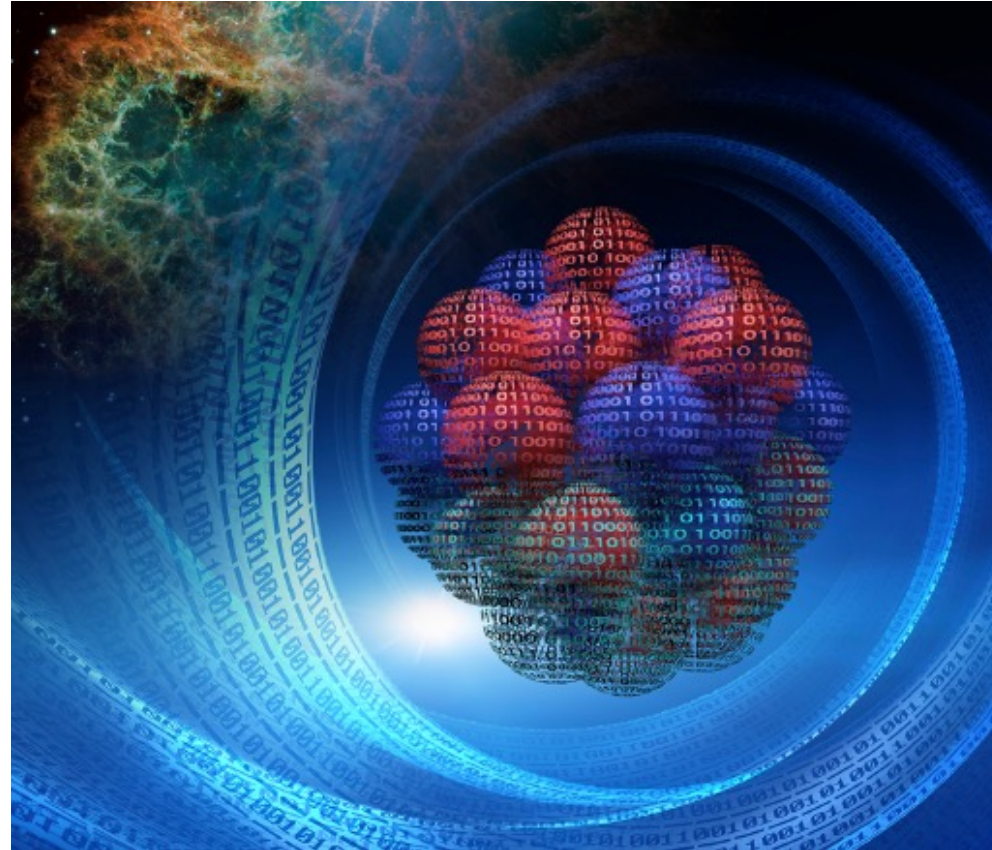


Computing nuclei and nuclear reactions



Thomas Papenbrock

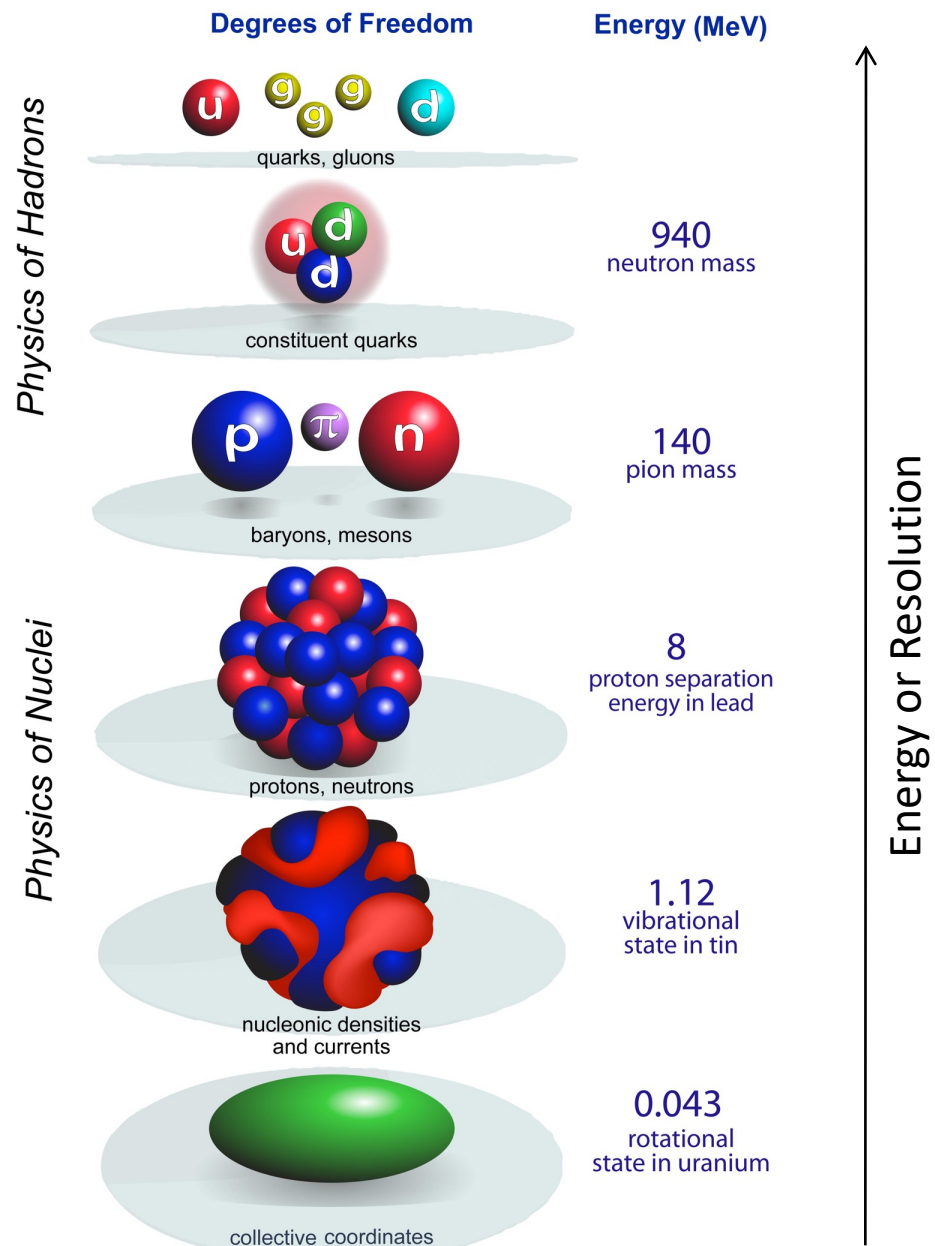
University of Tennessee & Oak Ridge National Laboratory

