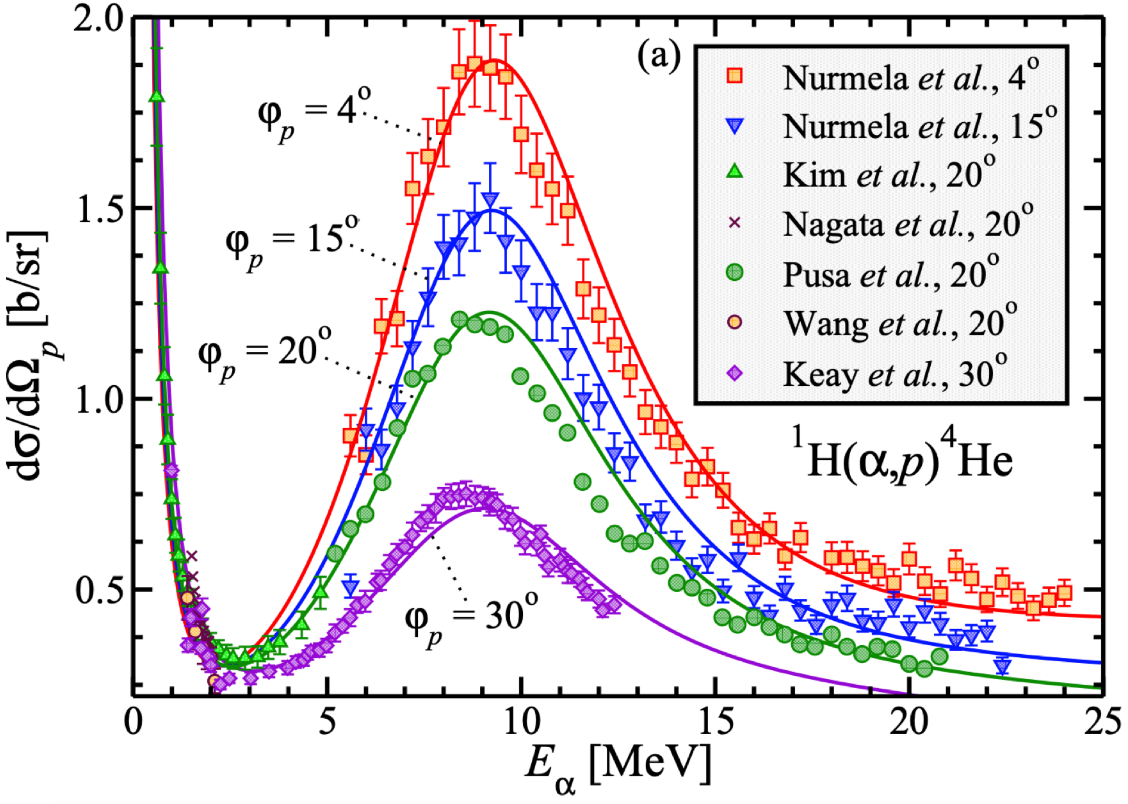
$$\left(\begin{array}{c|c} \mathcal{H}_{\mathcal{P}\mathcal{P}} & \mathcal{H}^{(0)}_{\mathcal{P}\mathcal{Q}} \\ \hline \mathcal{H}^{(0)}_{\mathcal{Q}\mathcal{P}} & \mathcal{H}^{(0)}_{\mathcal{Q}\mathcal{Q}} \end{array}\right)$$



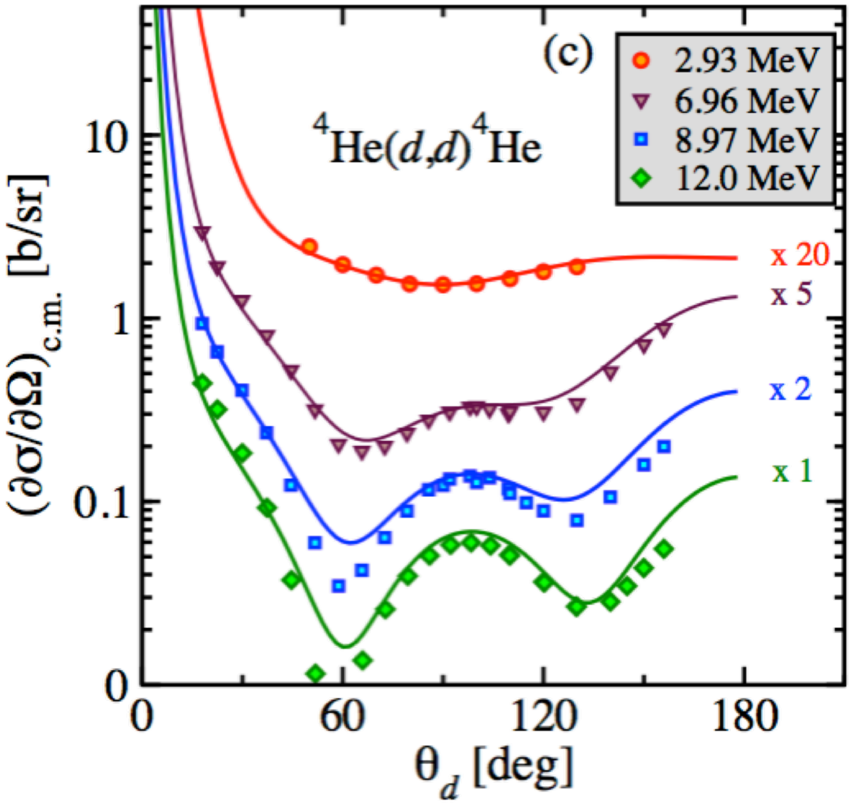
- Need to re-construct the interaction potential seen by the two fragment nuclei.
- Internal P-space Hamiltonian contains interaction potential
- External Q-space only has free components $T + V_{\mathrm{Coul}}$

Can we make accurate predictions?
Nucleon and deuterium elastic scattering on ^{4}He

PRC 90, 061601(R)



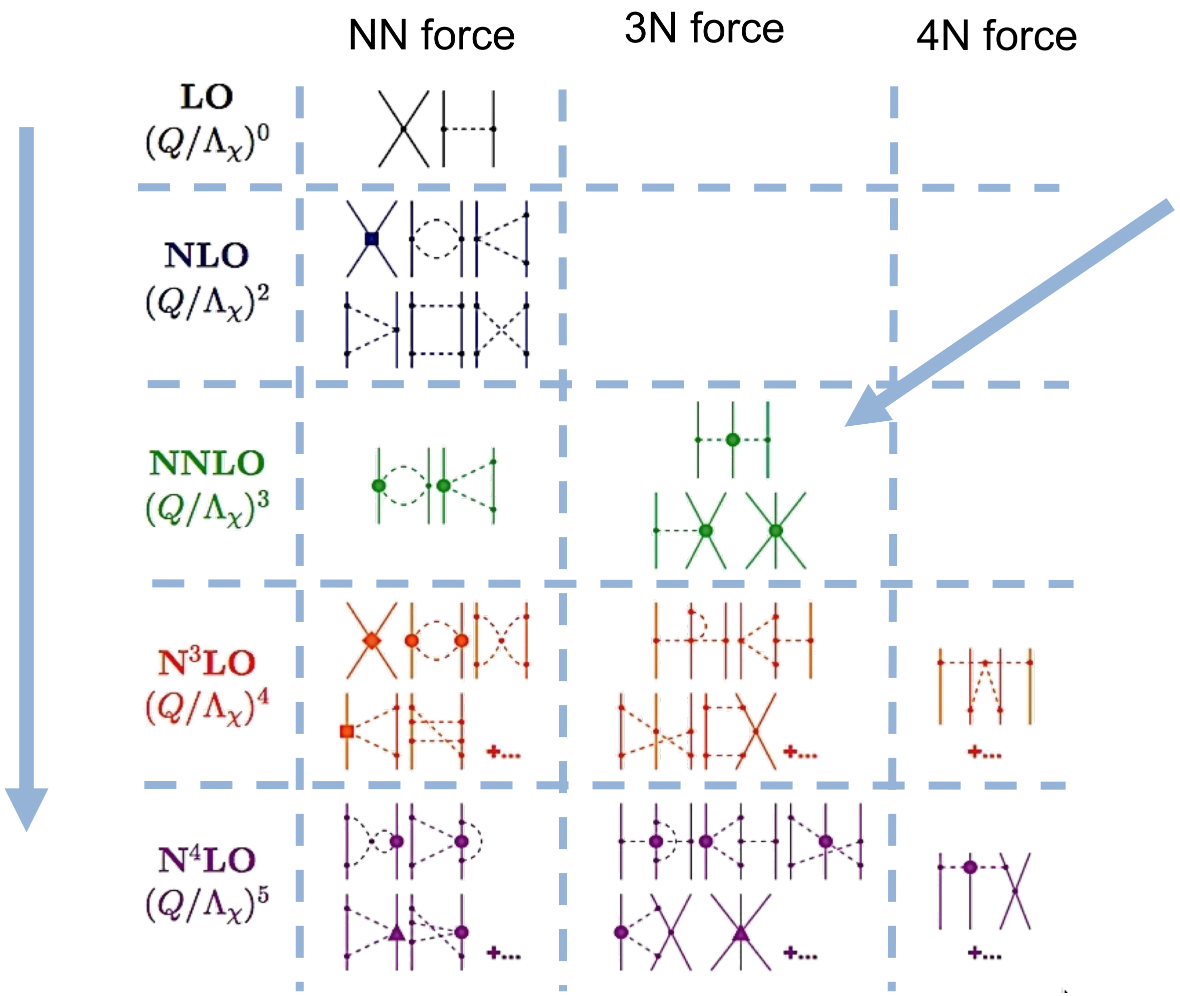
PRL114, 212502



But what about uncertainties? And heavier projectiles?

Chiral effective field theory interactions provide a direct link between the nuclear interactions and QCD.

Systematic expansion of the nuclear force means quantifiable uncertainties!

