Towards α-clustering and α-induced reactions within the no-core shell model with continuum

Kostas Kravvaris, Sofia Quaglioni, Kevin Quinlan, Kyle Wendt, Petr Navratil

LLNL-PRES-806181

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

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Nuclear Clustering is found throughout the mass chart.

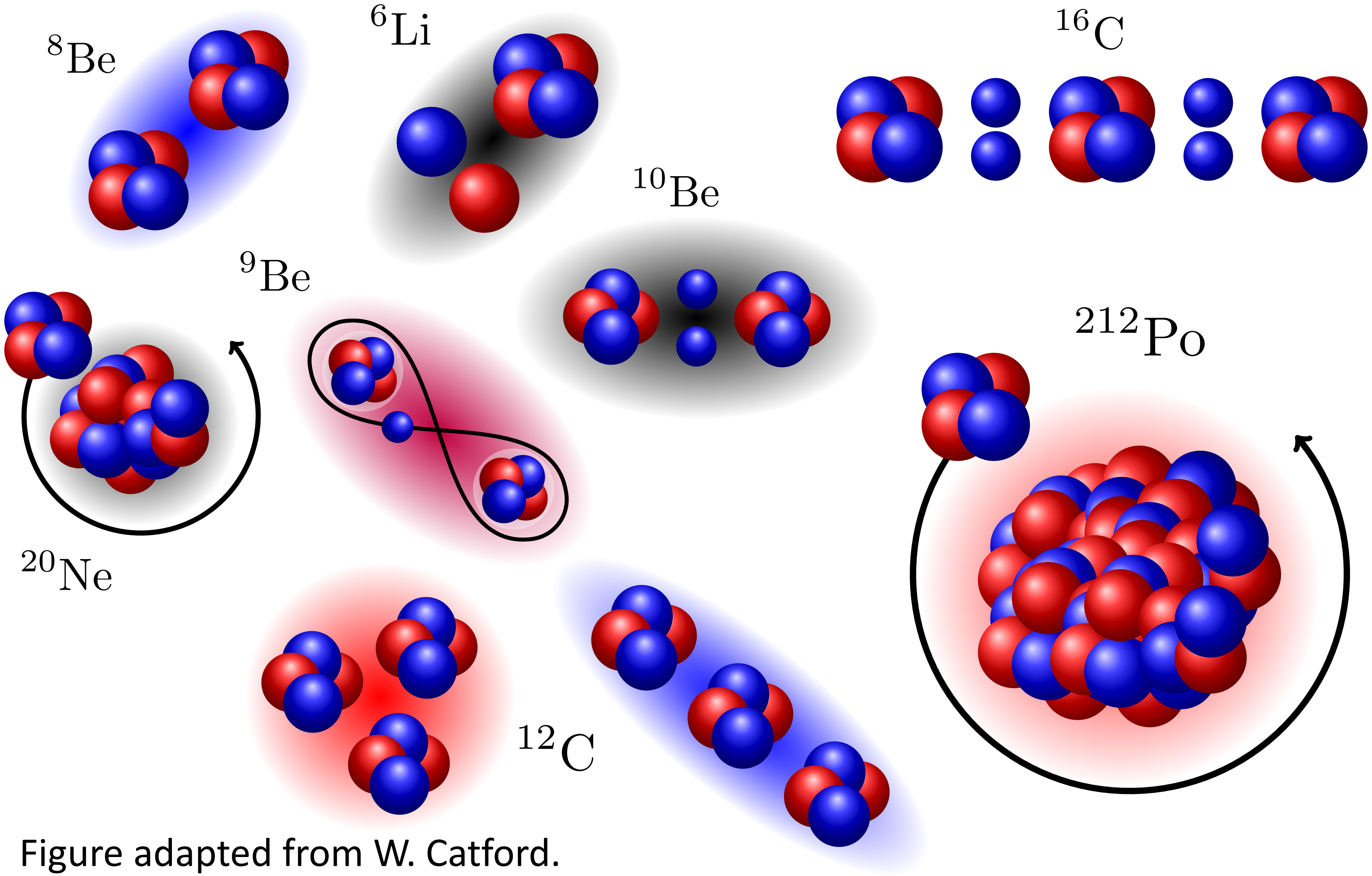
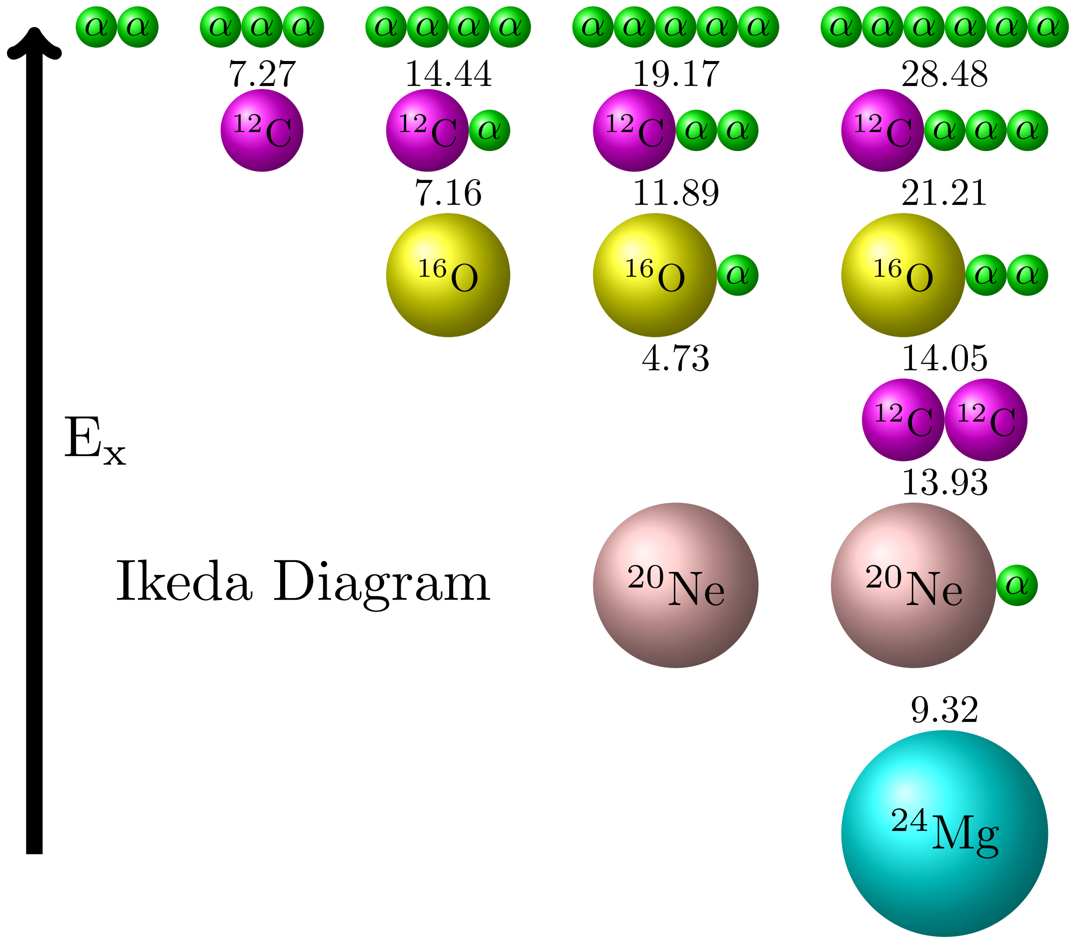
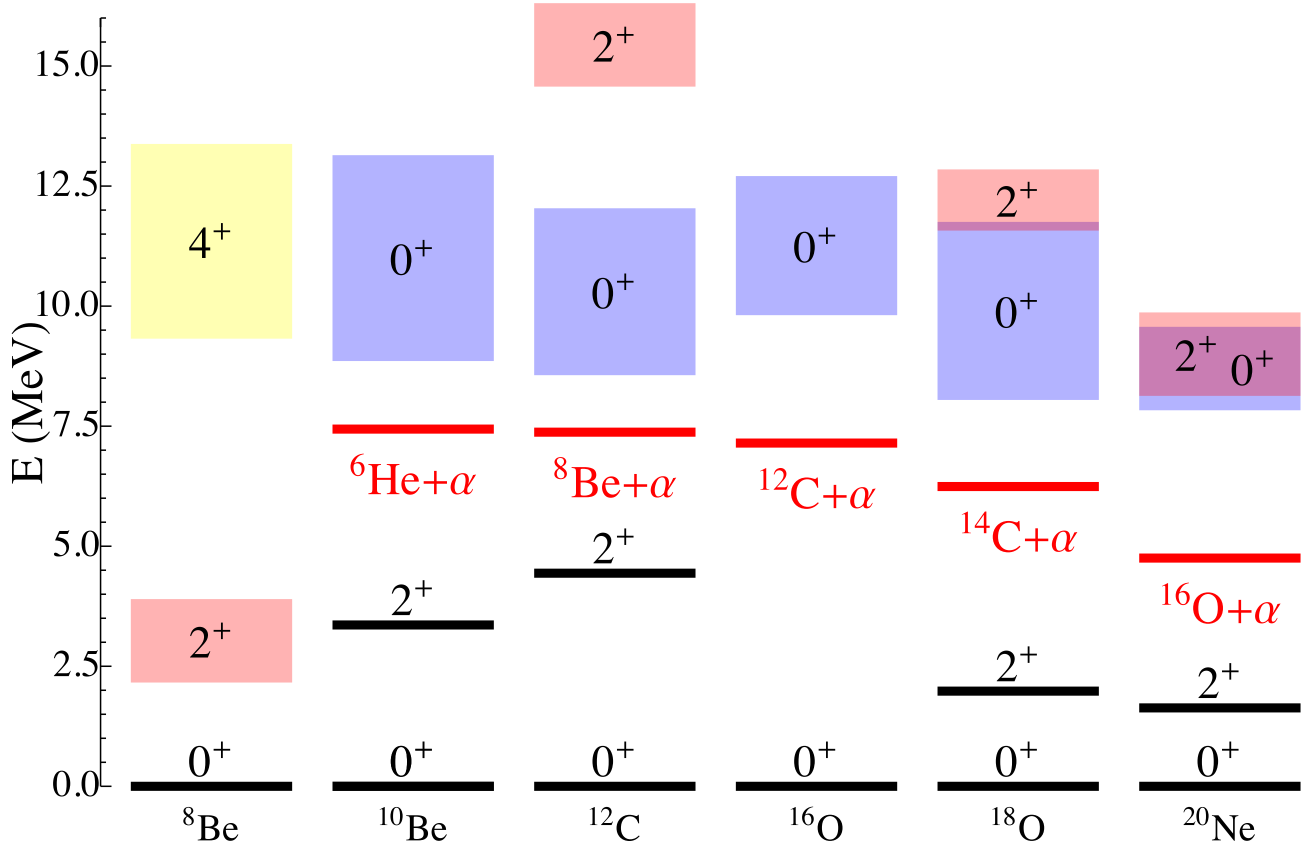