Future Trends in Nuclear Physics Computing

Stony Brook University, Sep 28, 2022

Work supported by the US Department of Energy

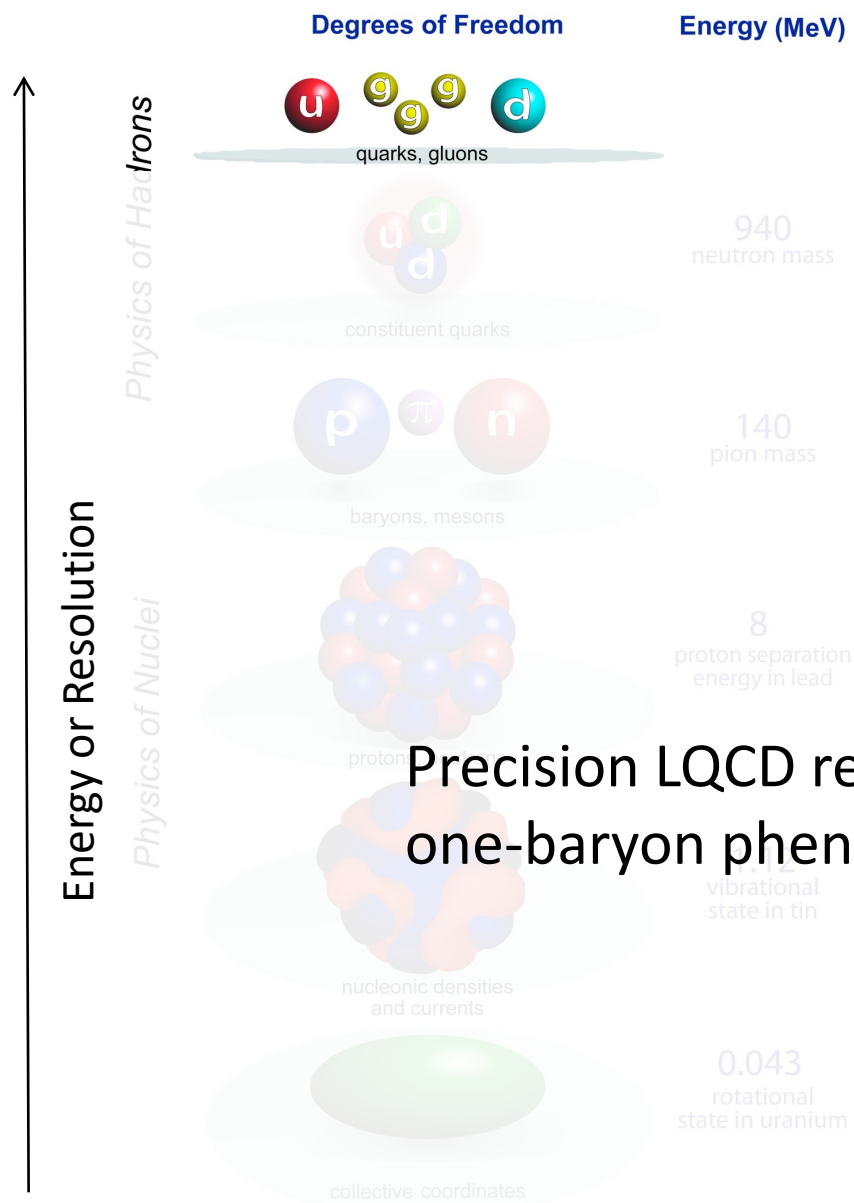
Energy scales and relevant degrees of freedom



- Multiple separation of scales
- Opportunities for effective field theories (EFTs)
- EFTs replaced various models
- Ideas from EFT and RG impacted nuclear theory
- Precision computations and uncertainty estimates / quantification

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Precision lattice QCD computations



Precision LQCD results for one-baryon phenomena!