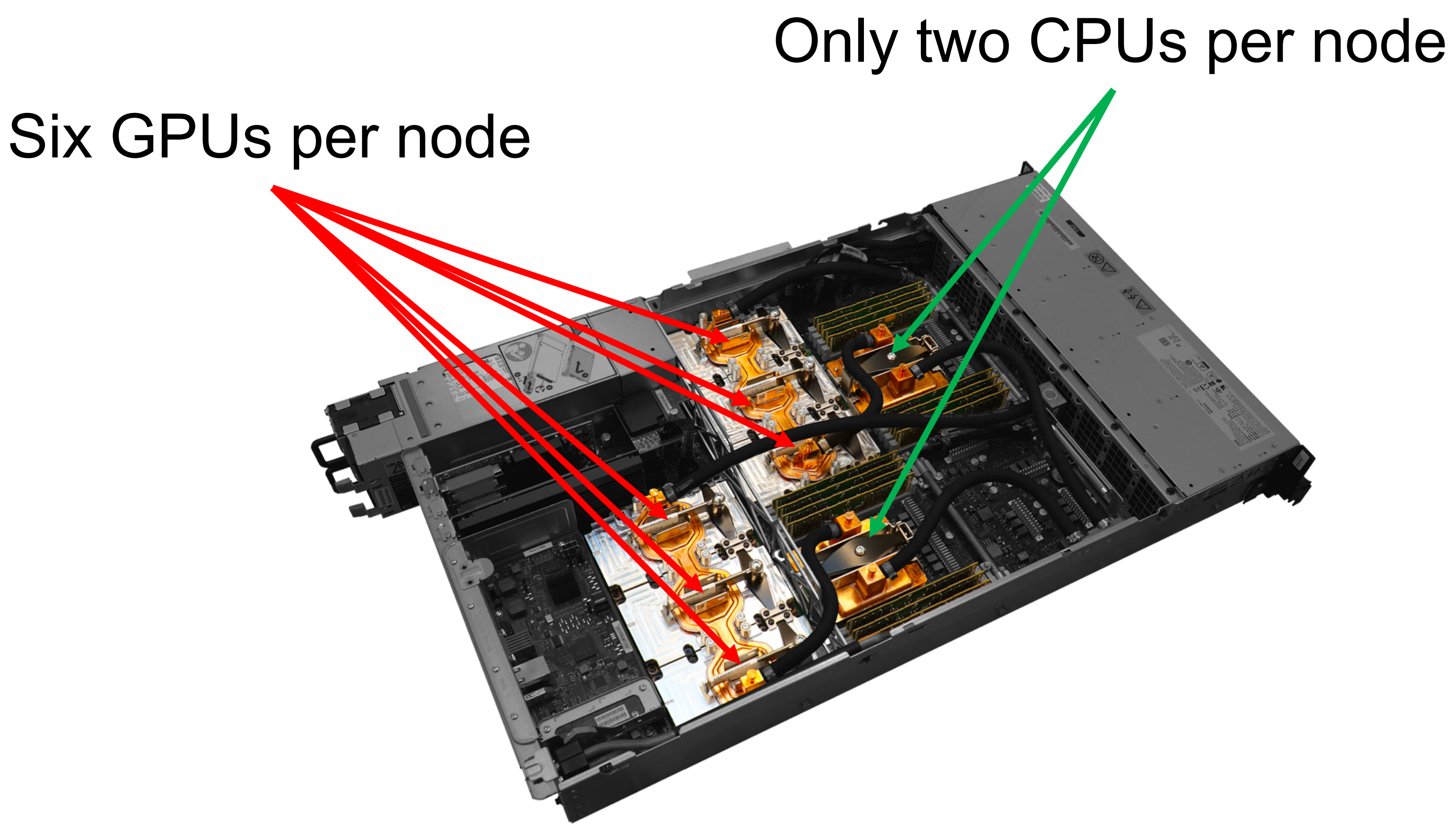


Few diagrams means few parameters that must be constrained from experiments.

Many-nucleon forces appear organically.

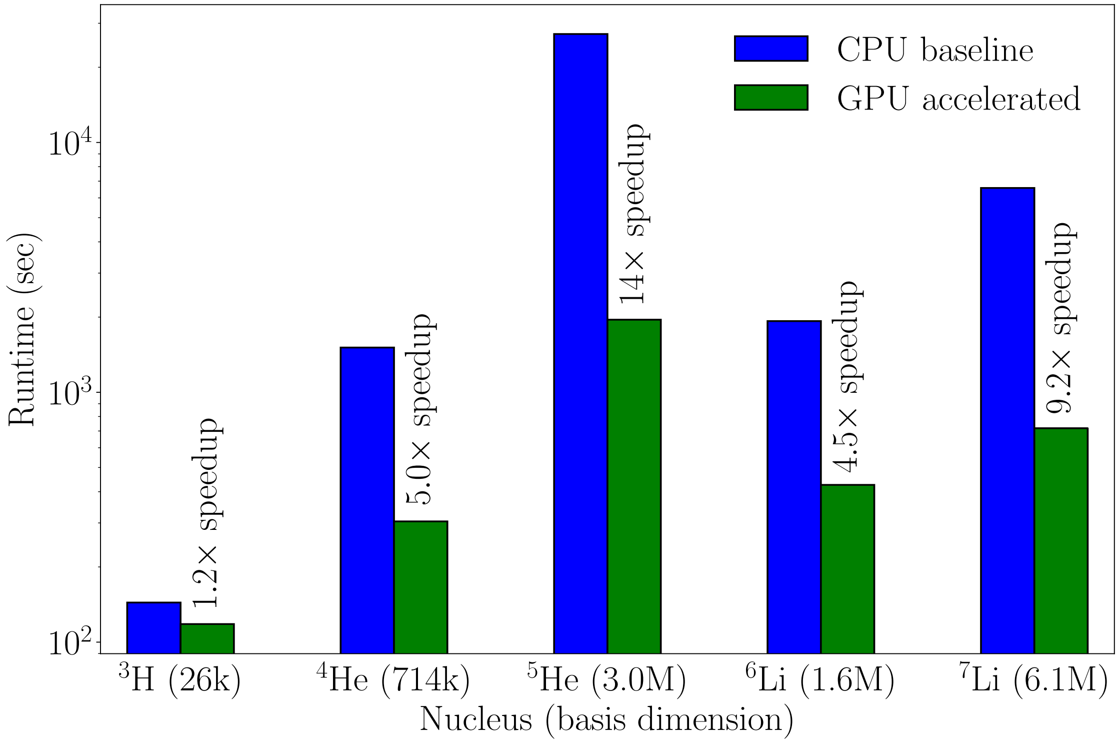
Three-Nucleon forces make calculations order-of-magnitude more expensive.

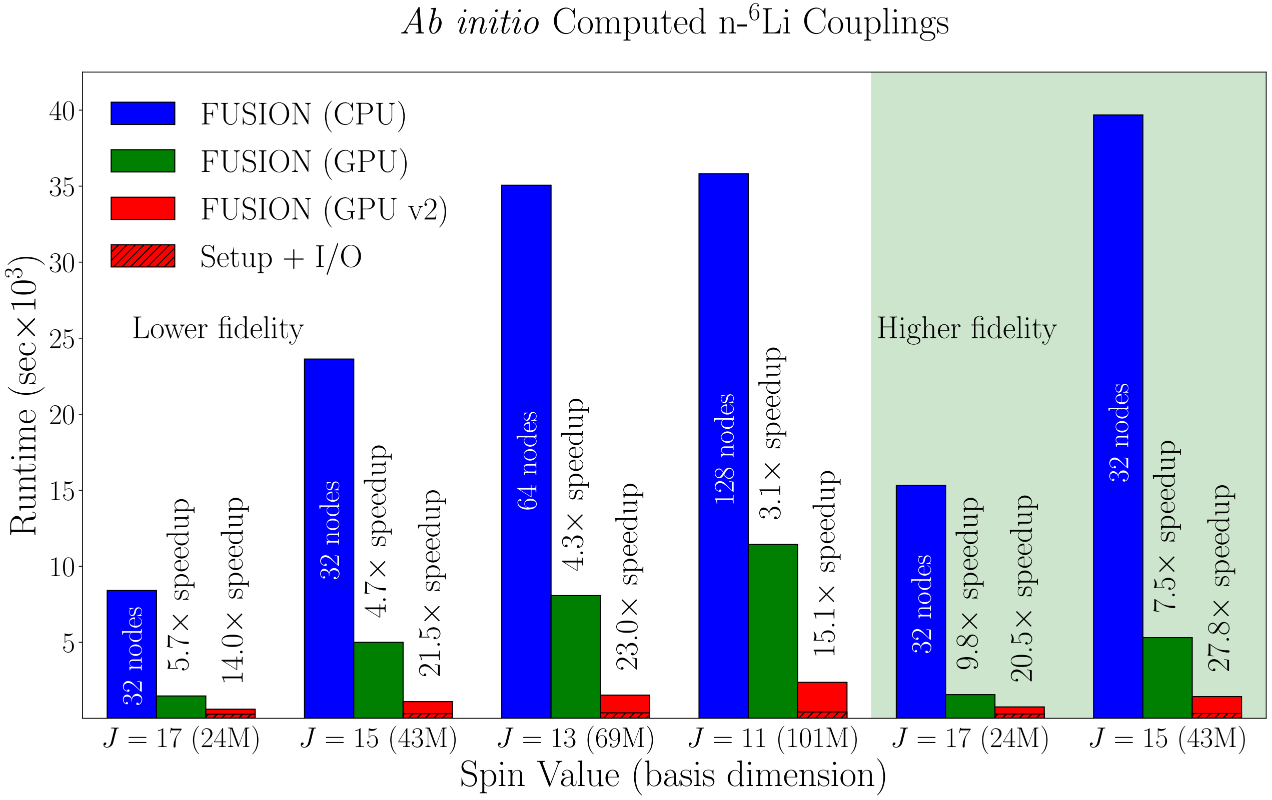
In the past few years there has been a revolution in HPC architectures with the introduction of general-purpose GPUs