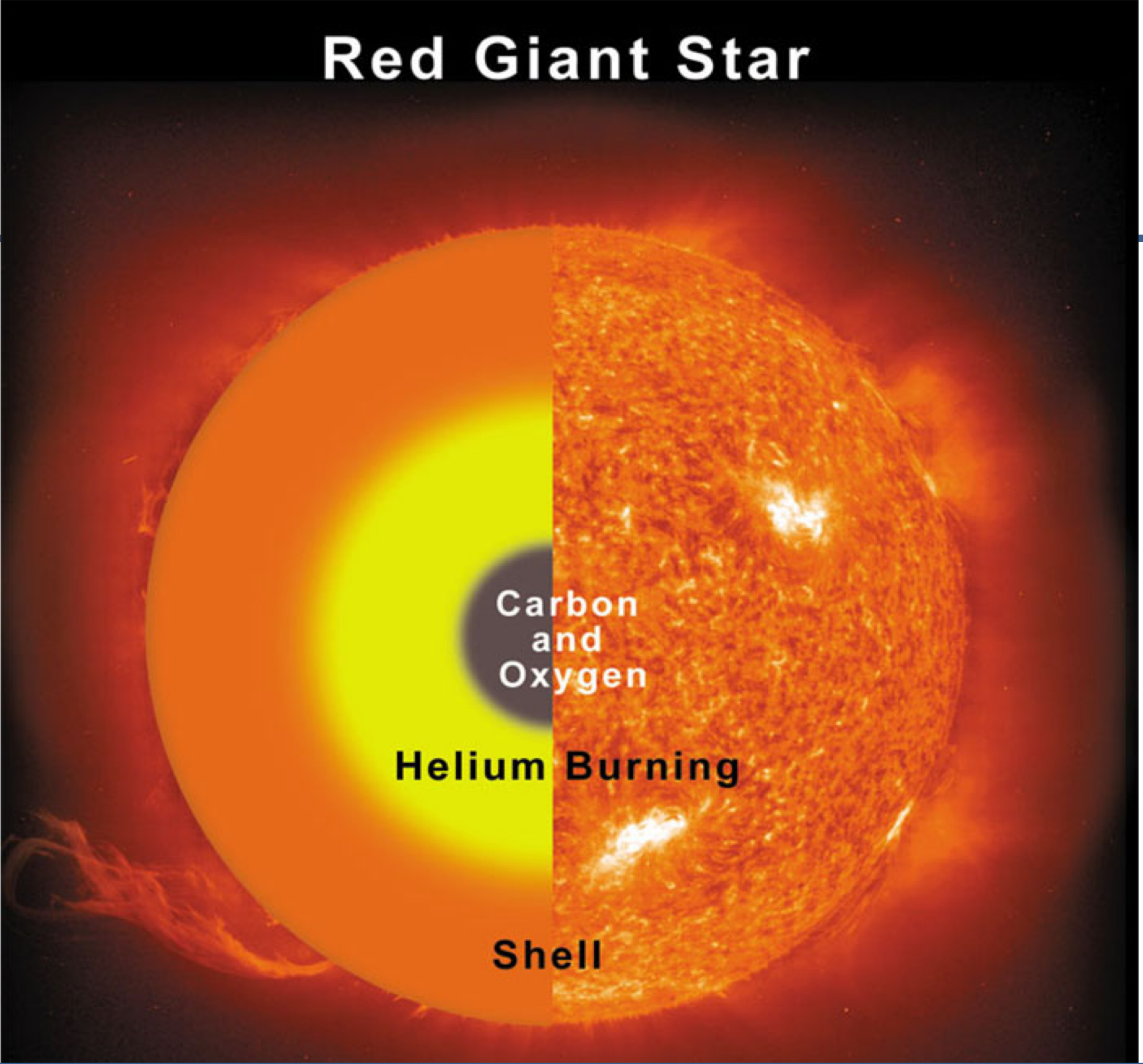
Figure adapted from W. Catford.

- Emergent phenomenon where substructures are formed within a nucleus.
- Appears throughout the mass chart but is most prevalent in light nuclei.
- Alpha particles play a major role due to large binding energy.

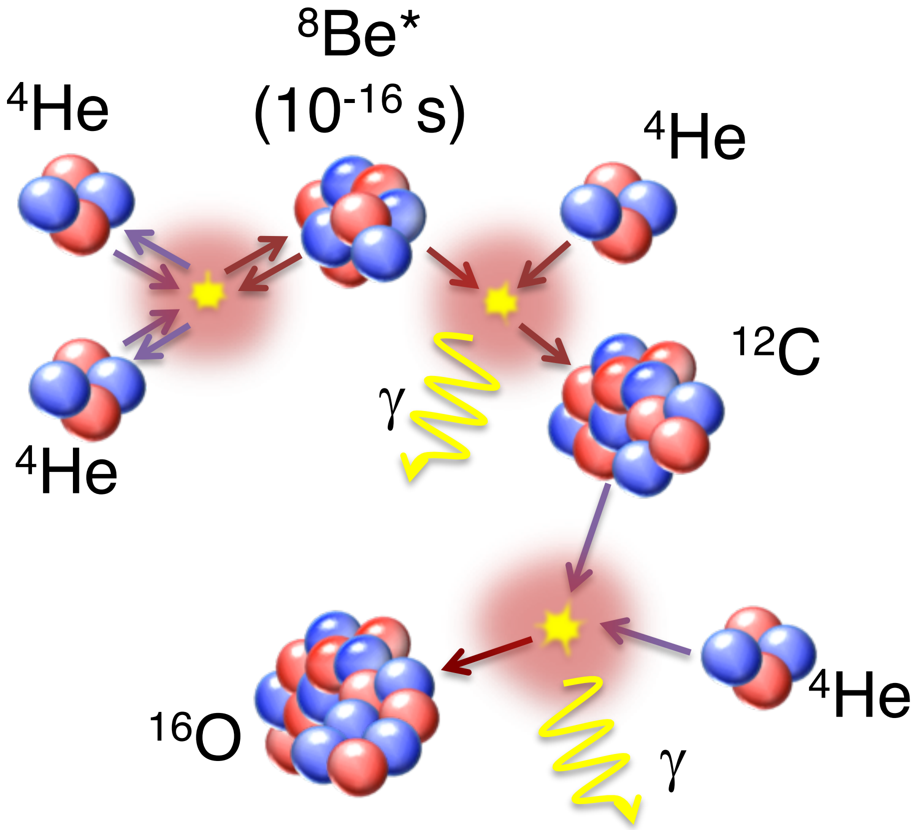
Cluster states throughout the energy spectrum.







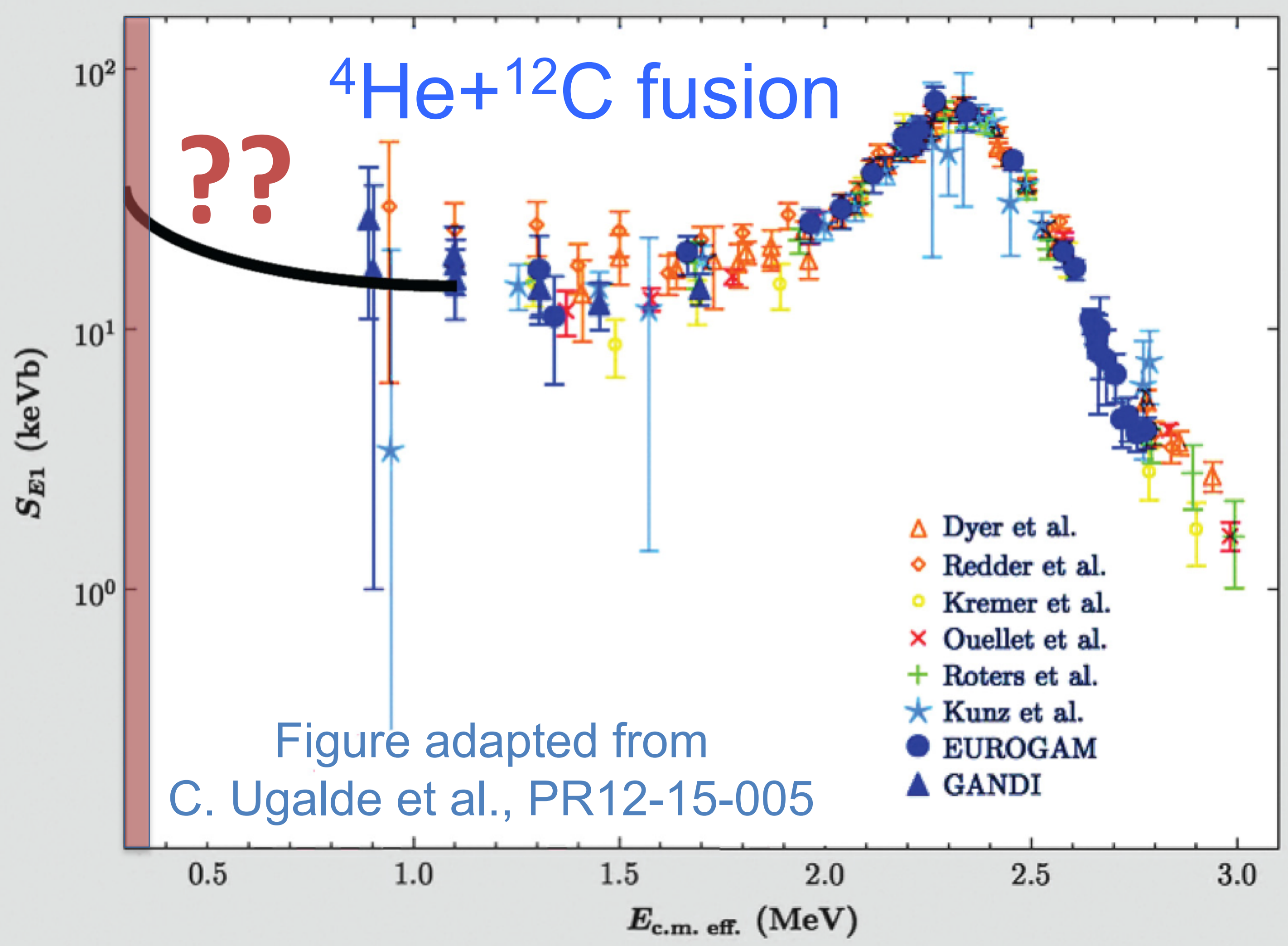
Cluster states strongly influence reaction rates