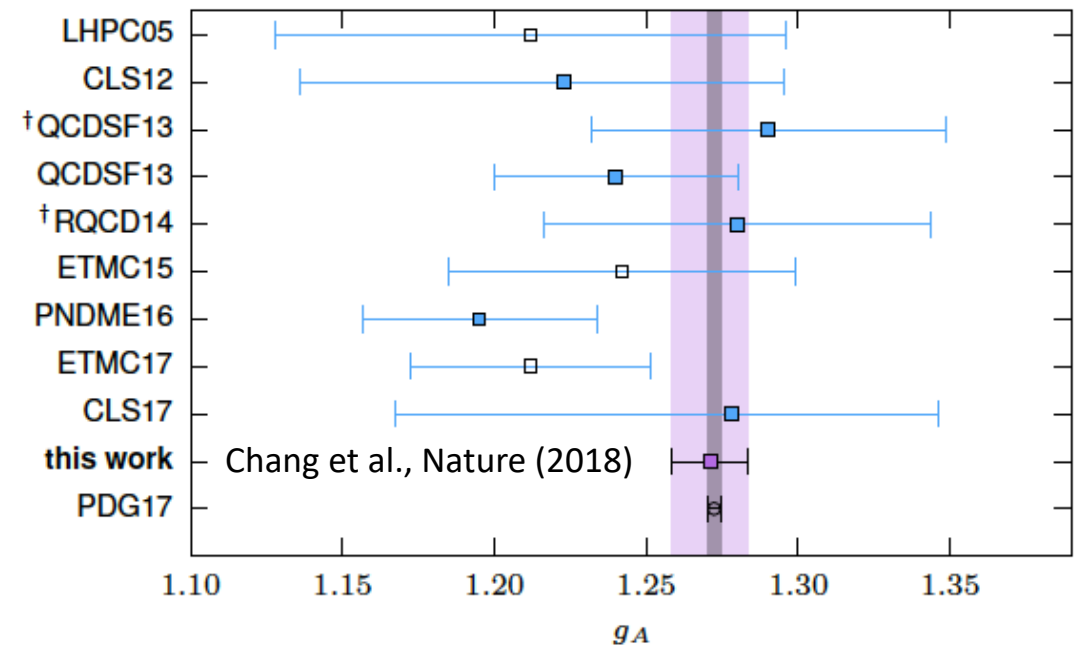
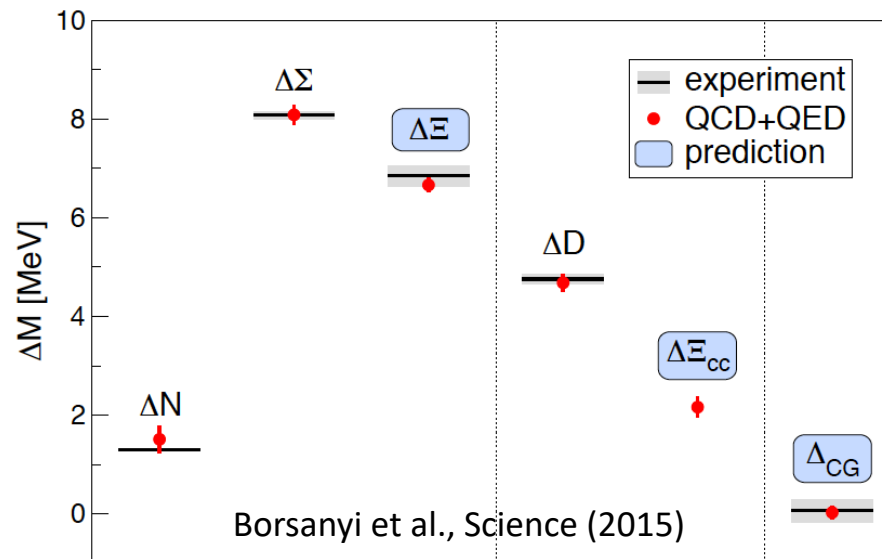
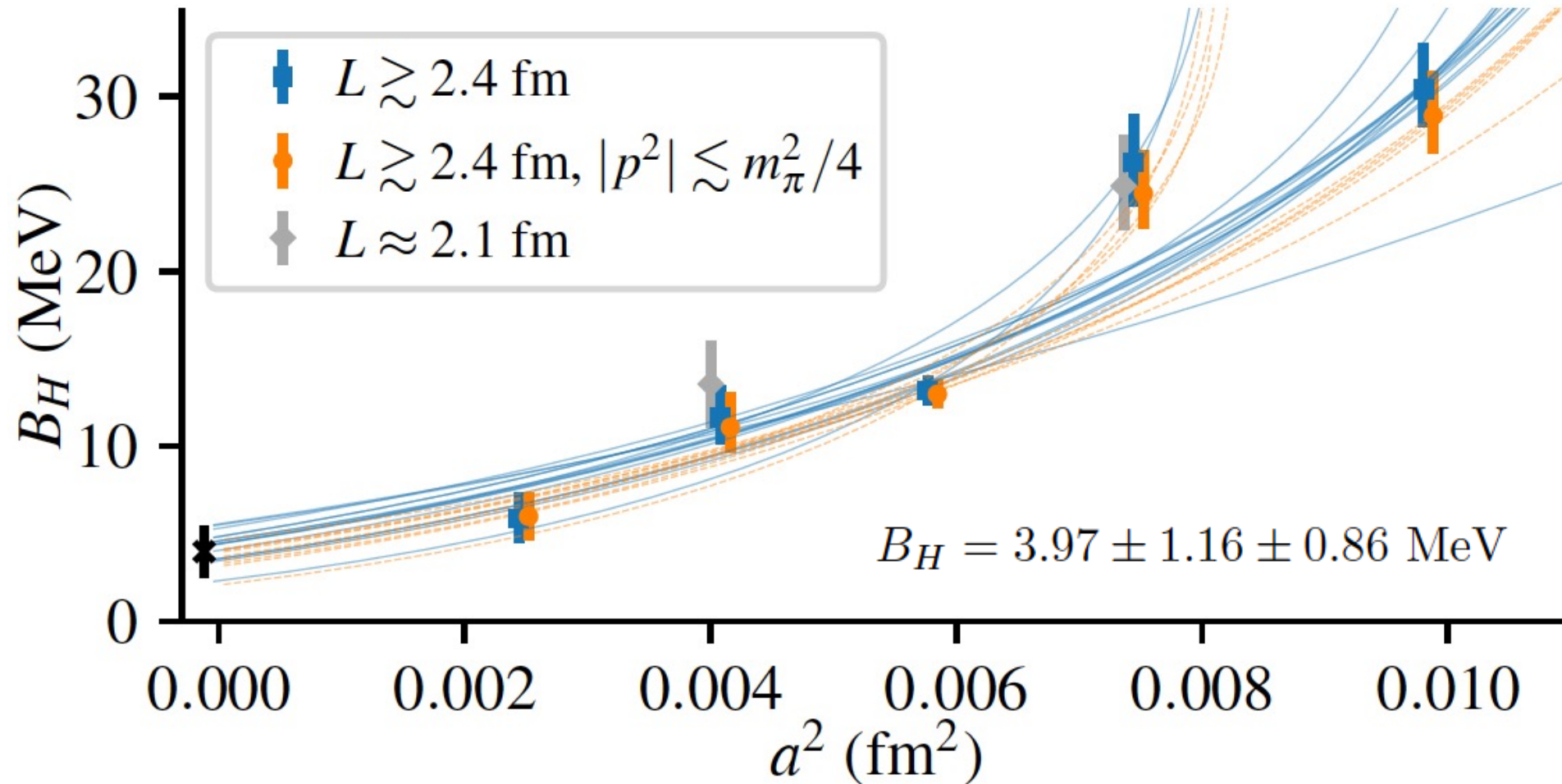