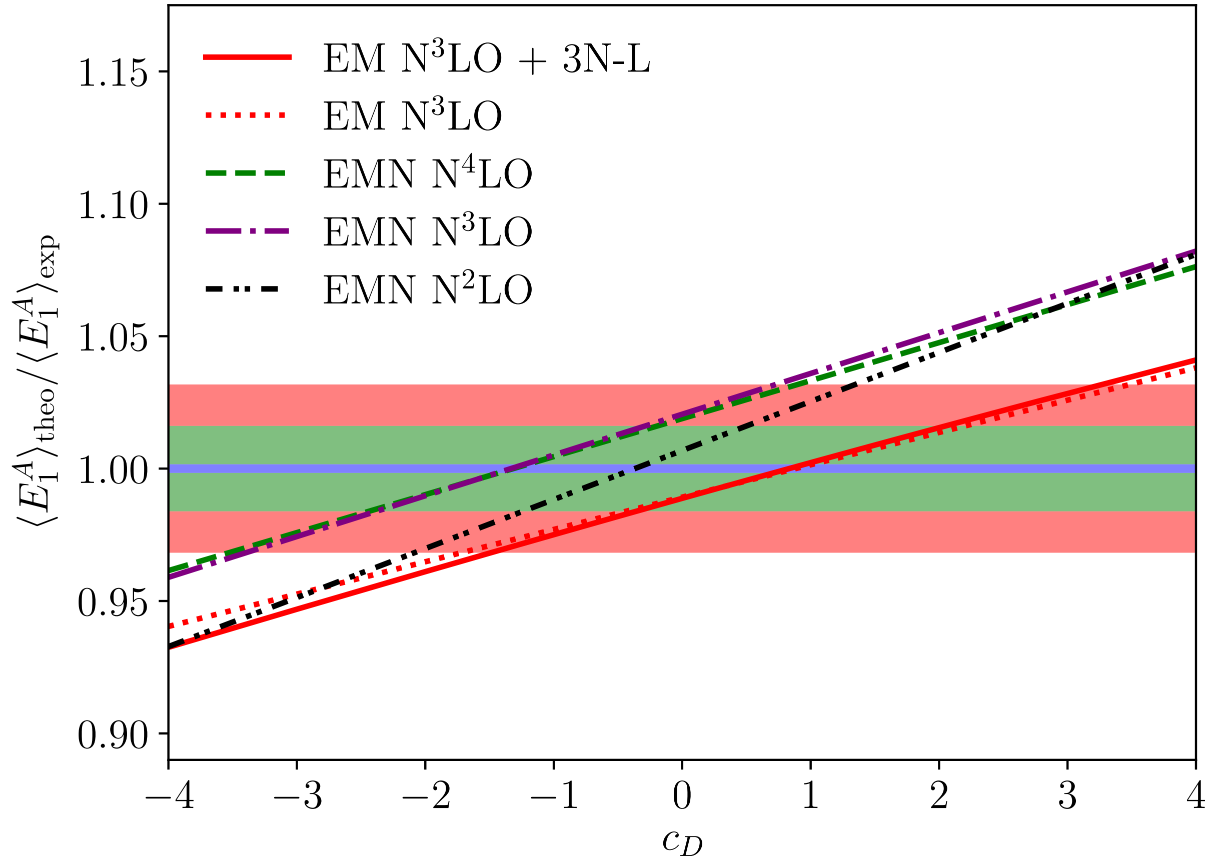
The majority of available compute power is now offloaded

High-Performance Computing is essential for ab initio theory. Novel architectures allow for previously impossible calculations.

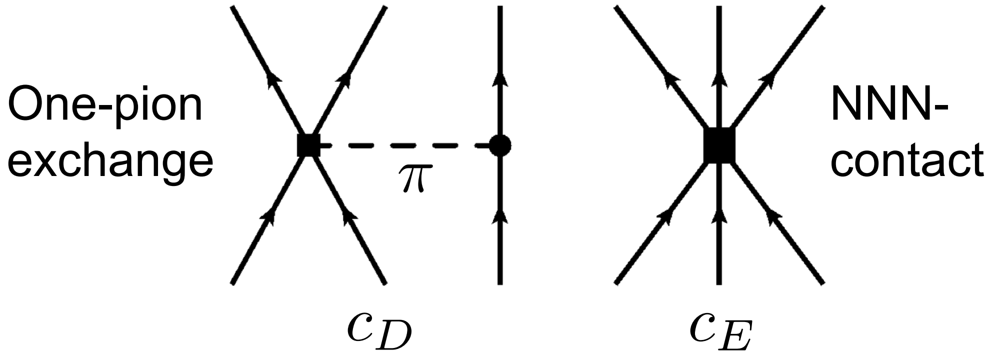


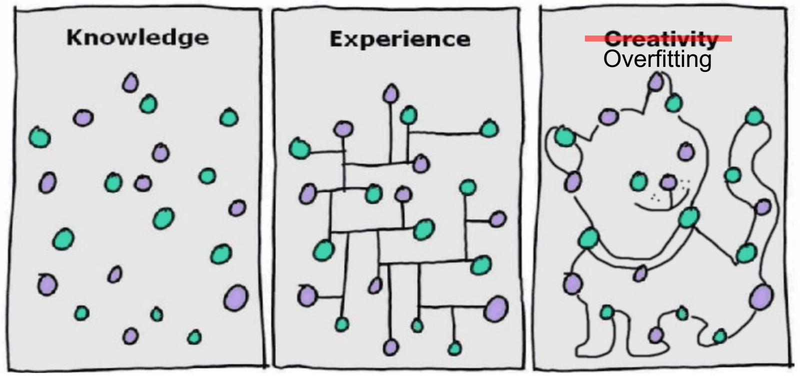


Determining low-energy constants from three-body observables



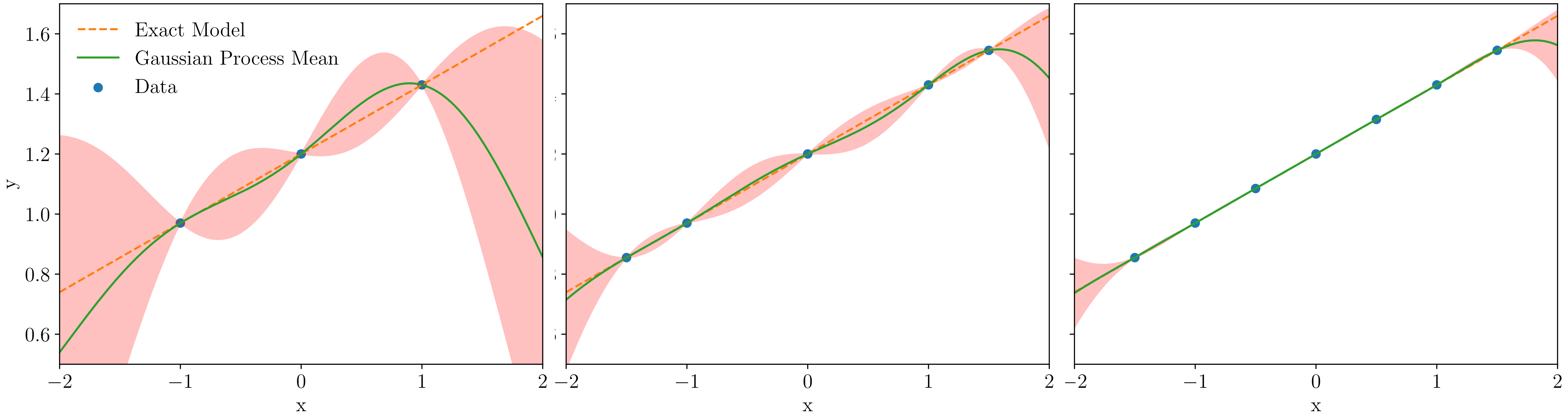
Entem & Machleidt, Phys. Rev. C **68**, 041001(R)
Entem, Machleidt & Nosyk Phys. Rev. C 96, 024004 (2017)





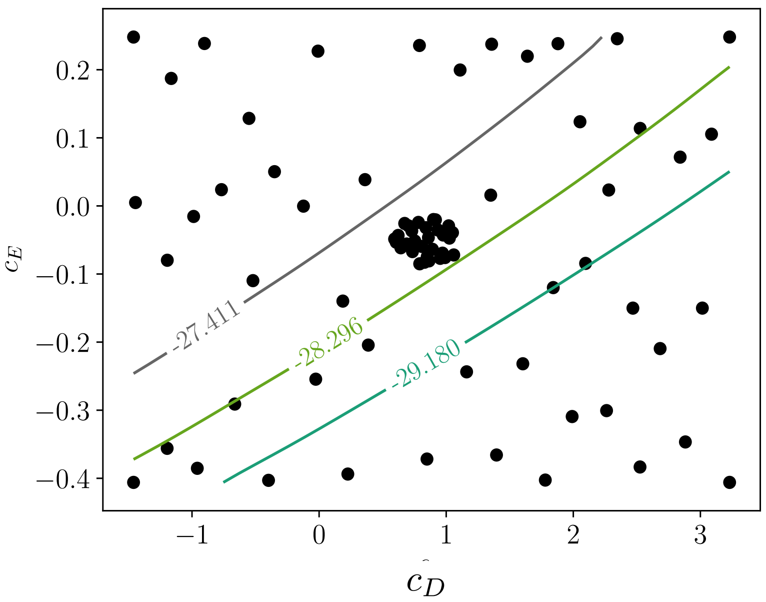
$$\chi^2 = \sum \frac{\left(O^{th} - O^{exp}\right)^2}{\sigma^2_{\rm exp} + \sigma^2_{\rm th}}$$