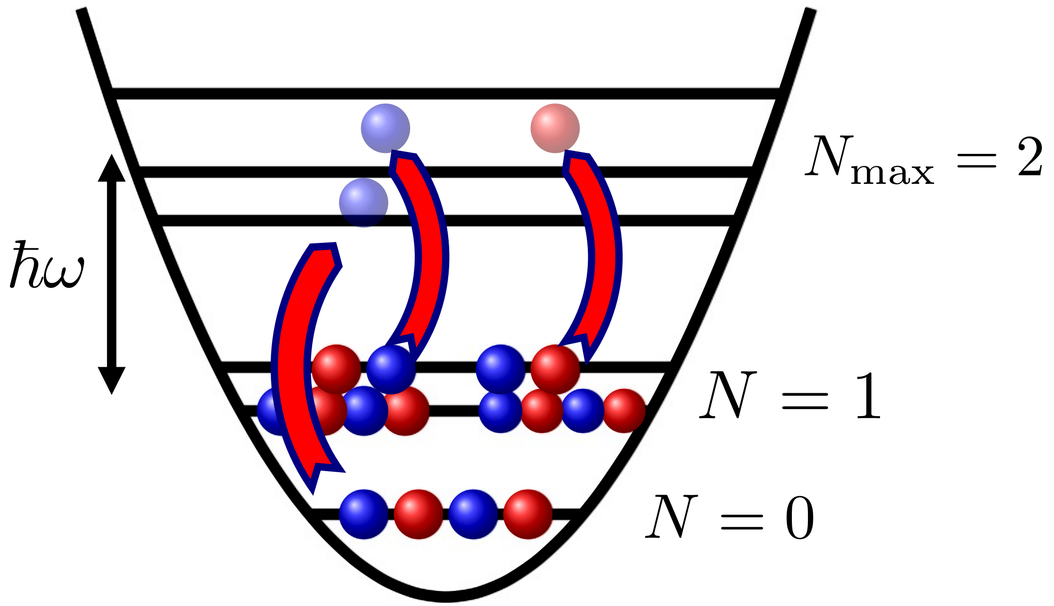
"Not only important for the development of the chemical building blocks of life but also for the entire scheme and sequence of nucleosynthesis events as we imagine them now." (2015 LRP)

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

- Direct measurements at 300 keV (helium burning conditions) so far impossible
- Major hurdle in precisely determining carbon-to-oxygen ratio produced in stars, introduces large uncertainties in stellar-evolution models and in the predictions of stellar nucleosynthesis



For a complete ab initio description we need both structure…

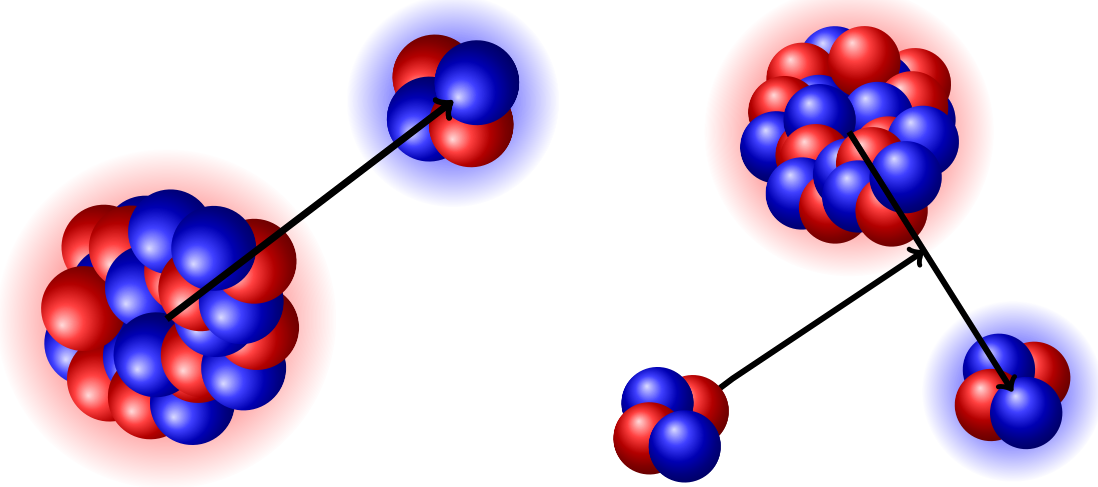


Configuration Interaction
No Core Shell Model (NCSM)

- 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

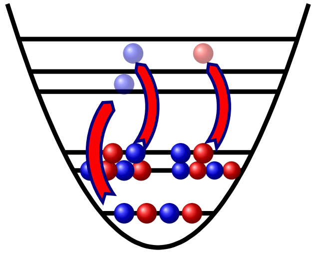
- The CI picture is no longer sufficient to describe the many-body system.
- We need to expand the basis with collective excitations targeting the cluster effects.



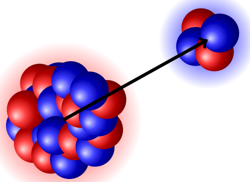
Discrete structure information input

Continuous dynamical input (clustering/reactions)

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



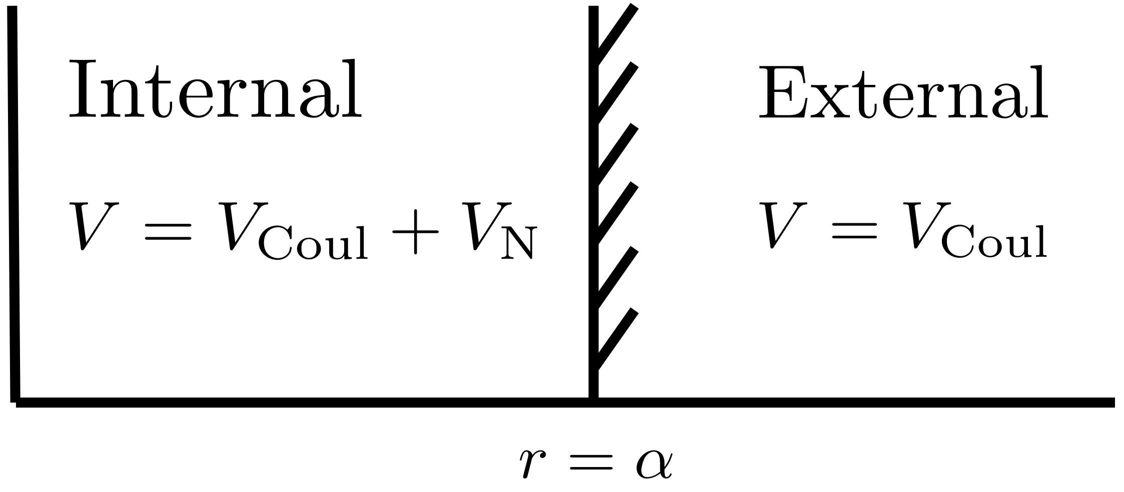
$$\rangle + \sum_{\nu} \int dr u_{\nu}(r) |$$



$$\rangle$$

Solving for the unknowns with the R-Matrix.

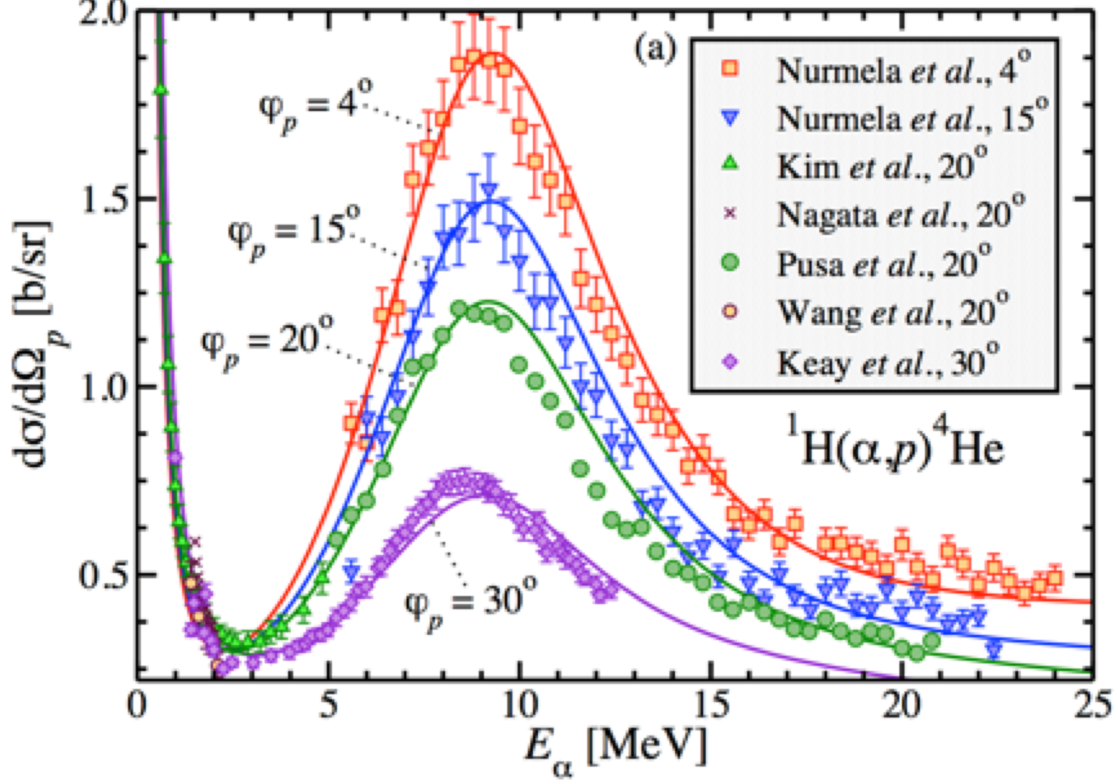
$$\left(\begin{array}{c|c} \mathcal{H}_{\mathcal{P}\mathcal{P}} & \mathcal{H}^{(0)}_{\mathcal{P}\mathcal{Q}} \\ \hline \mathcal{H}^{(0)}_{\mathcal{Q}\mathcal{P}} & \mathcal{H}^{(0)}_{\mathcal{Q}\mathcal{Q}} \end{array}\right)$$