Fig.: Bertsch, Dean, Nazarewicz (2007)

Towards Lattice QCD computations of hadron bound states

H-baryon, hypothetical six-quark bound state $uuddss$, computed at $m_\pi = m_K = 420$ MeV



Computing nuclei from QCD ...

Does nuclear binding increase or decrease with increasing pion mass?

The computation of light nuclei from lattice QCD is uncertain, see, e.g., discussion in [Drischler, Haxton, McElvain, Mereghetti, Nicholson, Vranas, Walker-Loud, arXiv:1910.07961]

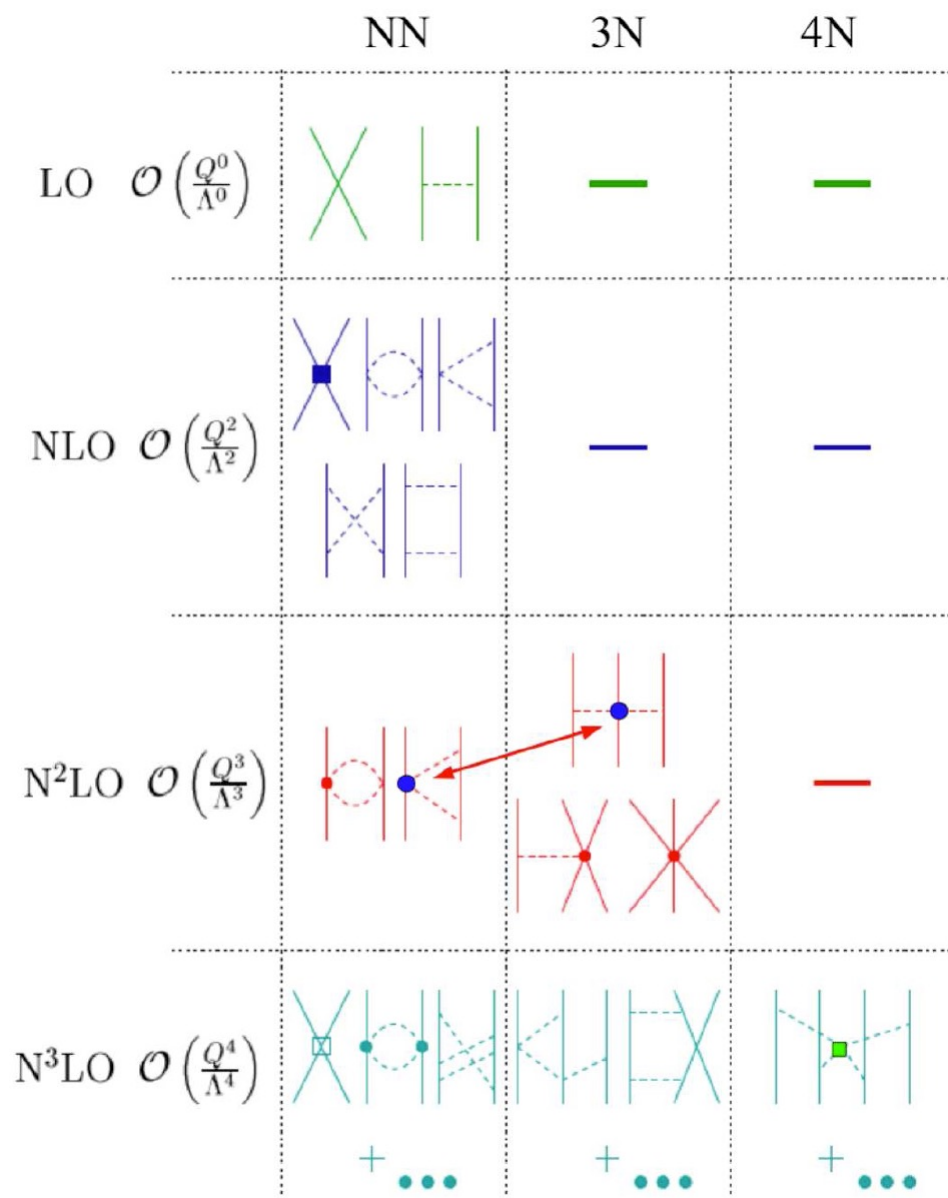
It is not clear, whether nuclear binding increases with increasing pion mass [see, e.g., NPLQCD collaboration] or whether it decreases [see, e.g., HAL QCD collaboration].

Effective field theories ready to be matched to lattice QCD data; compute nuclei as heavy as ^{40}Ca , see [Barnea et al, Phys. Rev. Lett. (2015); Contessi et al, Phys. Lett. B (2017); McIlroy et al Phys. Rev C (2018); Bansal et al., Phys. Rev. C 98, 054301 (2018)]

Uncertainties in the two-hadron system impede progress in linking nuclei to lattice QCD