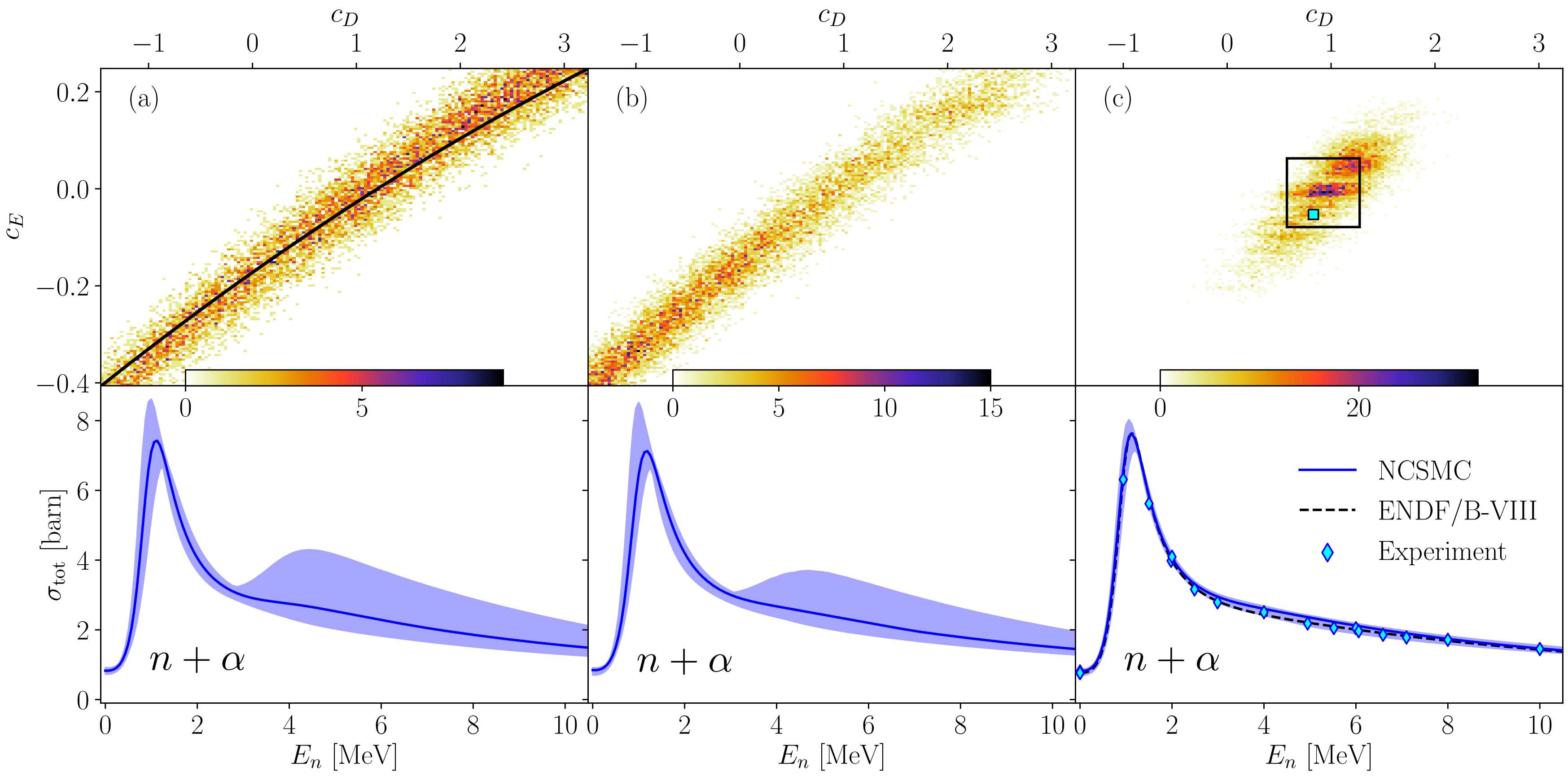
Gaussian Processes can act as systematically improvable emulators for expensive calculations



Each calculation could take hours to complete. Since the emulator's uncertainty is known, we know where to sample next.

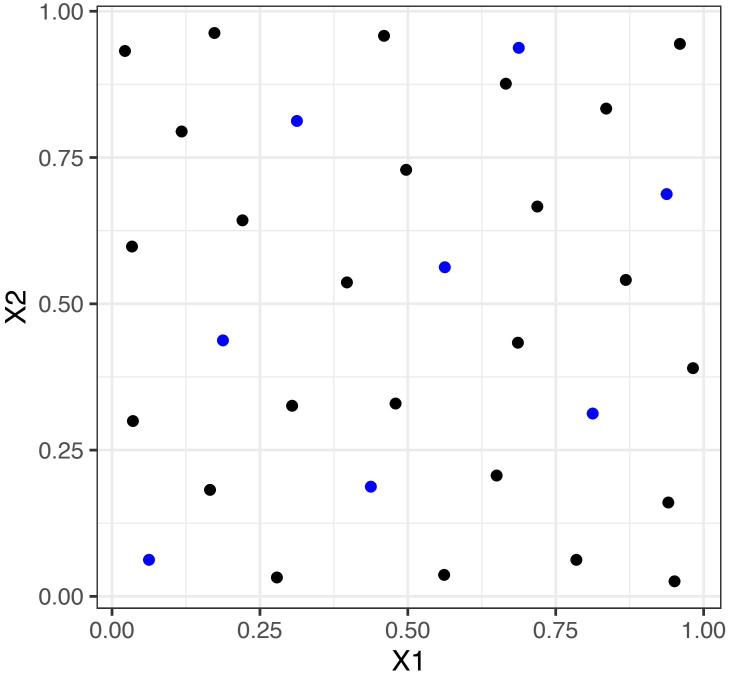
Significant speedups coupled with efficient emulators make uncertainty quantification of theoretical predictions possible.

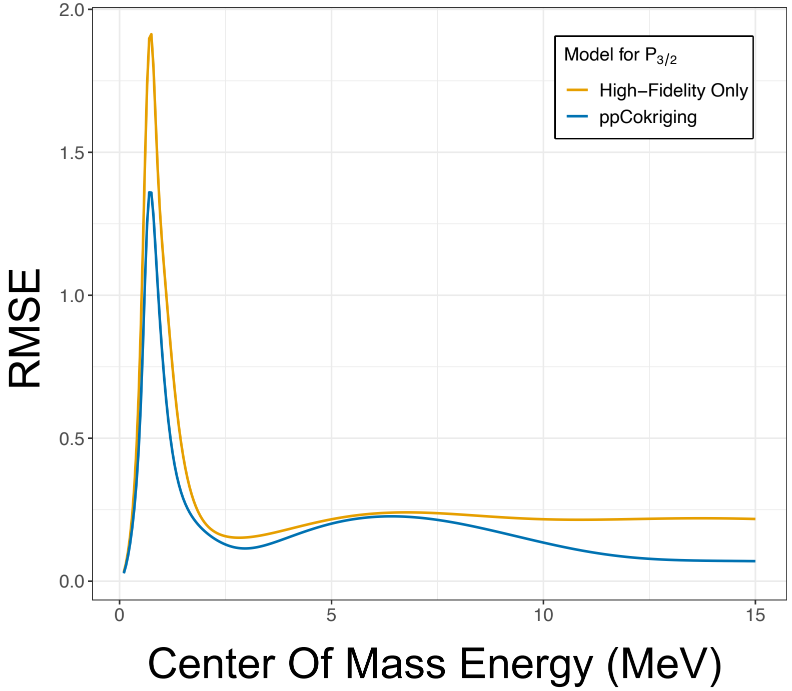


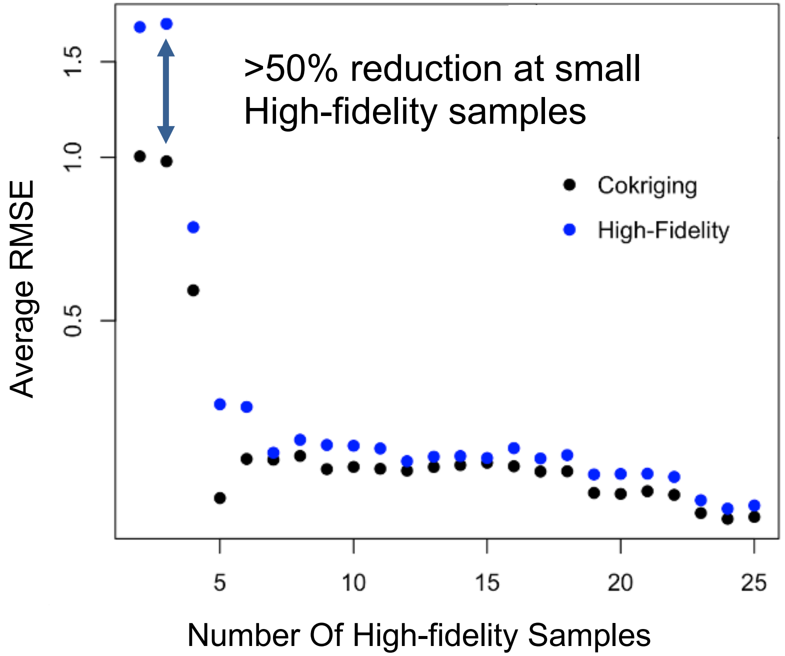


Phys. Rev. C **102**, 024616 (2020)

Mixed-fidelity modeling can be used for computationally expensive reactions.







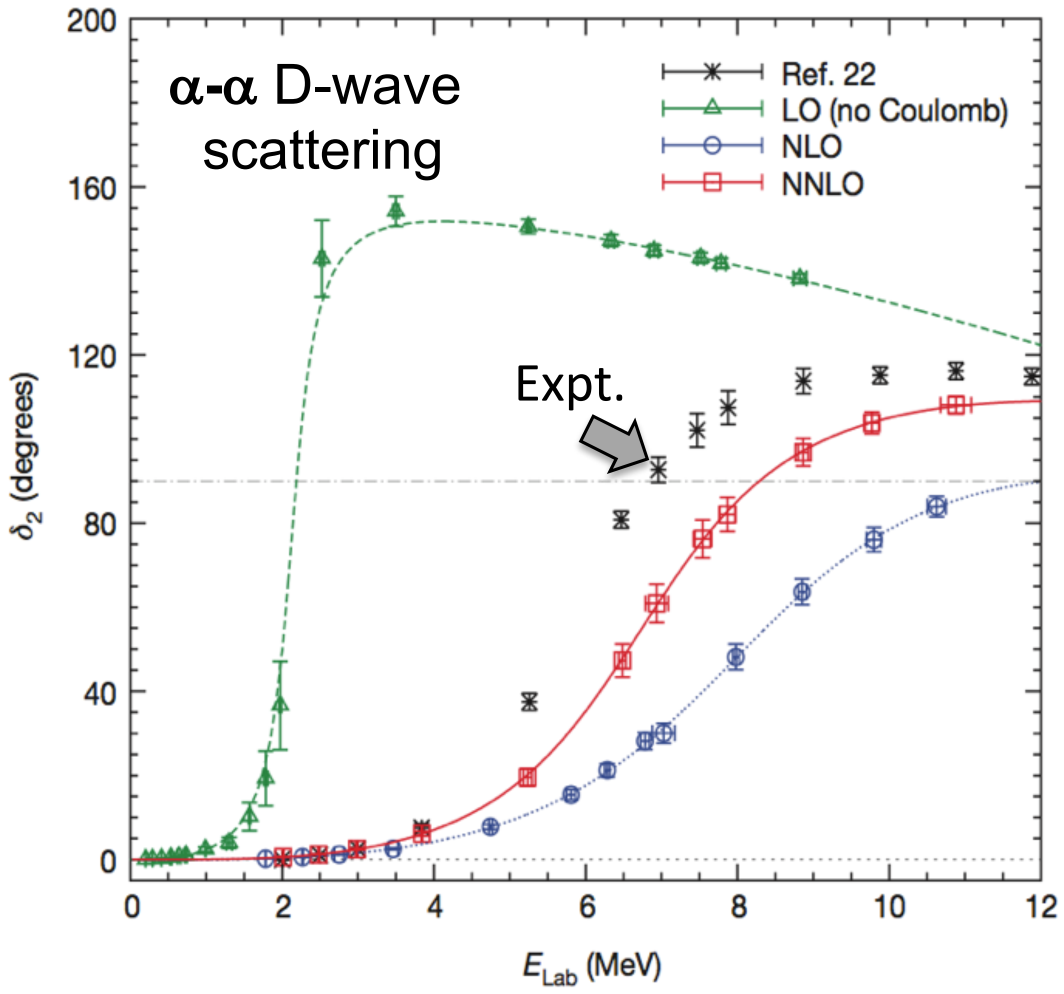
In close collaboration with Kevin Quinlan (LLNL)

Can ab initio theory treat He burning reactions?