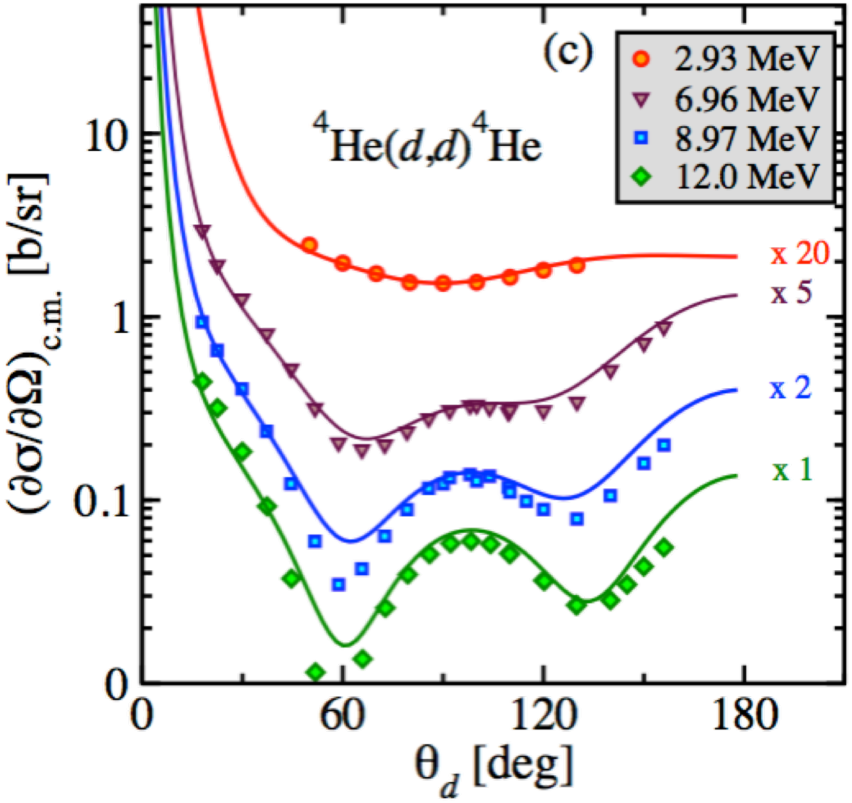
- Need to re-construct the interaction potential seen by the two fragment nuclei.
- Internal P-space Hamiltonian contains interaction potential
- External Q-space only has free components $T + V_{\mathrm{Coul}}$

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

PRC 90, 061601(R)



PRL114, 212502

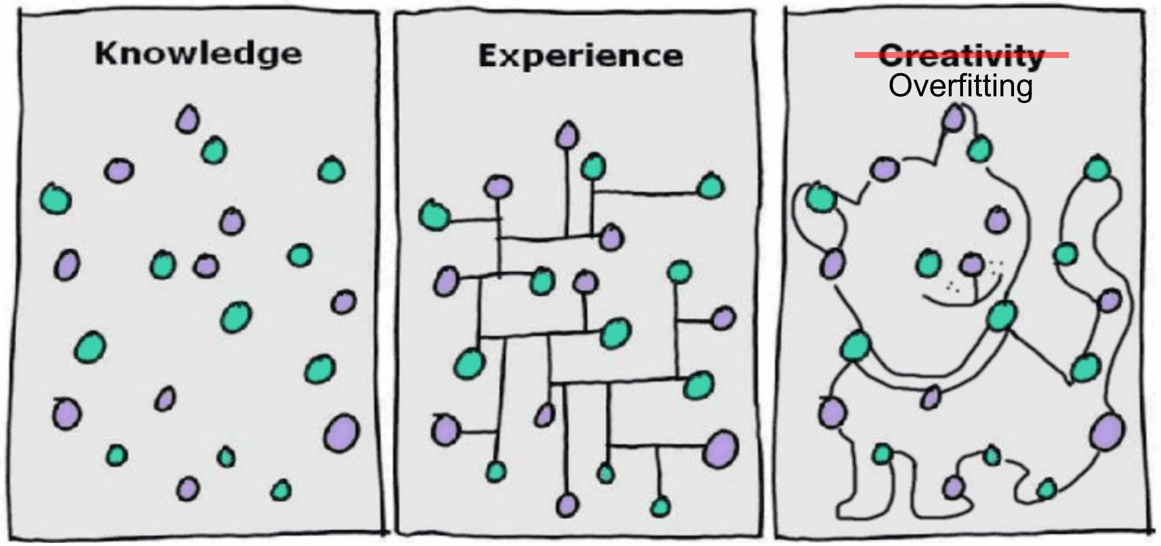


But what about uncertainties? And heavier projectiles?

Sources of uncertainty in ab initio calculations of many-body reactions.

- Uncertainty arising from approximations done in the solution of the many-body problem. –Make as few assumptions as possible, and if we must, make one, be sure to have it under control.

- Uncertainty from un-converged calculations due to limited computer power. –Pick something we know is converged or try to quantify the expected change.

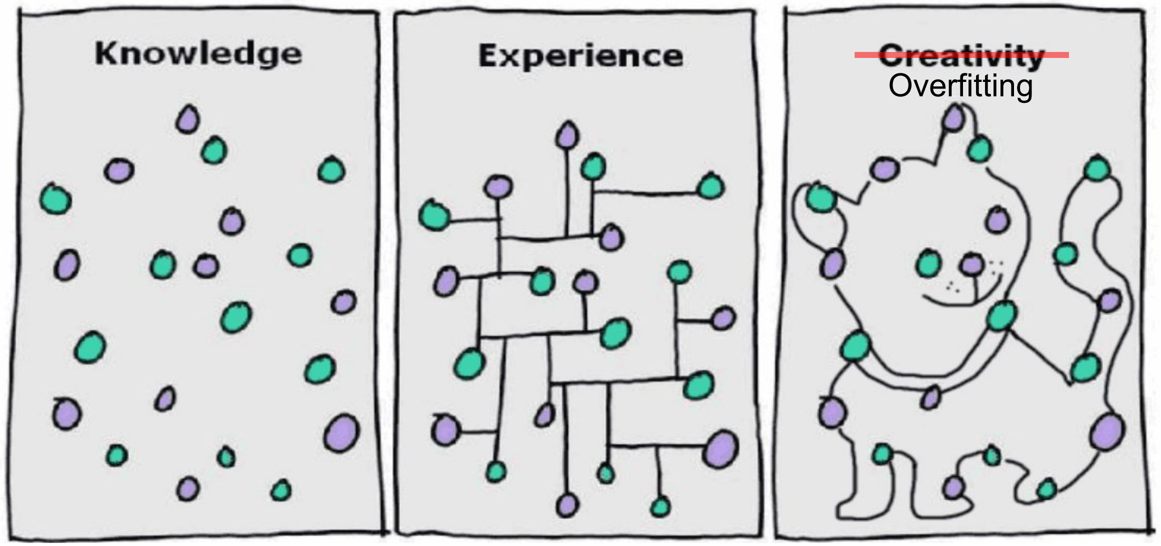


$$\chi^2 = \sum \frac{\left(O^{\mathrm{th}} - O^{\mathrm{exp}}\right)^2}{\sigma^2_{\mathrm{exp}} + \sigma^2_{\mathrm{th}}}$$

Sources of uncertainty in ab initio calculations of many-body reactions.

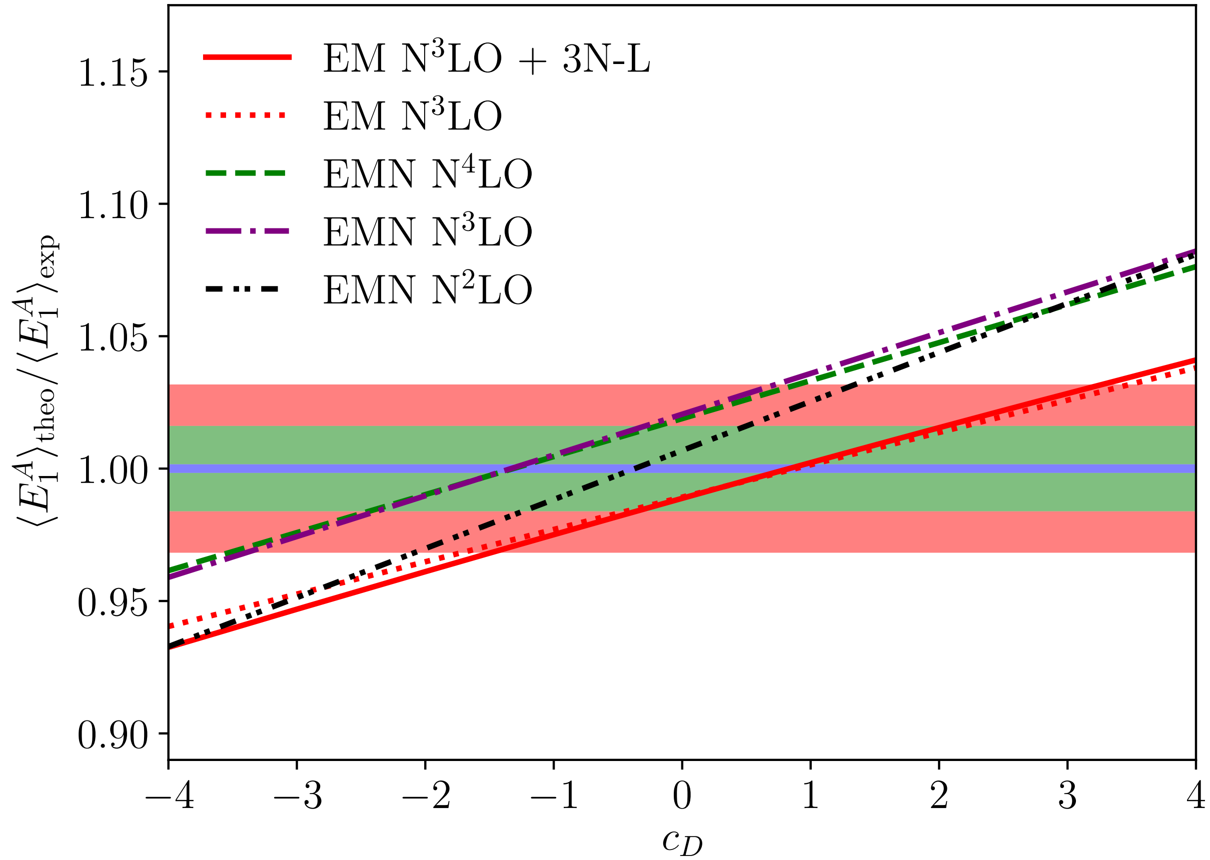
- Uncertainty in the underlying interaction, arising from missing physics, in terms of EFT truncation, exclusion of 4N-forces at N3LO, etc. –Not much we can do to correct for it but, it can be quantified!

- Uncertainty from poorly determined values for LECs, either due to absence of, or large uncertainties in, experimental data. –It can be quantified, if we can propagate it, and if we are not in a very bad minimum.