Nuclear forces from chiral effective field theory

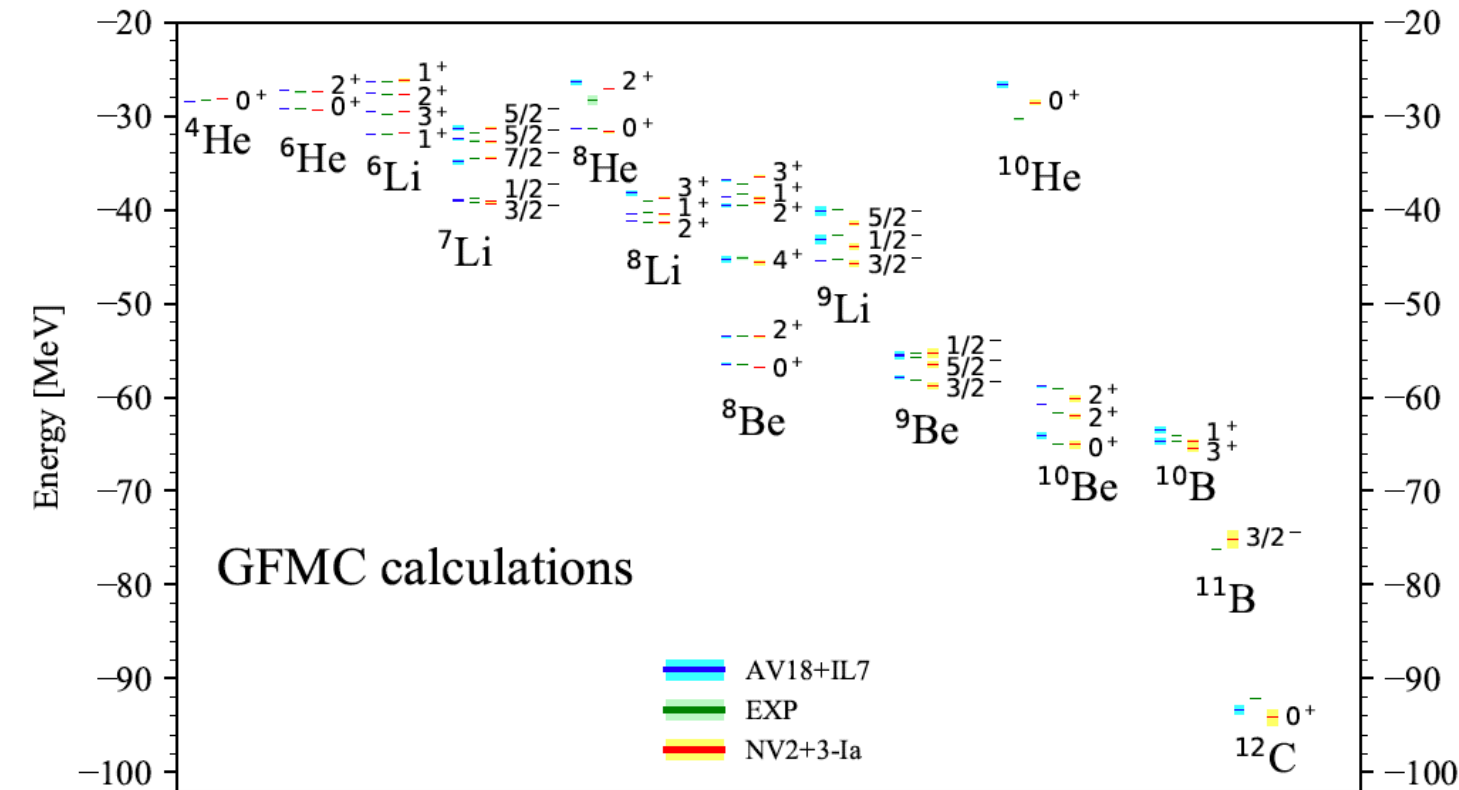
[Weinberg; van Kolck; Epelbaum, Gloeckle, Meissner; Entem & Machleidt; ...]



- Higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard *et al.* 2007; Krebs *et al.* 2012; Hebeler *et al.* 2015; ...]
- Implemented in continuum and on lattice [Borasoy *et al.* 2007]
- Local / non-local formulations [Gezerlis *et al.* 2013]
- Propagation of uncertainties [Navarro Perez 2014]
- Delta degrees of freedom “Norfolk V” [Piarulli et al 2015, 2016, ...]
- Semilocal potentials [LENPIC collab. 2019, 2020, ...]
- Different optimization protocols [Ekström *et al.* 2013; 2015; ...]

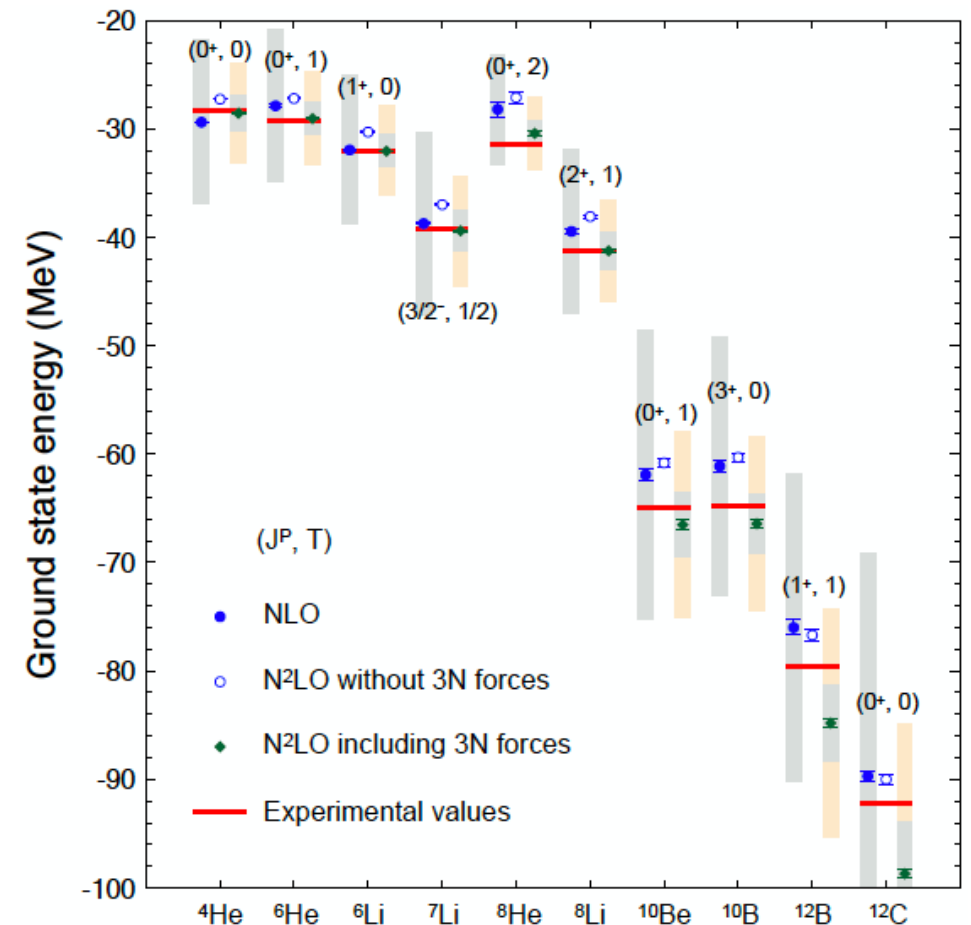
Much improved understanding and handling via renormalization group transformations [Bogner *et al.* 2003; Bogner *et al.* 2007]