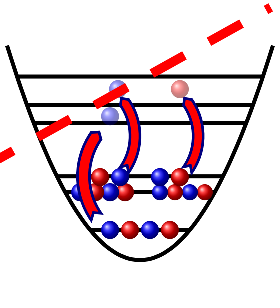
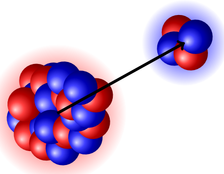
Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111

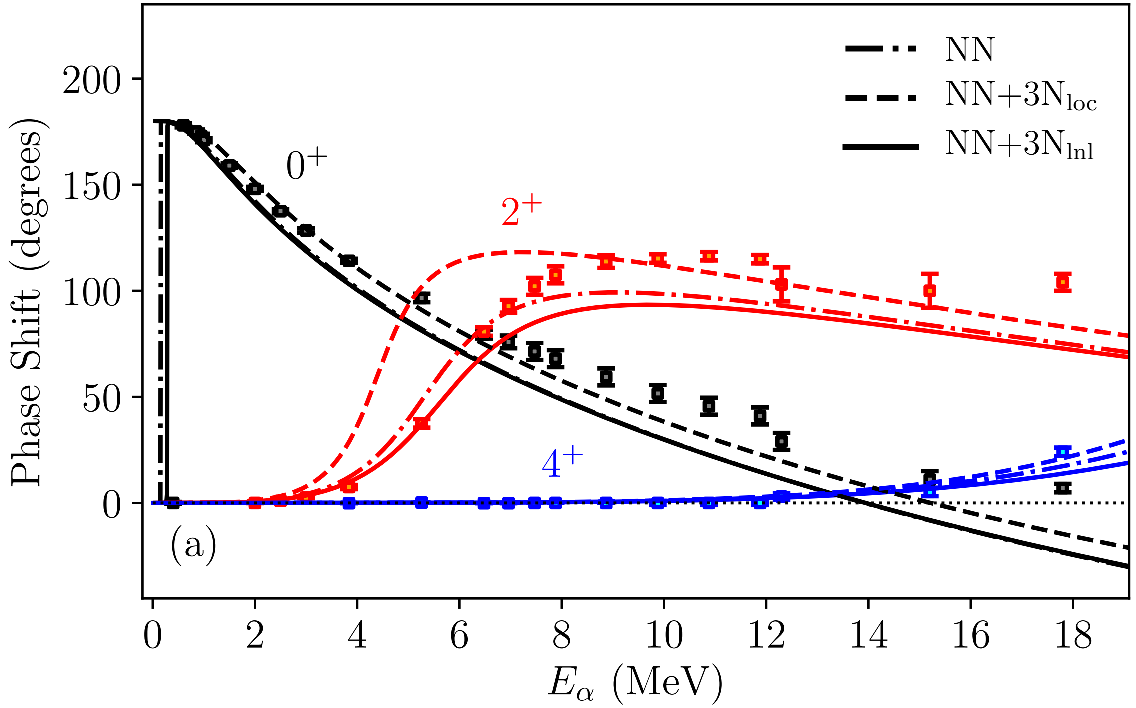
Nuclear Lattice EFT with the Adiabatic Projection Method

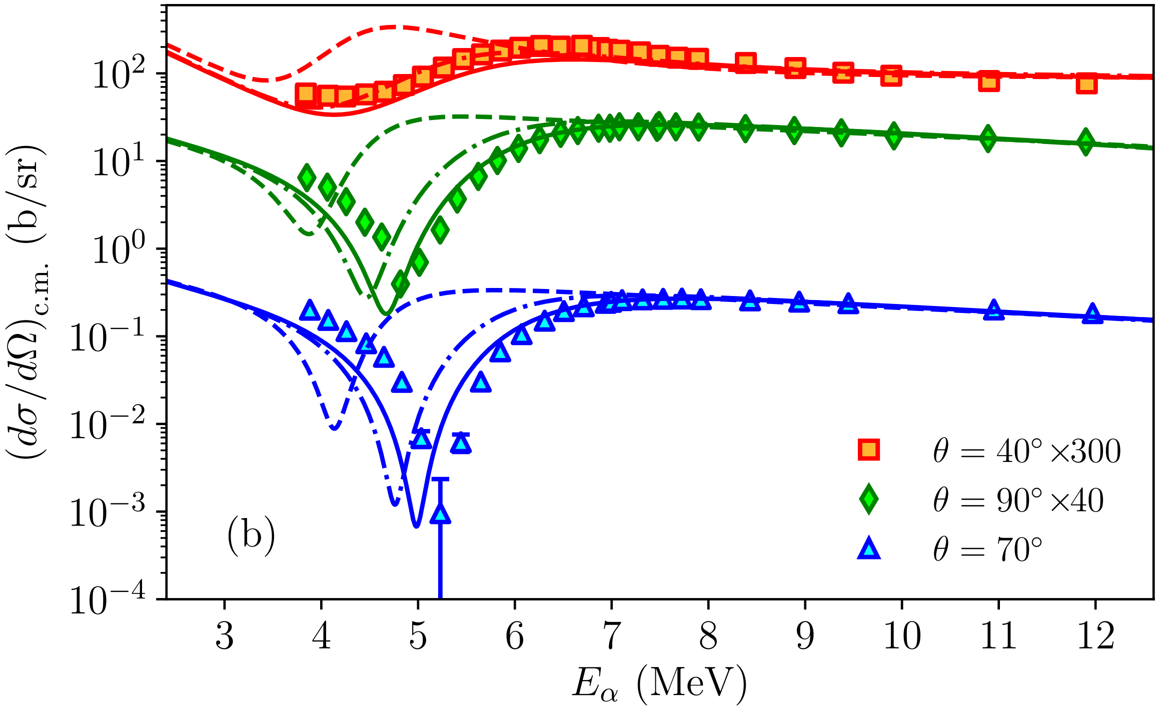
- Promising results for ^{4}He+^{4}He scattering
- Favorable computational scaling (~A^2)
- ^{4}He+^{12}C fusion becoming possible!
- Extensions to enable treatment of three-cluster dynamics required before the method can be applied to the triple-^{4}He fusion process



Current status for α-α scattering

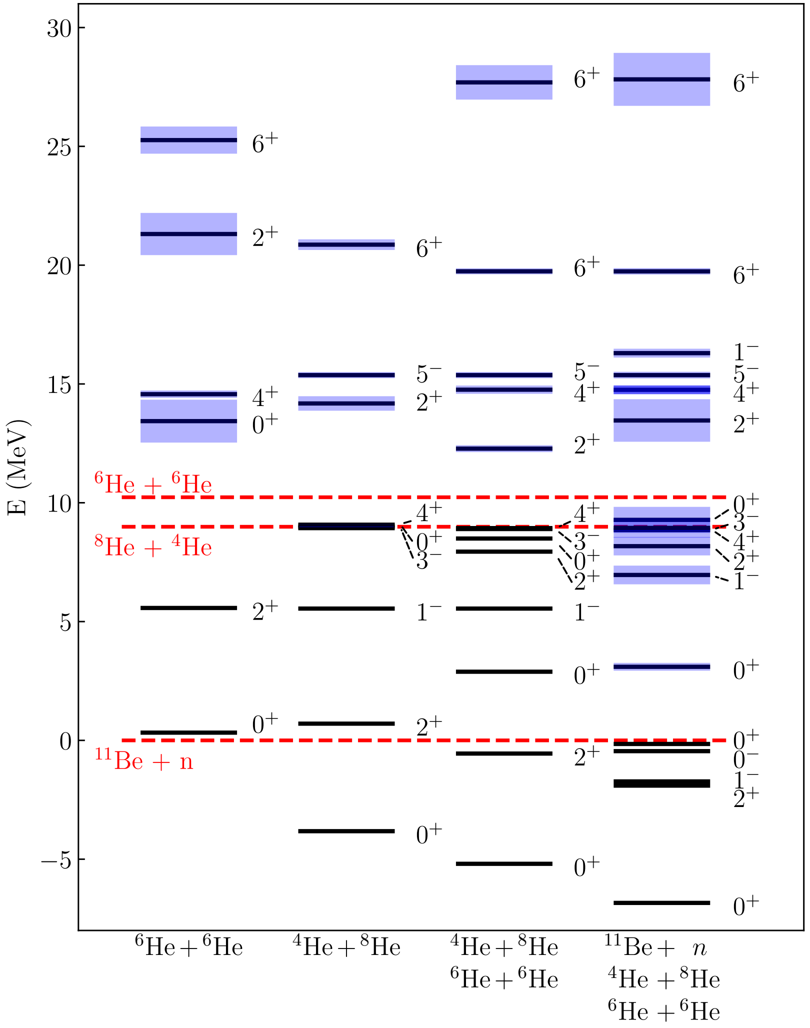
$$\Psi = \sum_{\lambda} c_{\lambda} \Big|$$  $$\Big\rangle + \sum_{\nu} \int dr\, u_{\nu}(r) \Big|$$  $$\Big\rangle$$