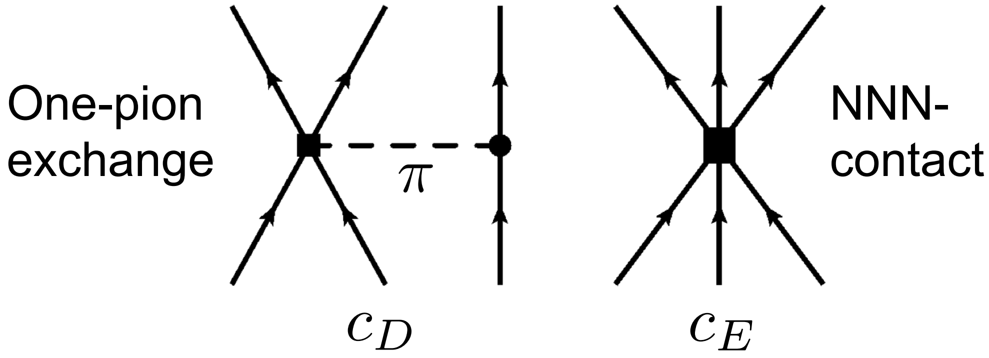


$$\chi^2 = \sum \frac{\left(O^{\mathrm{th}} - O^{exp}\right)^2}{\sigma^2_{exp} + \sigma^2_{\mathrm{t}h}}$$

Determining low-energy constants from three-body observables



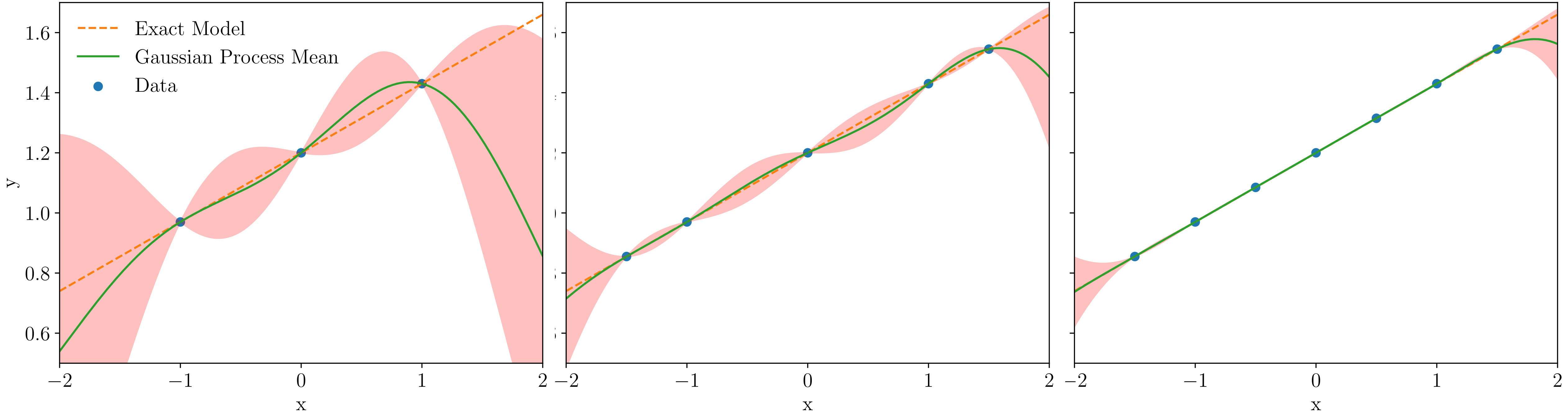
Entem & Machleidt, Phys. Rev. C **68**, 041001(R)
Entem, Machleidt & Nosyk Phys. Rev. C 96, 024004 (2017)



- Estimating theoretical uncertainties is not easy (or pleasant!)

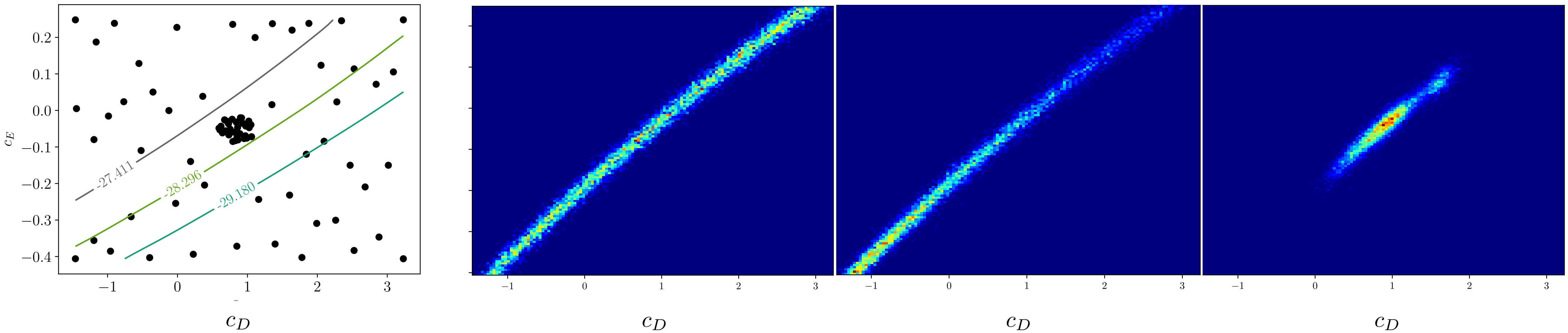
- Even at large chiral order, the theoretical uncertainty completely dominates over experiment, leading to large confidence intervals.

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.

Gaussian Process Models for uncertainty quantification.



Start from small number of design runs and train a GP

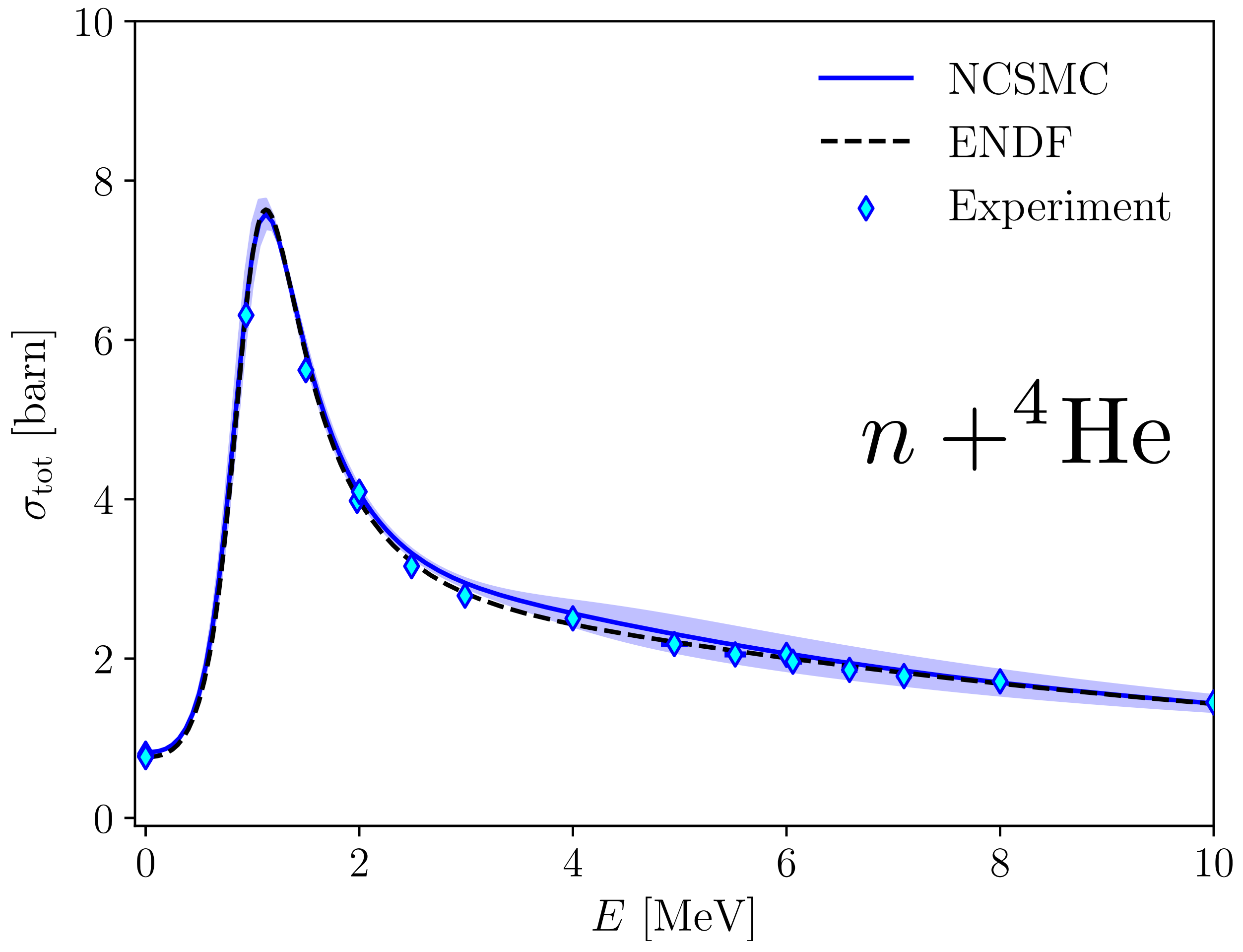
Sample posterior fitting to ^{4}He Binding energy.

Add ^{4}He charge radius: Narrower band.

Add resonance information: Clearer posterior!

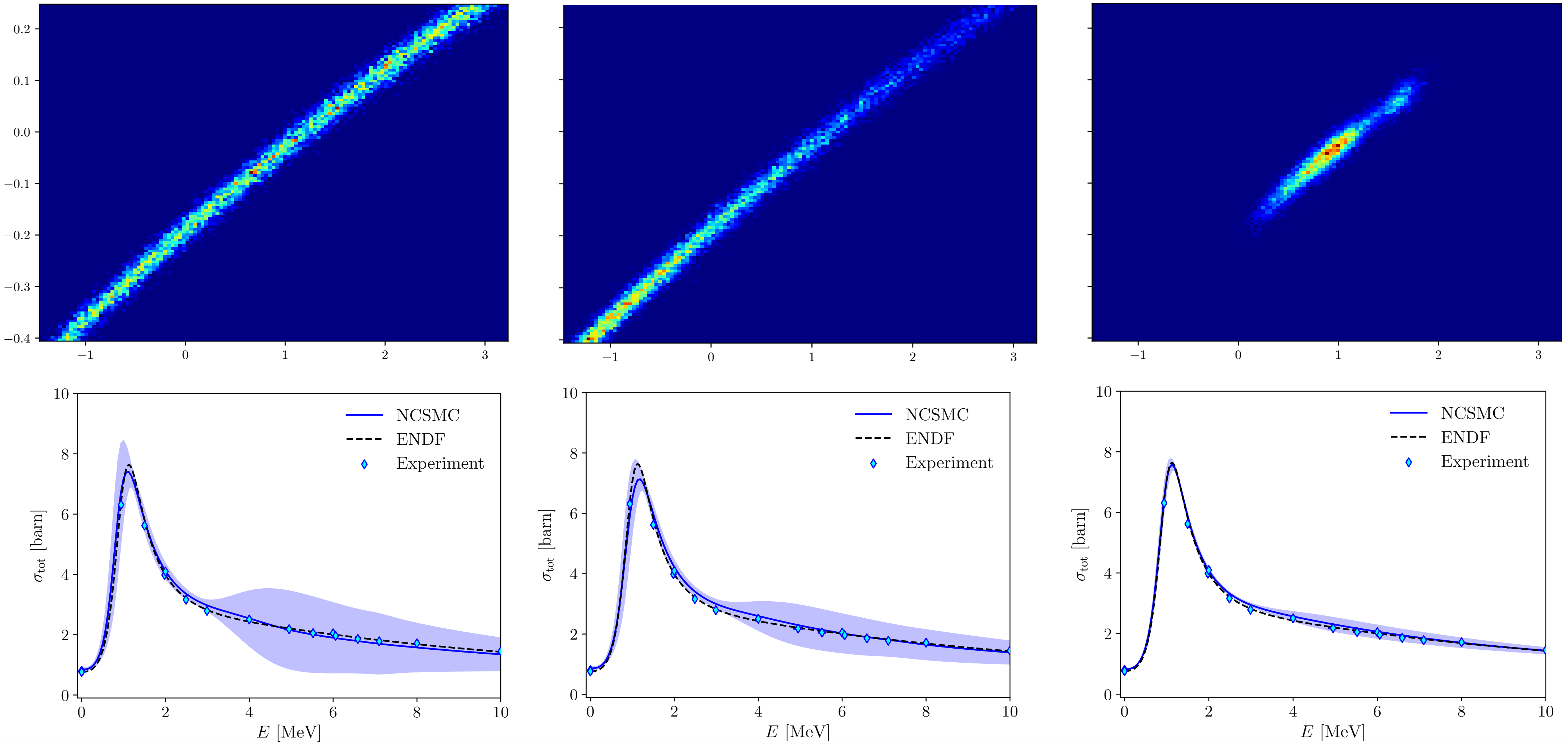
Including many-body reaction observables gives better confidence intervals