Ab initio computations of light nuclei



Energies in light nuclei from Δ -chiral EFT and Argonne potentials, compared to data.

Piarulli et al, Phys. Rev. Lett. 120, 052503 (2018)



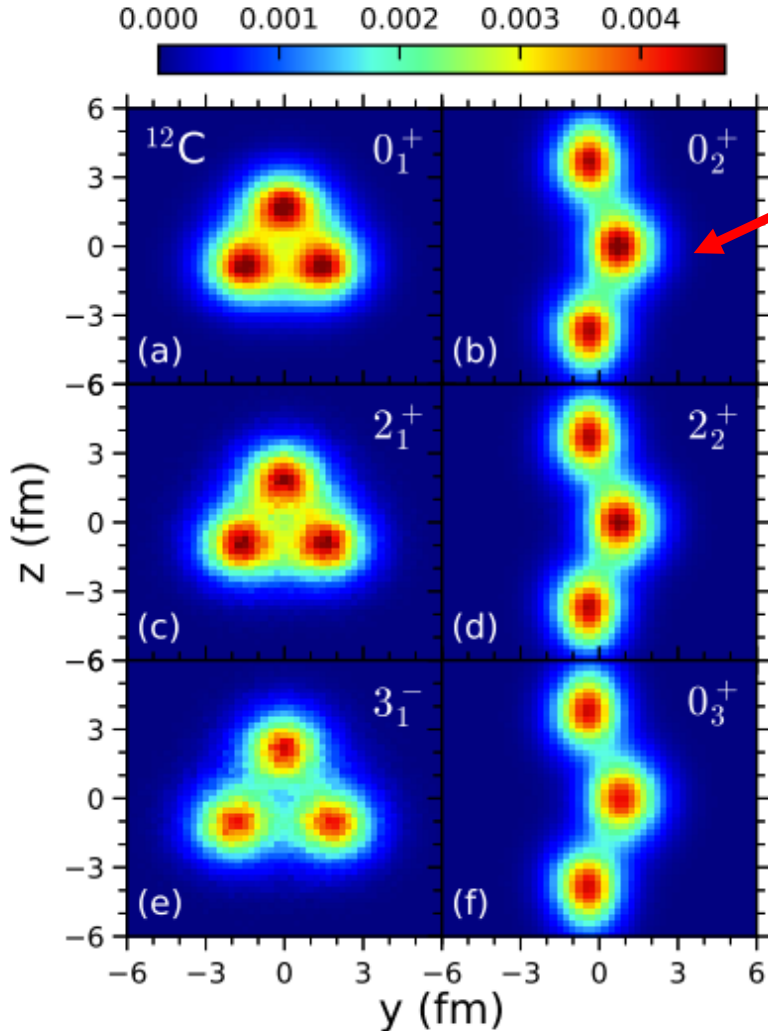
Ground-state energies of light nuclei from semi-local chiral EFT and compared to data.

Maris et al, Phys. Rev. C 103, 054001 (2021)

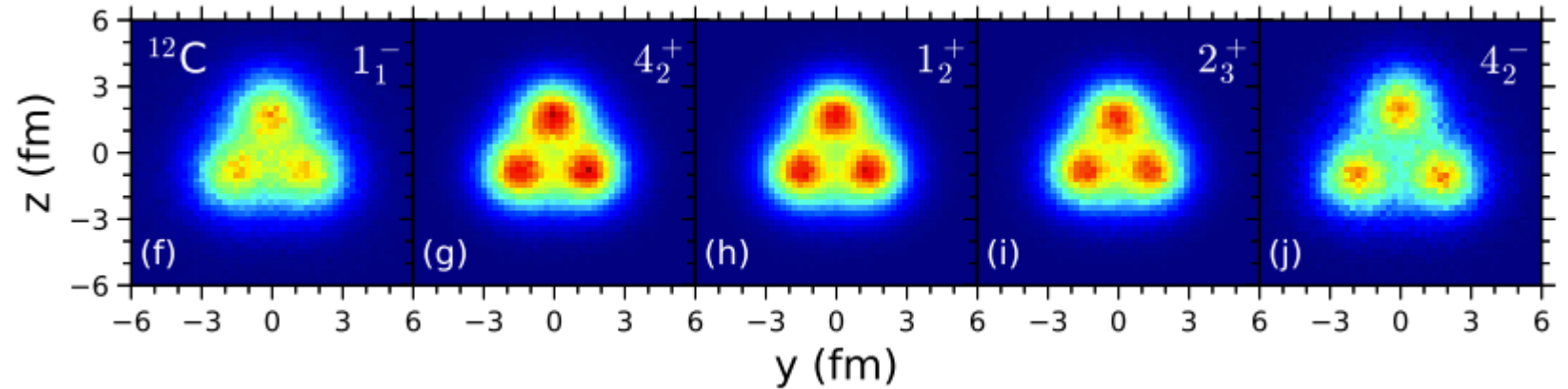
Charge radii still a challenge for $A > \approx 16$