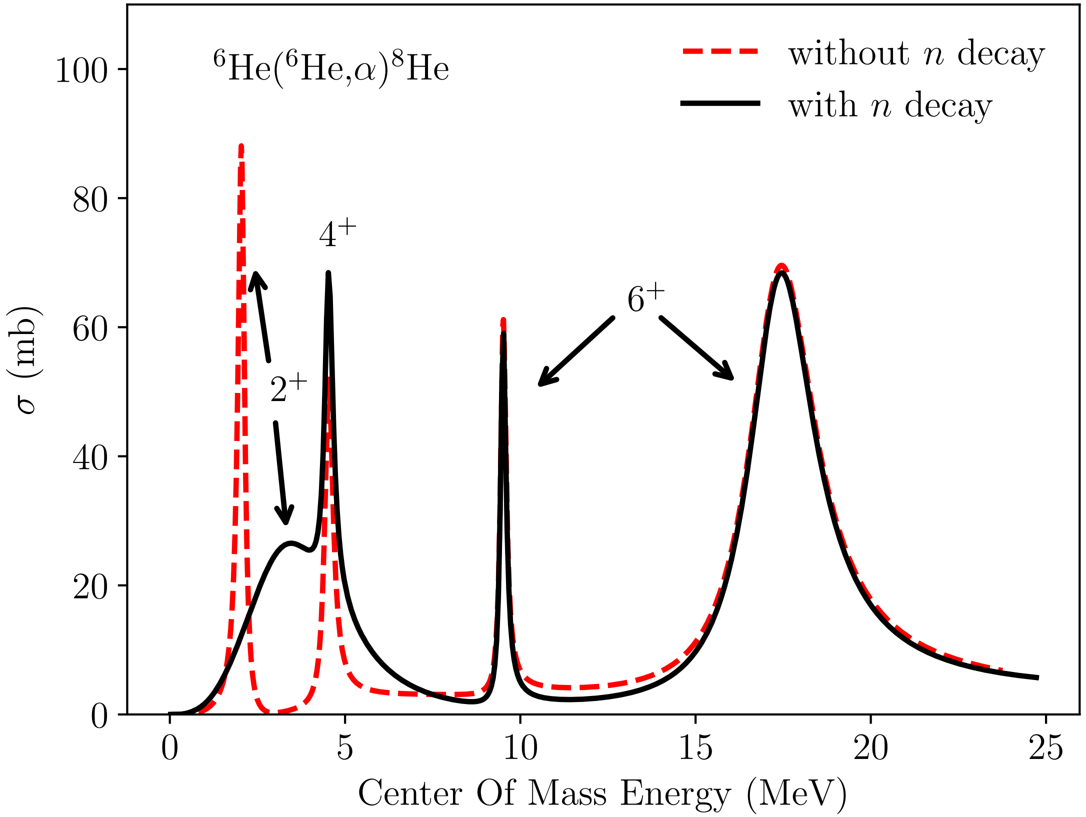




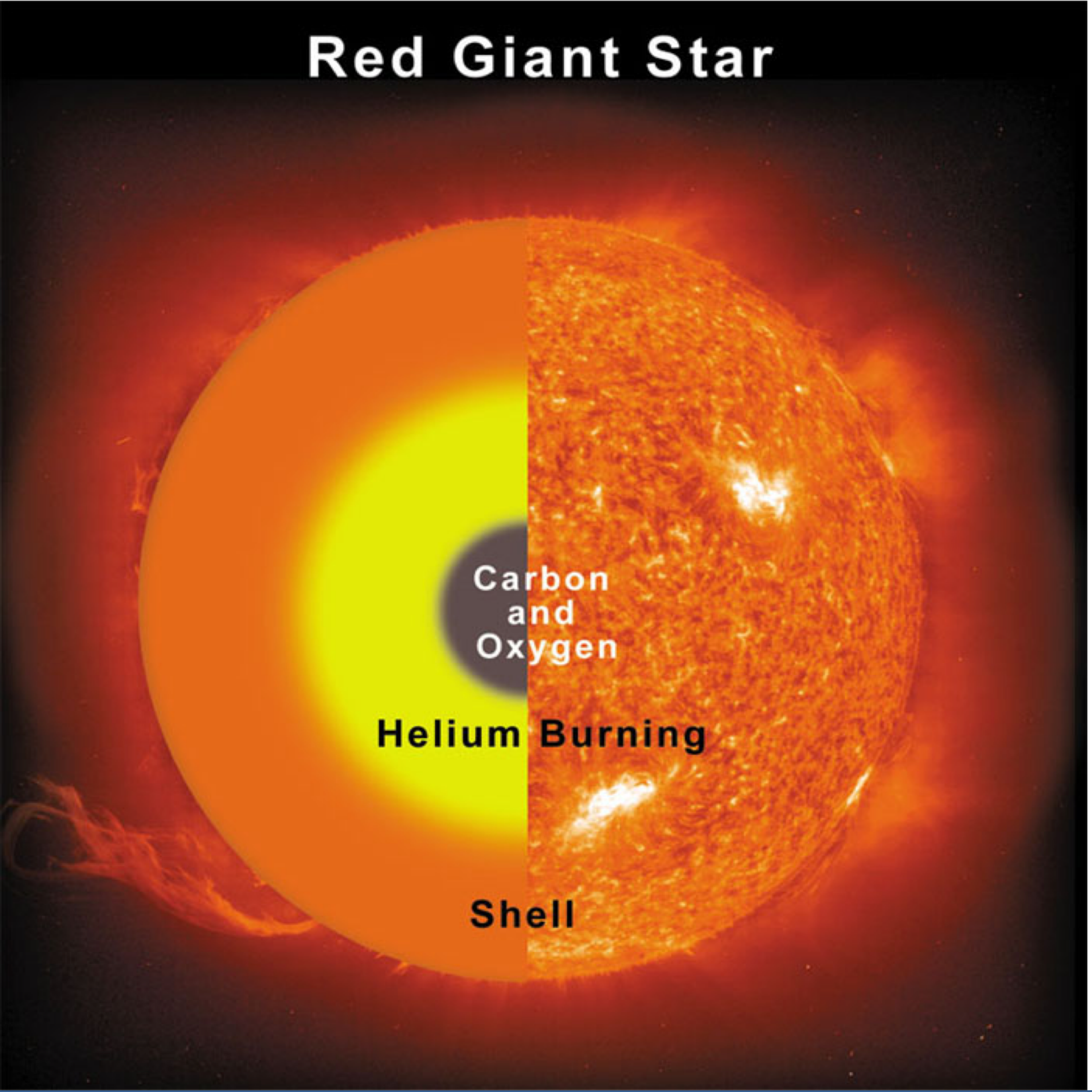
arxiv:2012.00228

Clustering and reactions with p-shell projectiles

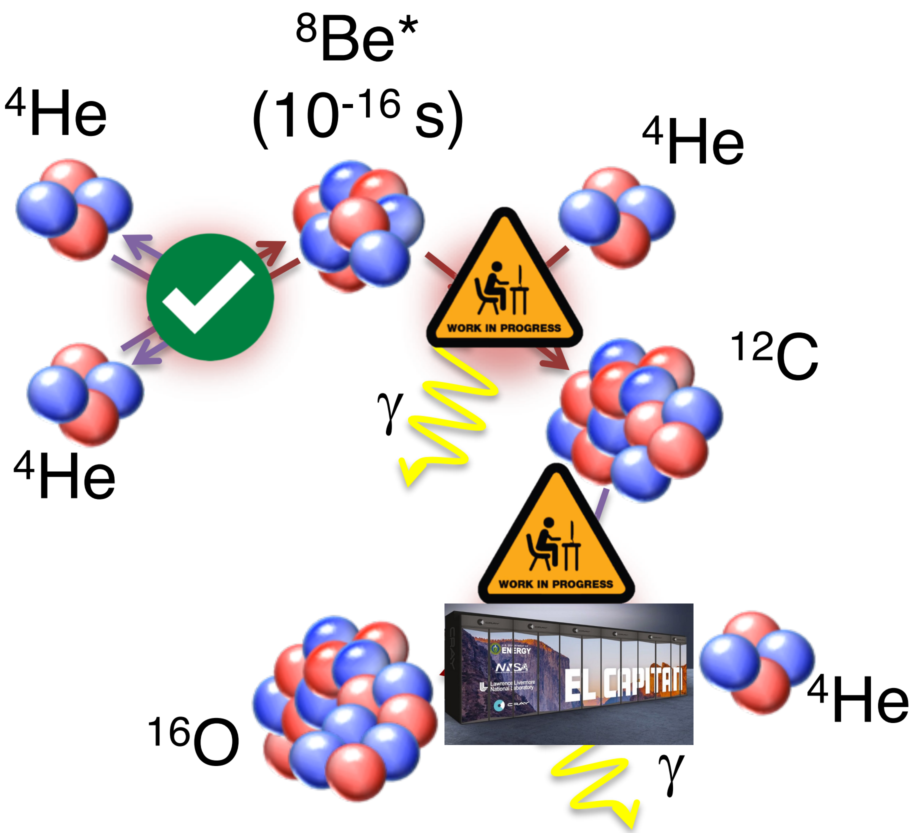




arxiv:2012.00228

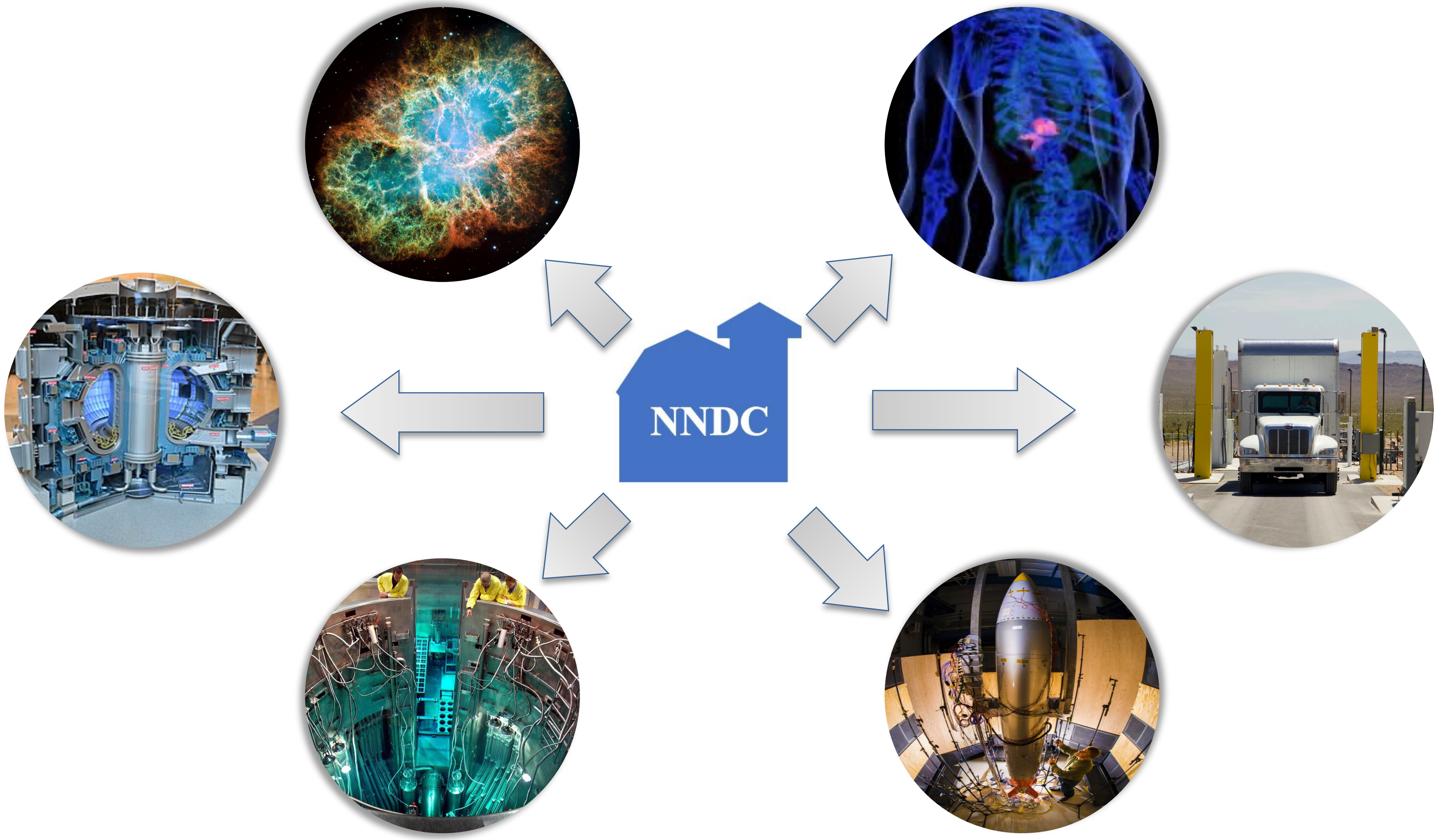


Reaction rates of solar cross sections determine element abundancies in the universe

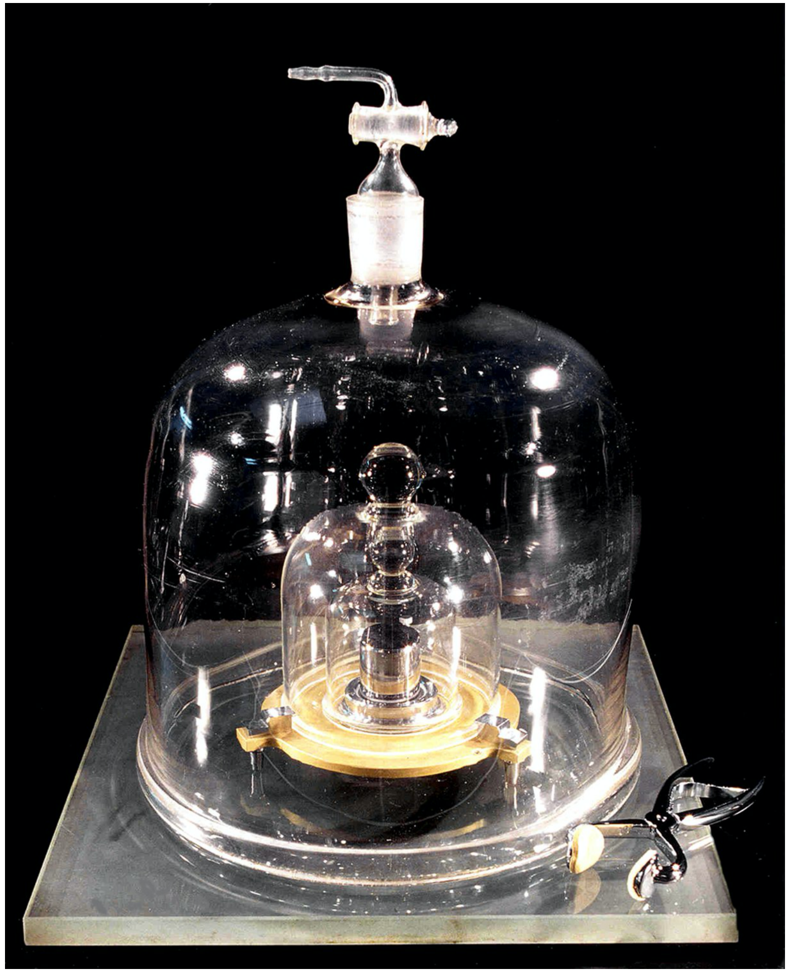