Cross section predictions with quantified uncertainty.



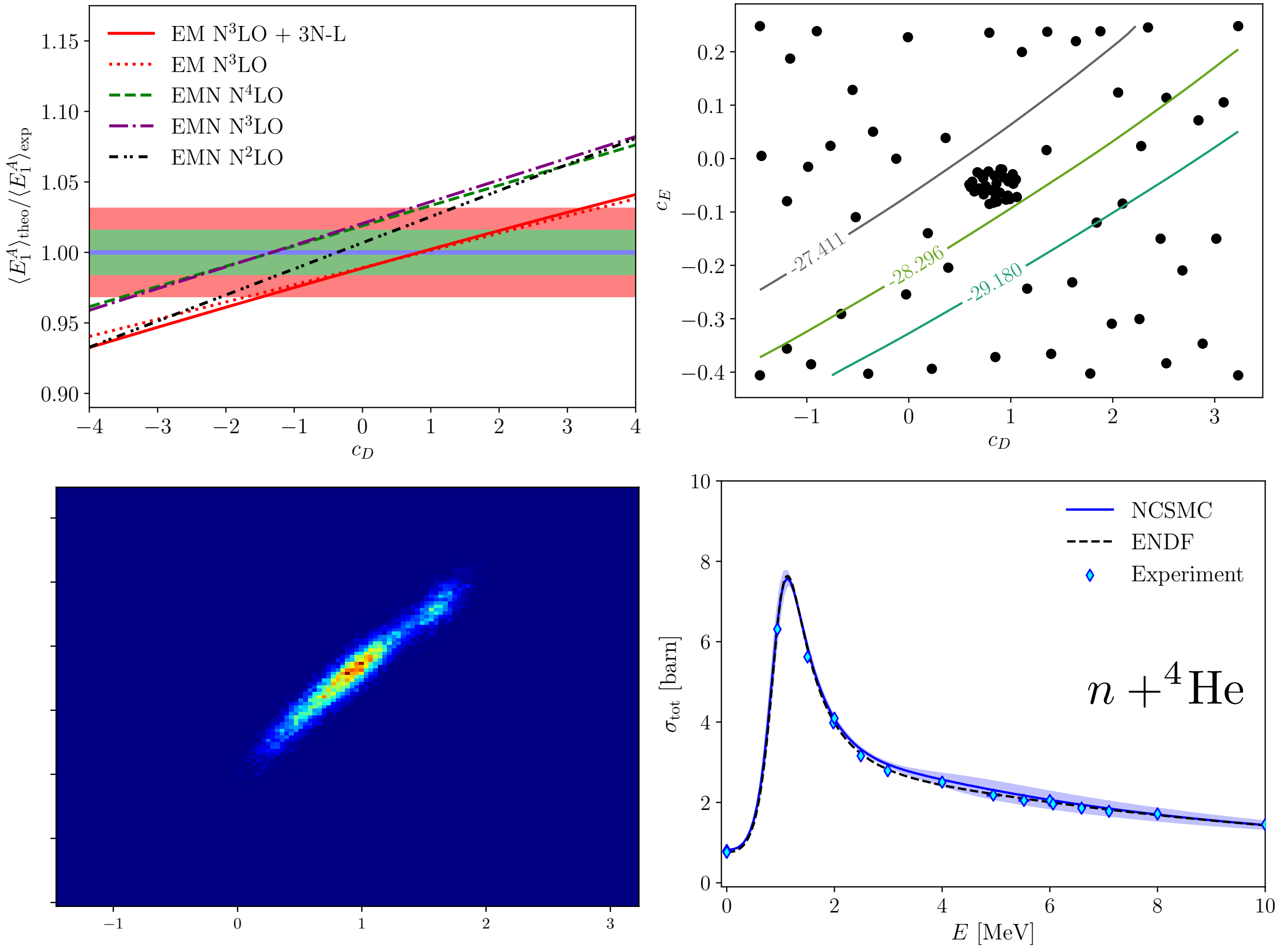
- New tools allow for robust uncertainty quantification.
- We now have a good handle for the range of validity of a theory: Good indication for what data to include next!
- Meaningful error bars are important for both theory and experiment.

Constrains in the parameters result in tighter confidence intervals for scattering observables.



Uncertainties in many-body scattering calculations: Summary.

- Incorporating theoretical uncertainties in the fitting process for the LECs leads to broader confidence intervals.
- Gaussian Processes allow for fast emulators using a (comparatively) small number of calculations.
- Doing MCMC on the emulator for posteriors of both the LECs as well as nuclear observables is then computationally feasible.

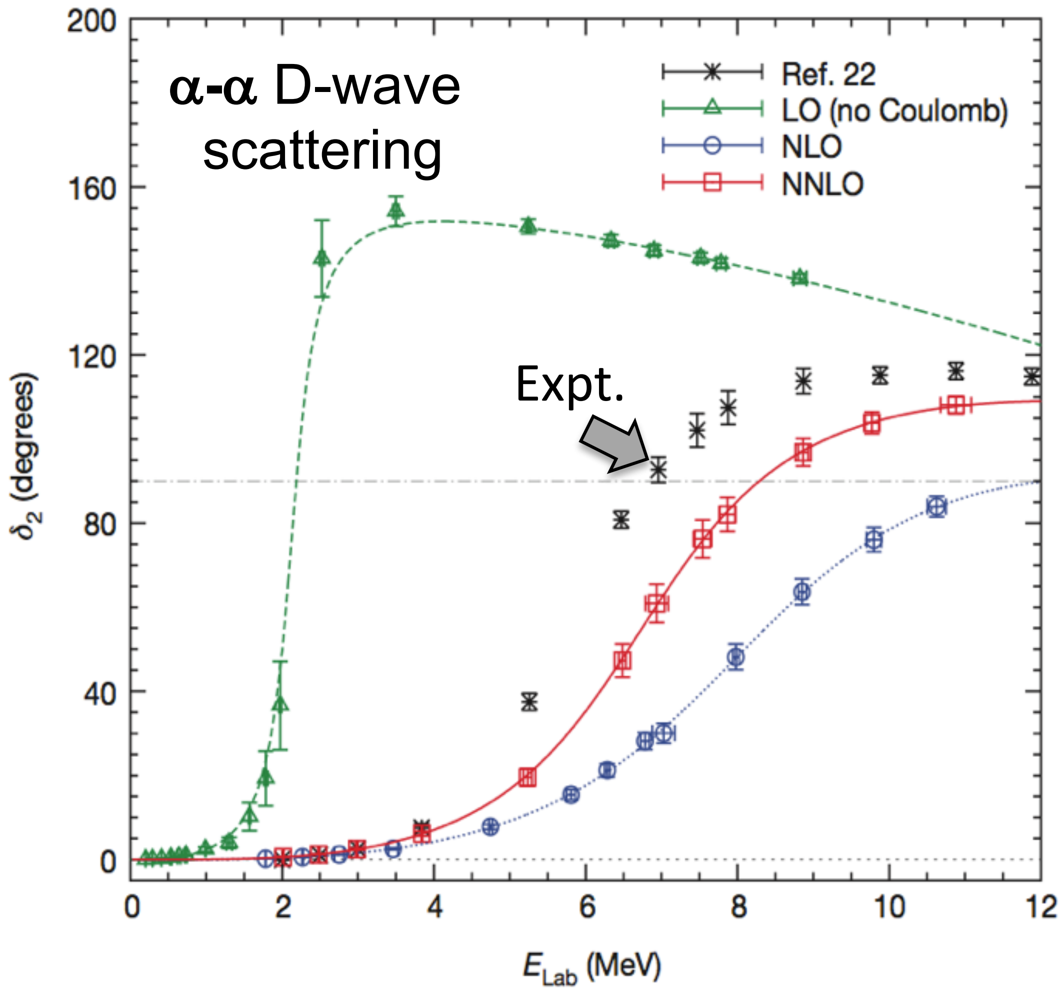


Can ab initio theory treat He burning reactions?