Clustering in nuclei

Lattice Effective Field Theory simulations of ^{12}C



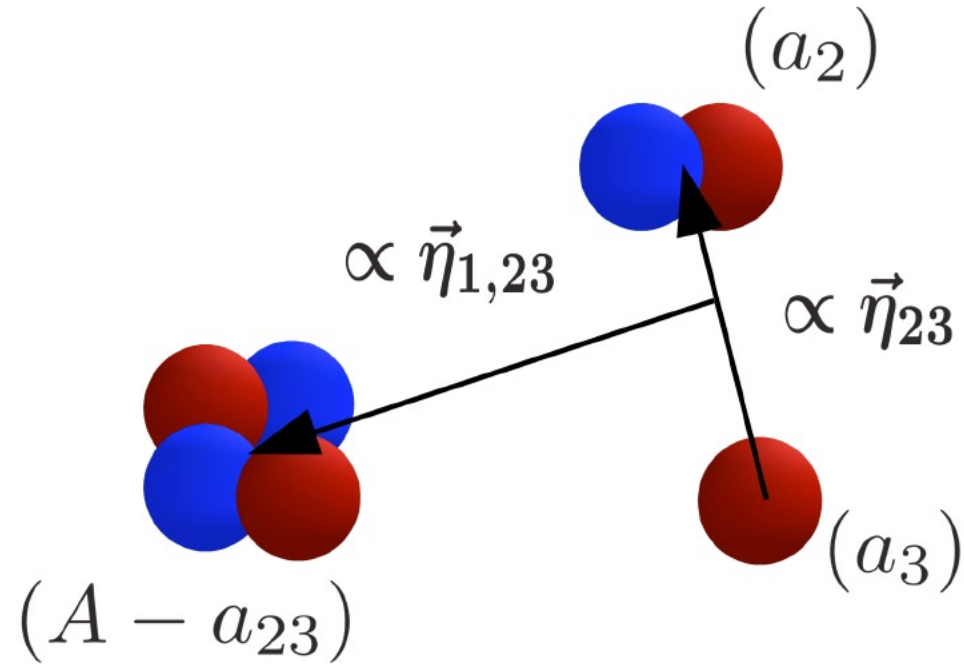
Hoyle State (triple α resonance)



Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)

Shen et al., arXiv:2202.13596 (2022)

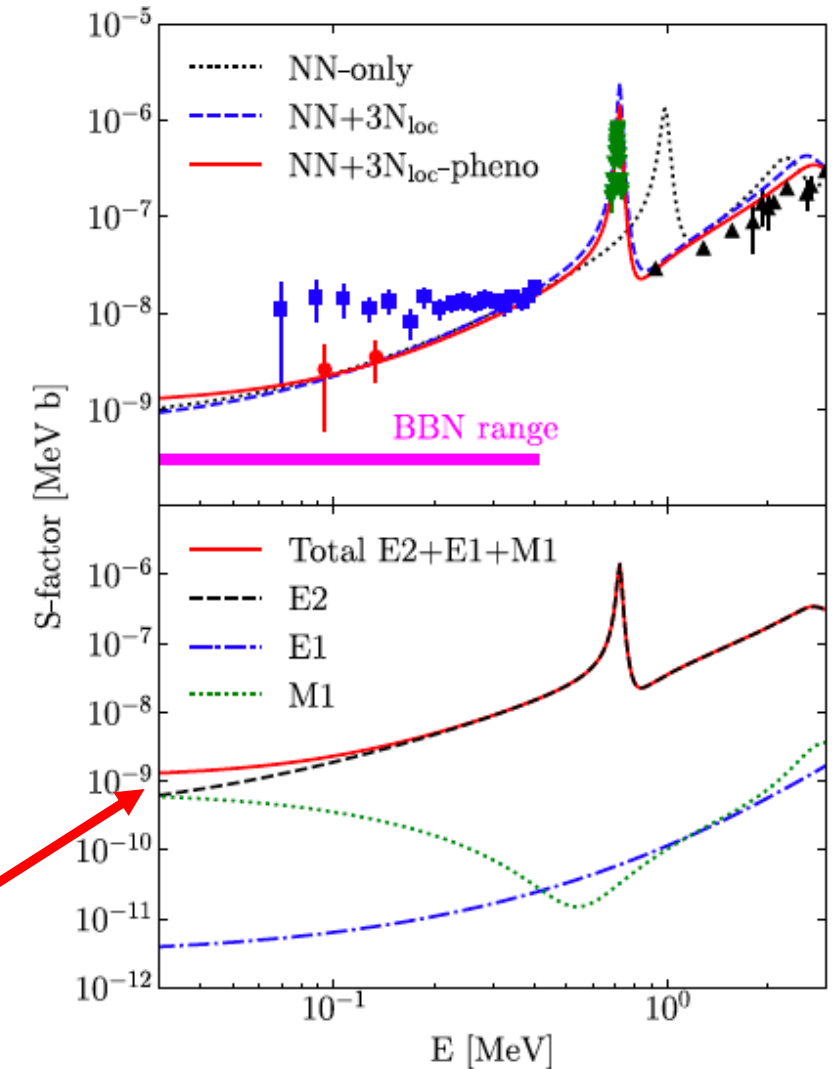
Nuclear astrophysics: Light ion reactions