"Not only important for the development of the chemical building blocks of life but also for the entire scheme and sequence of nucleosynthesis events as we imagine them now." (2015 LRP)

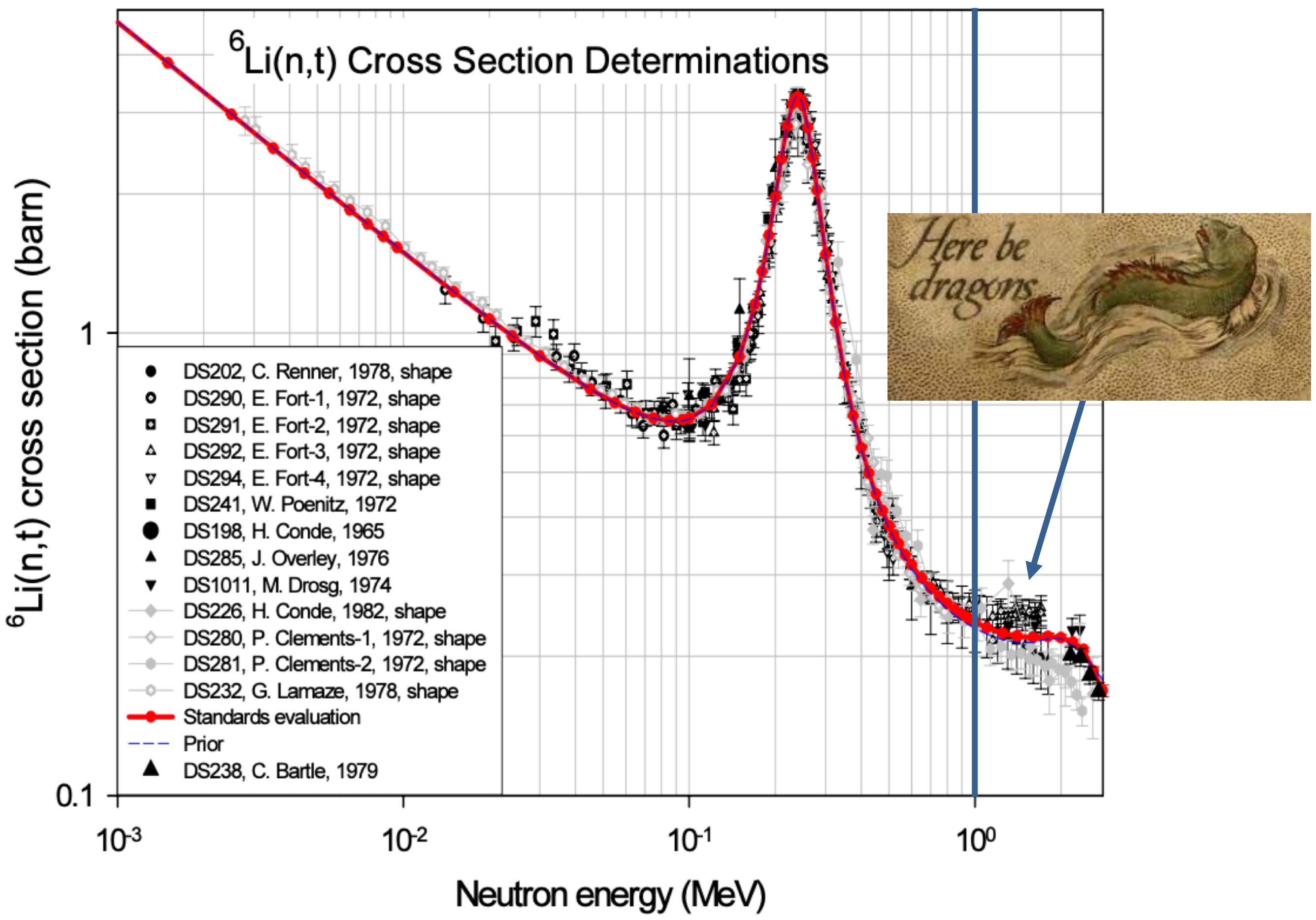
Nuclear data is ubiquitous in basic science and applications



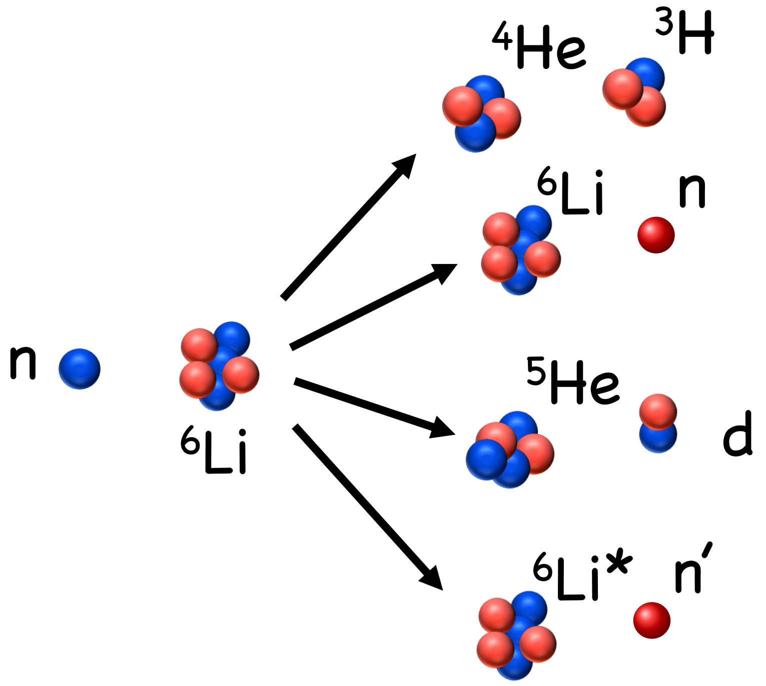
Neutron cross section standards are *working* standards. They are continually assessed, updated and improved.