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

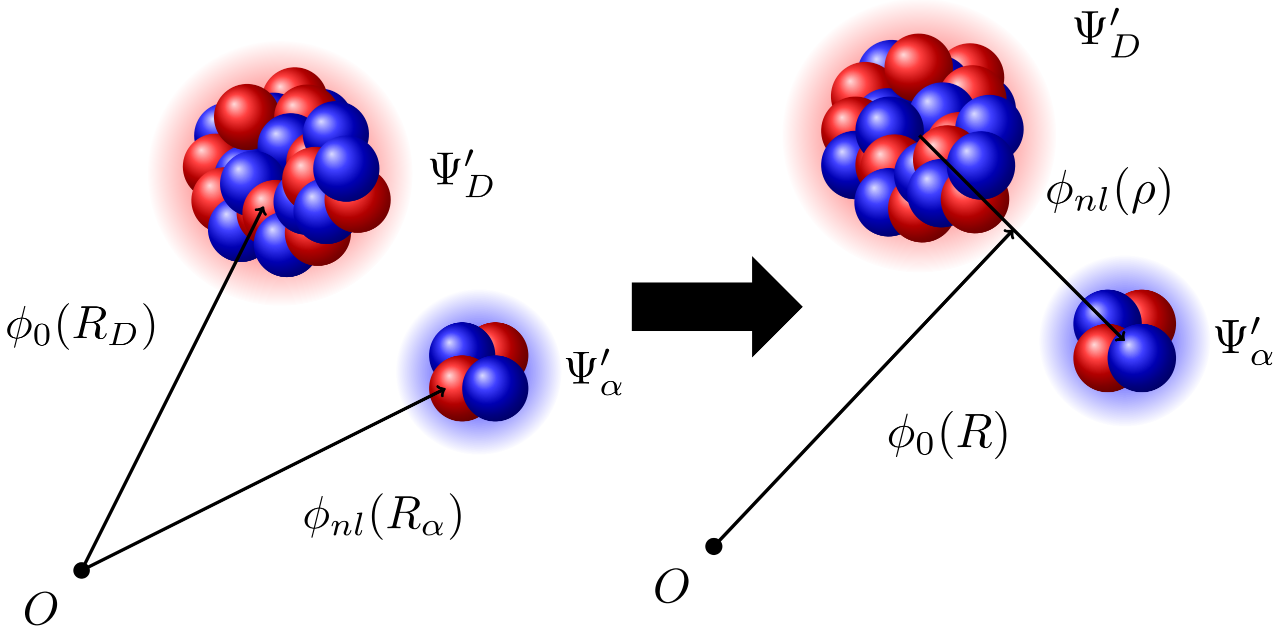
Nuclear Lattice EFT with the Adiabatic Projection Method

- 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



Building blocks for many-body reactions.

- Target/projectile wave functions are written in harmonic oscillator expansion.
- Need to remove spurious CM motion.
- In the harmonic oscillator basis this can be done exactly.



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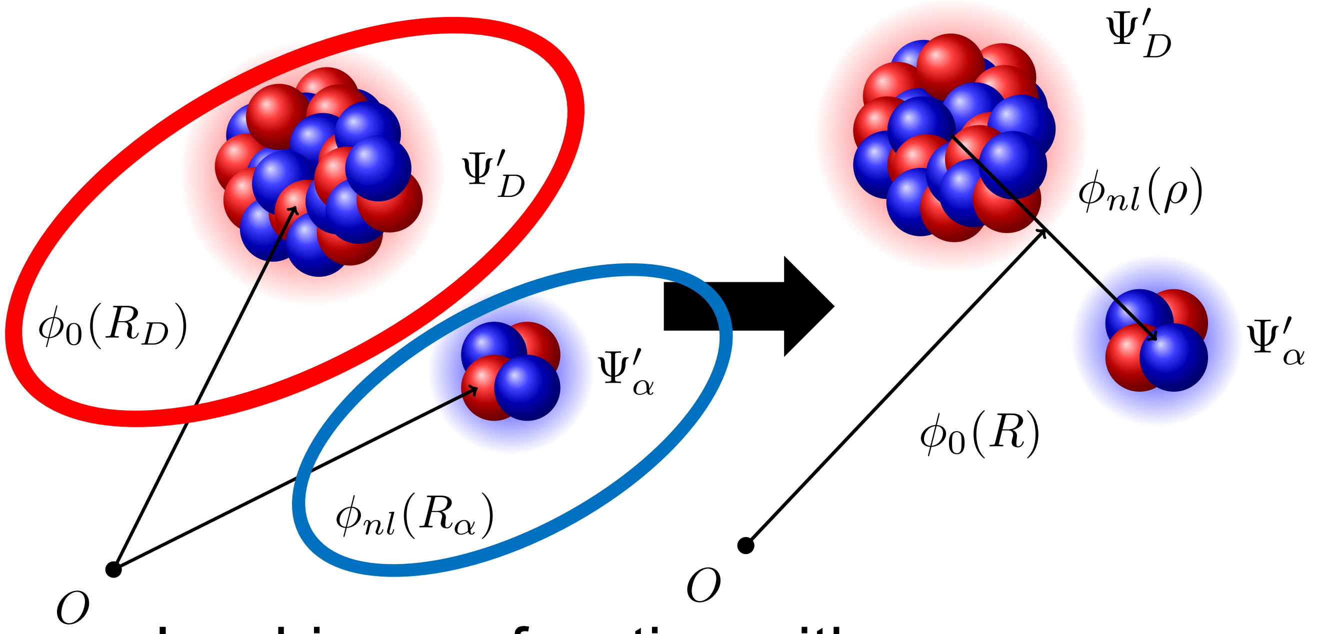
NCSM wave function for target



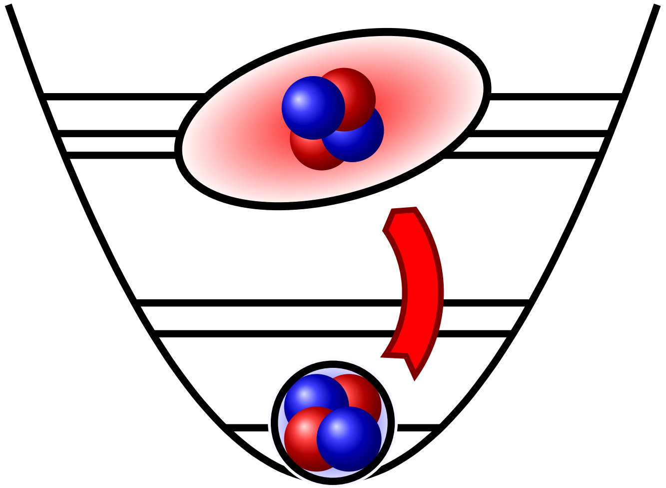
Jacobi wave function with attached center of mass for projectile

Developments to facilitate α-induced reactions.

KK. and A. Volya PRL 119, 062501, Phys. Rev. C 100, 034321

- NCSM wave functions already have a CM component we just need to control it to reach the desirable state.

- Full antisymmetrization is achieved by using second quantization formalism at all steps of the channel construction process.



$$E1 \sim R_{CM} \sim A^\dagger + A$$

nodes with $\left[A^\dagger \times A^\dagger\right]_0^{(0)}$

ℓ, m with $A_m^\dagger$

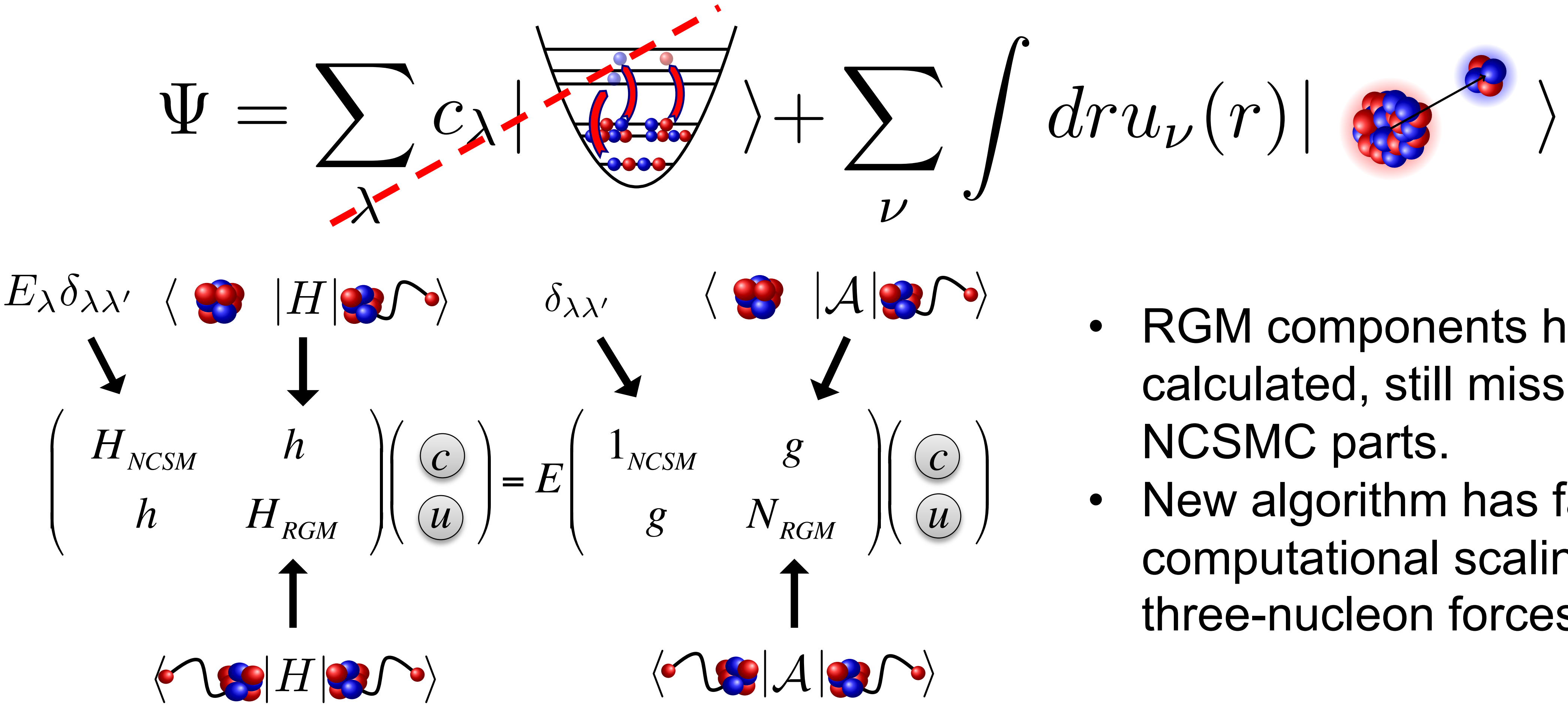
$$\mathcal{L}_m = \left[A^\dagger \times A\right]_m^{(1)}$$

$$|\Psi_\alpha\rangle = \Psi_\alpha^\dagger|\rangle = \sum_{\{m\}} X_m^\alpha a_{m_1}^\dagger a_{m_2}^\dagger a_{m_3}^\dagger a_{m_4}^\dagger|\rangle$$

$$|\Psi_\mathrm{D}\rangle = \Psi_\mathrm{D}^\dagger|\rangle = \sum_{\{m\}} X_m^\mathrm{D} a_{m_1}^\dagger a_{m_2}^\dagger \ldots a_{m_{A_\mathrm{D}}}^\dagger|\rangle$$

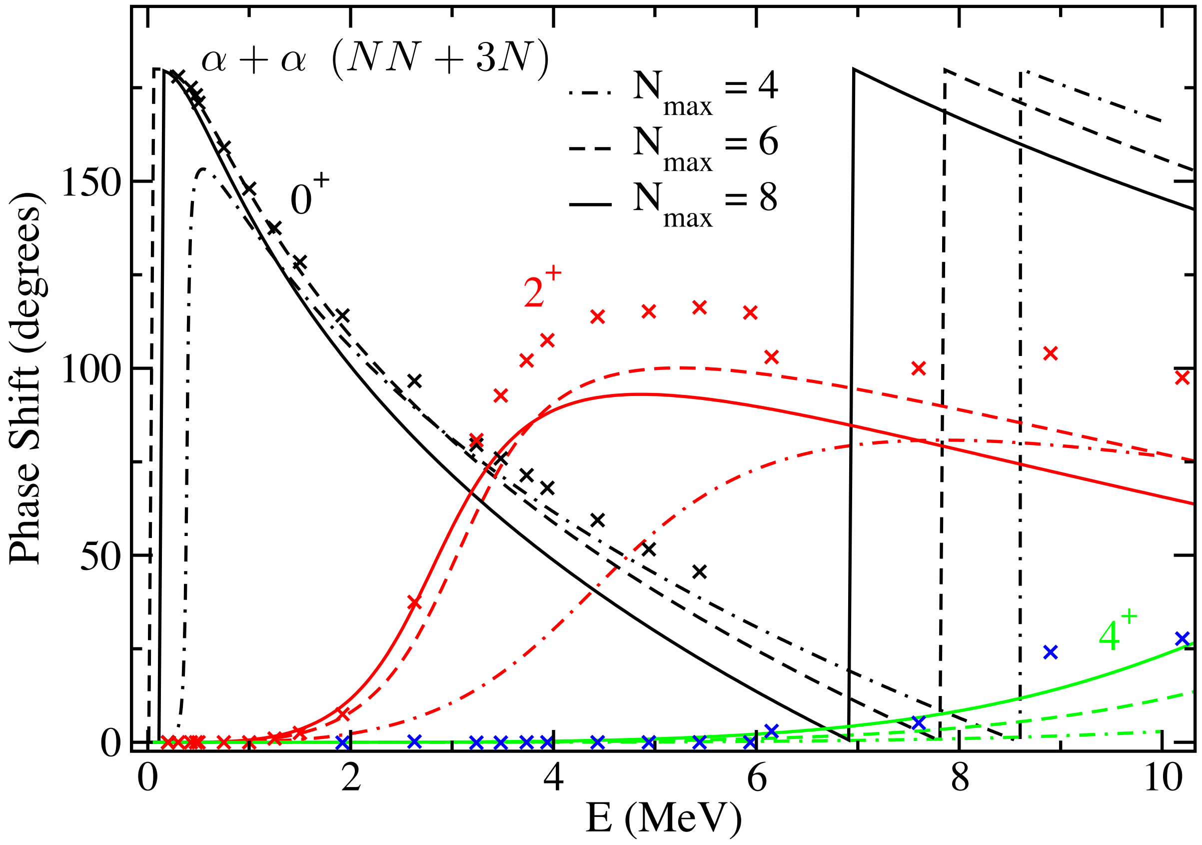
$$|\Psi_\mathrm{C}\rangle = \Psi_\alpha^\dagger \Psi_\mathrm{D}^\dagger|\rangle$$

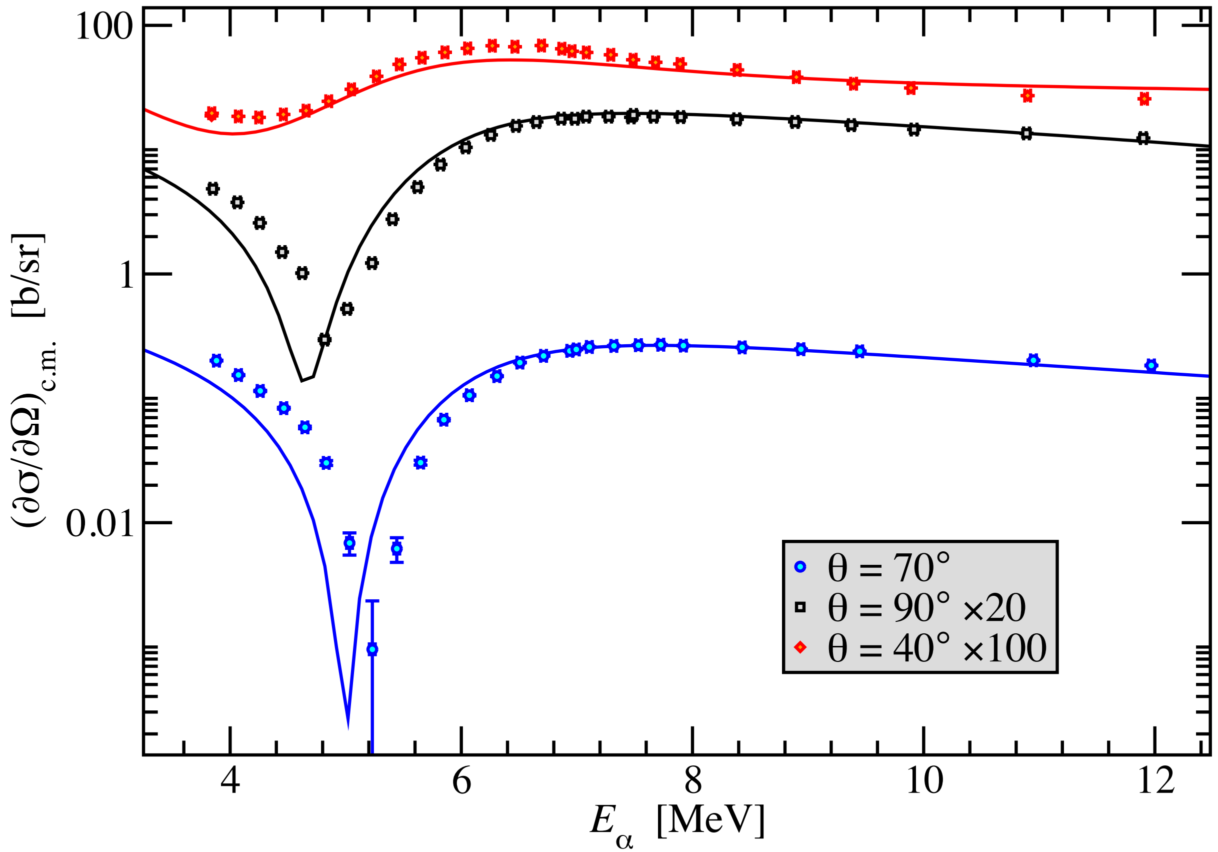
Current status for α-α scattering



- RGM components have been calculated, still missing some NCSMC parts.
- New algorithm has favorable computational scaling for three-nucleon forces.

Current status for α-α scattering

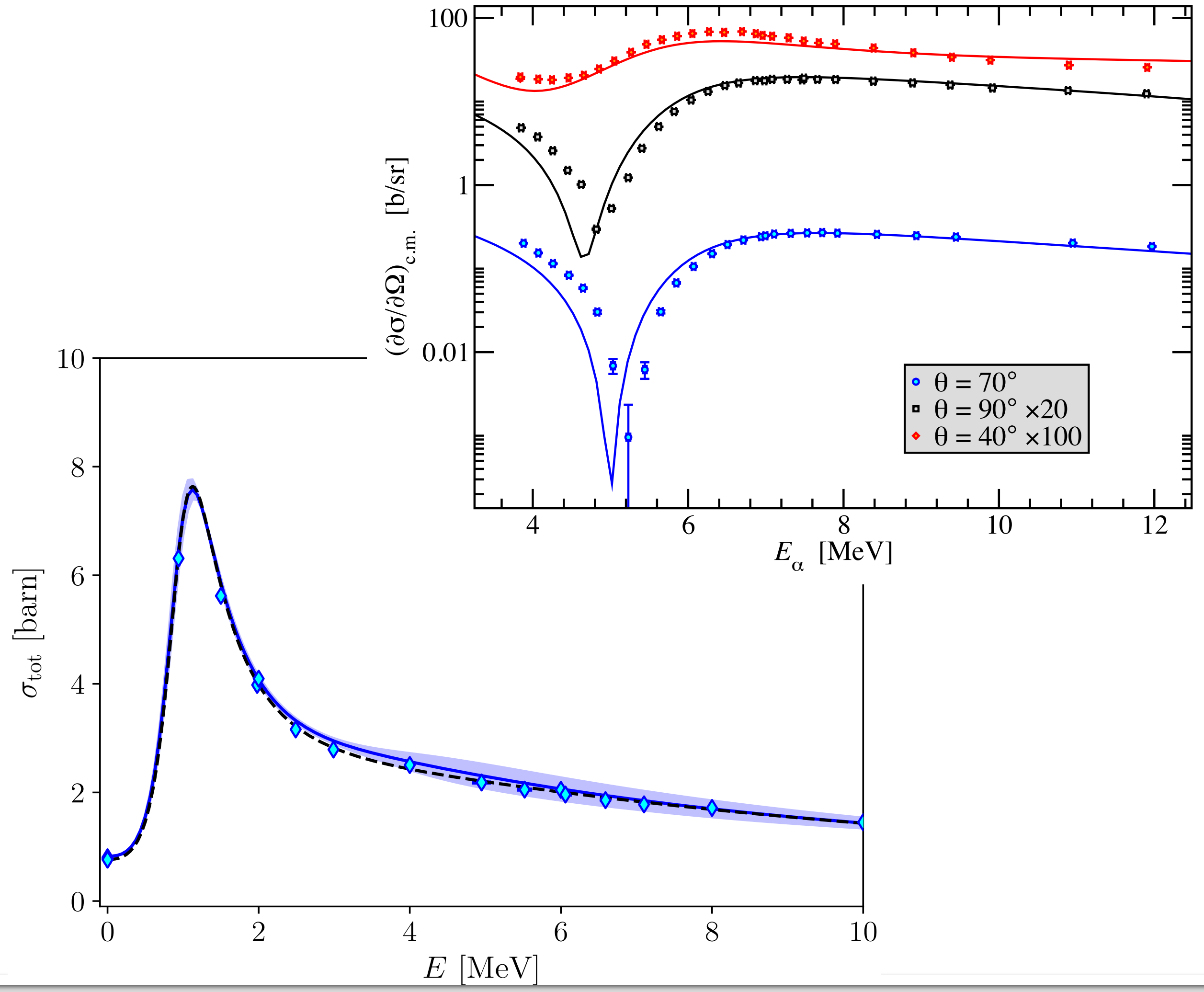




NN N3LO (Phys. Rev. C **68**, 041001(R)) hw = 24 MeV, SRG λ = 1.8 fm^-1, NNN N2LO

Conclusions

- We have made first steps towards a first-principles description of α-induced reactions.
- Role of three-nucleon forces is still under investigation.
- Ideally, we should be able to supplement theoretical predictions with confidence intervals. Emulators provide this framework.



Thank you!