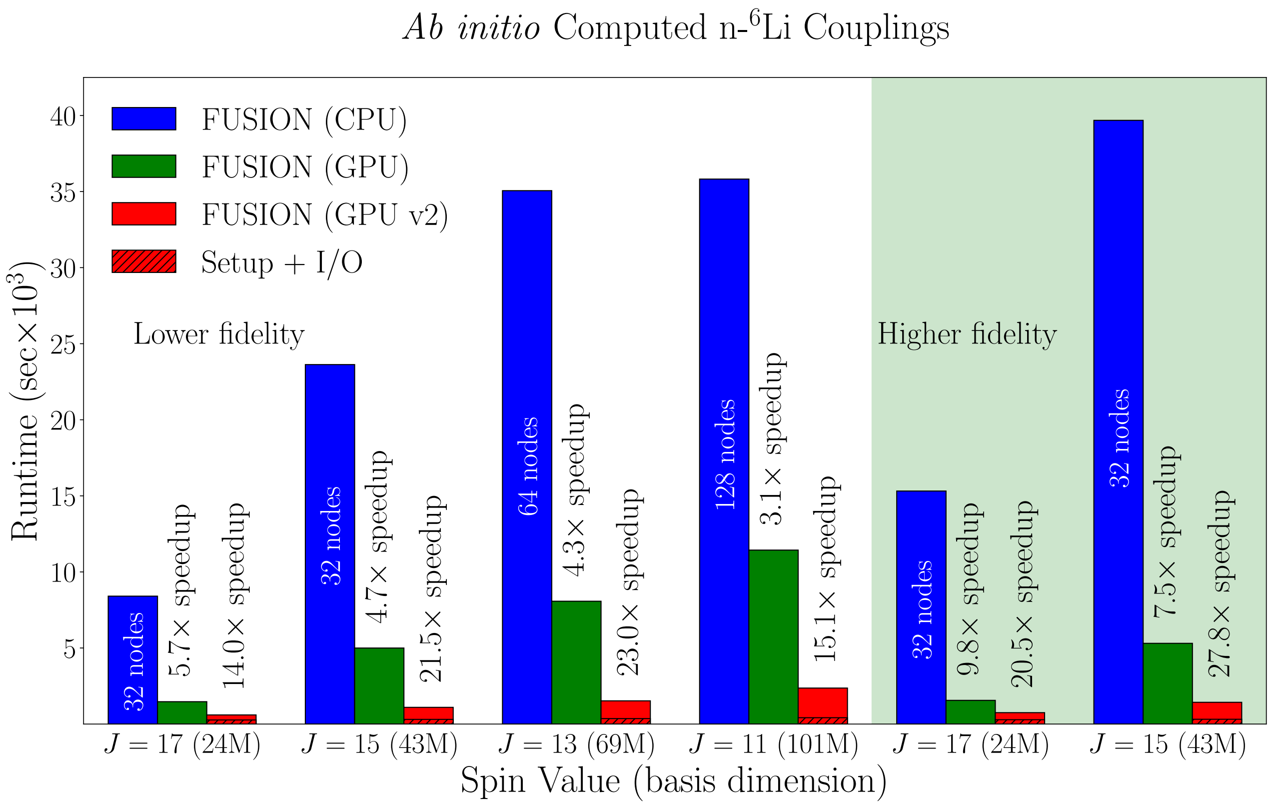


Carlson et al. Nuclear Data Sheets 110 (2009) 3215–3324



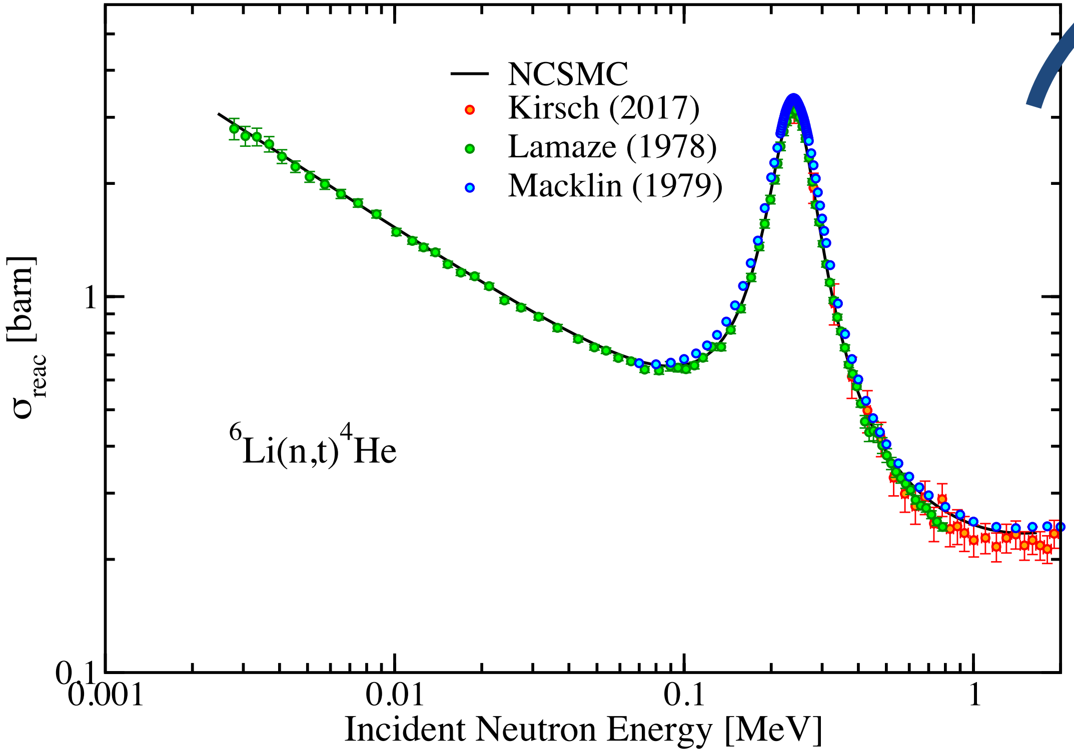
Going further: reactions with multiple open channels



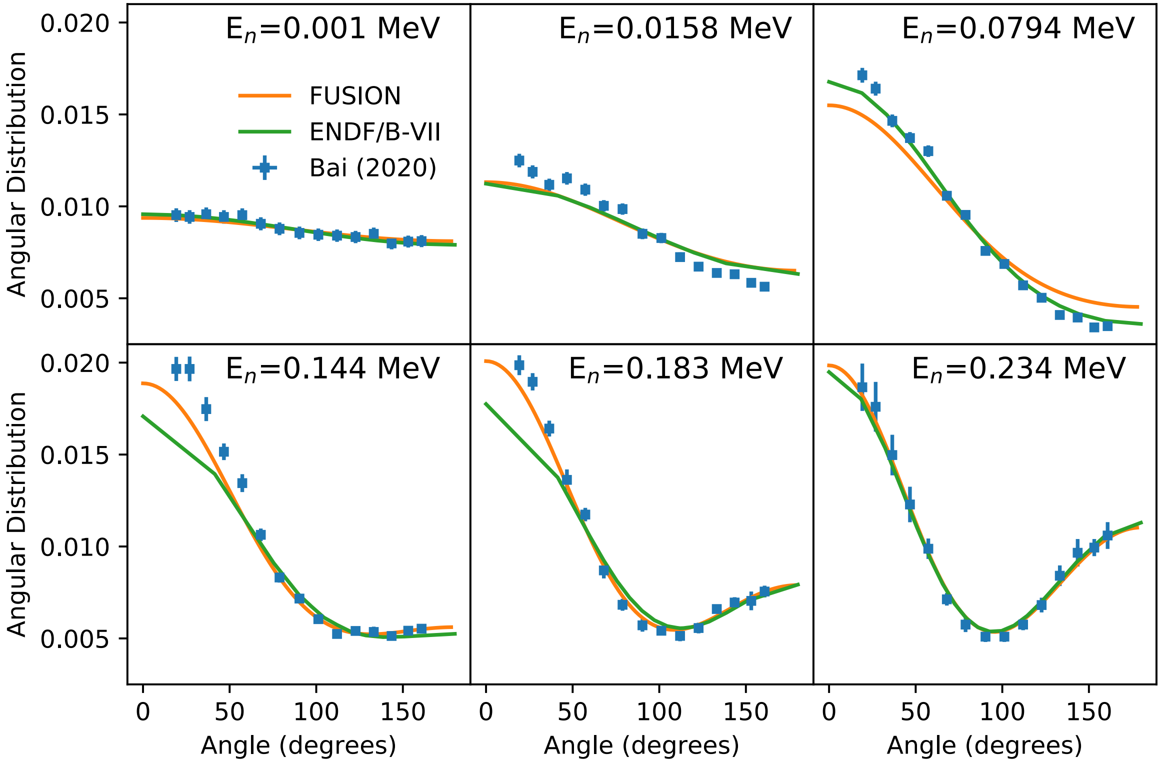


Ab initio nuclear reaction theory can provide an independent method for predicting standards cross sections

NCSMC parameters tuned to reproduce reaction cross section



Angular distributions are predicted with no further experimental input



Conclusions and prospects

- We have made first steps in dealing with α-clustering and α-induced reactions in an ab initio reaction theory setting.
- Reactions with p-shell nuclei as projectiles are becoming possible (α-transfer via ^{6}Li(X,d)Y 🙂)
- Theory predictions without some sense of the uncertainties involved are of limited use when it comes to comparing with precise experimental data.

Thanks to collaborators:
S. Quaglioni, P. Navratil, K. Quinlan, G. Hupin