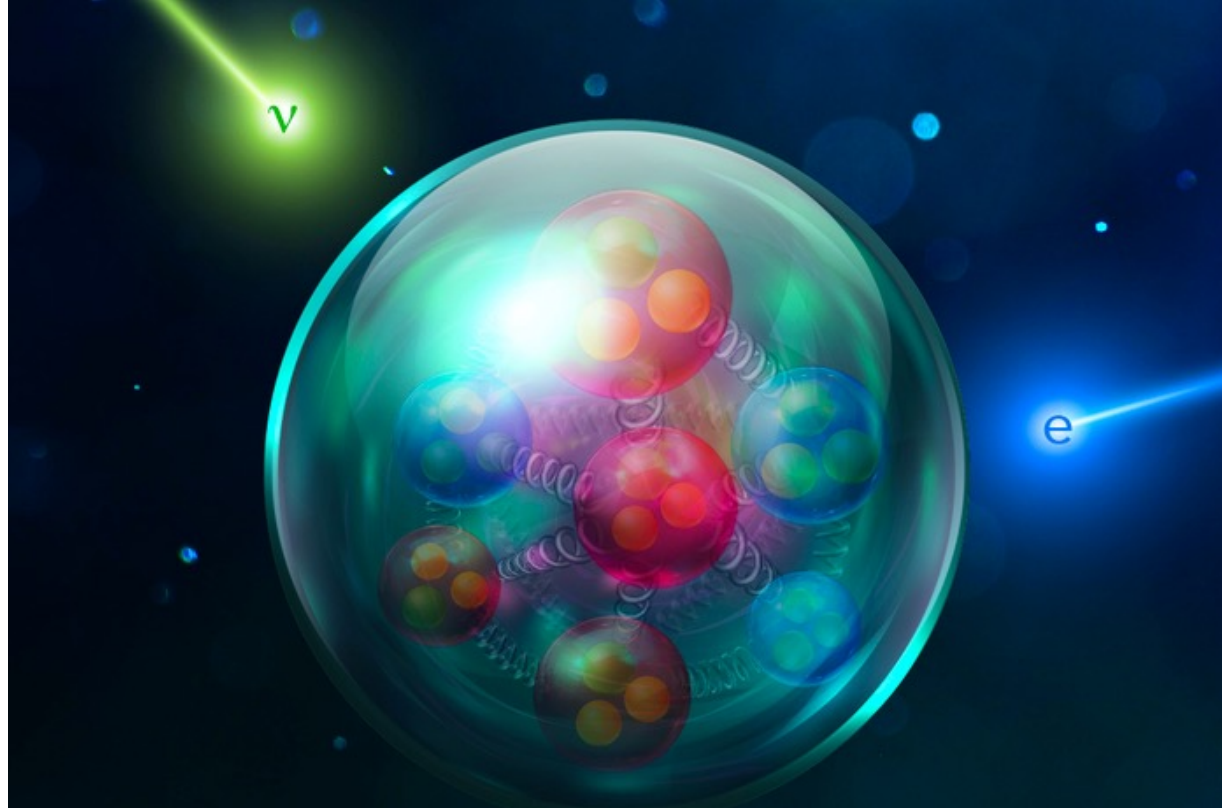
Structure of clusters computed microscopically
Anti-symmetry of all fermions included

Enhancement of the capture probability
below 100 keV due to M1 transitions

${}^4\text{He}(d,\gamma){}^6\text{Li}$ big bang radiative capture

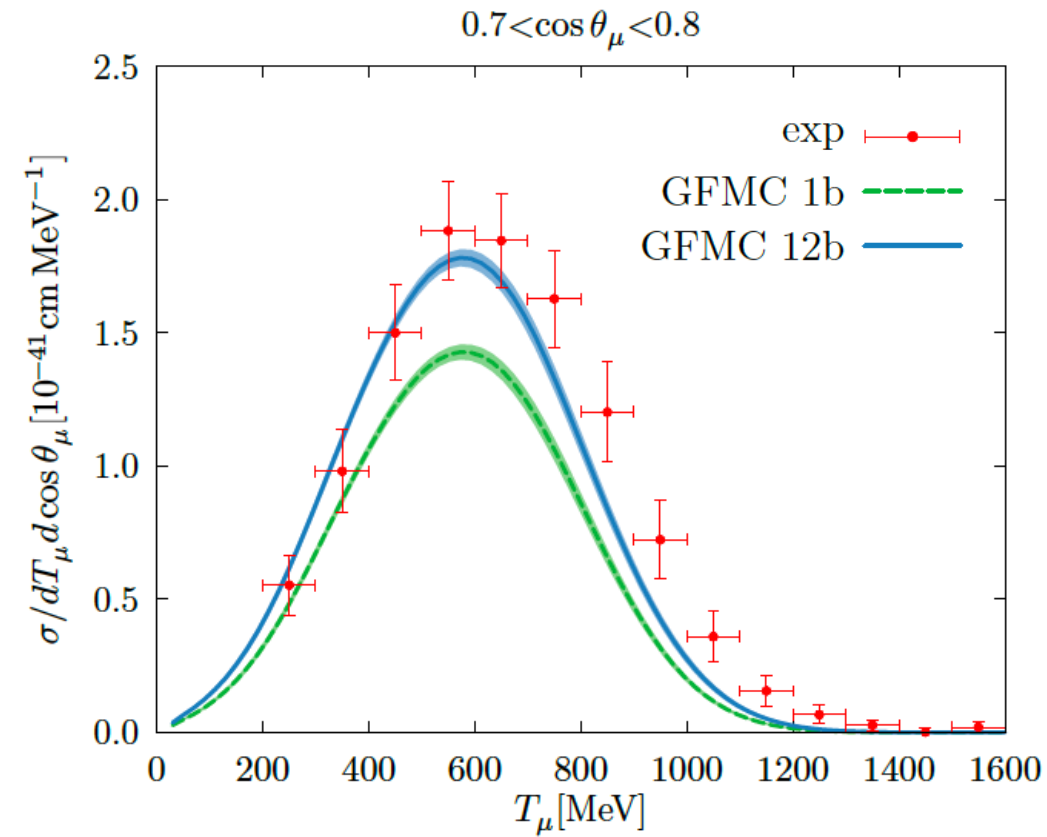


Progress in lepton-nucleus scattering



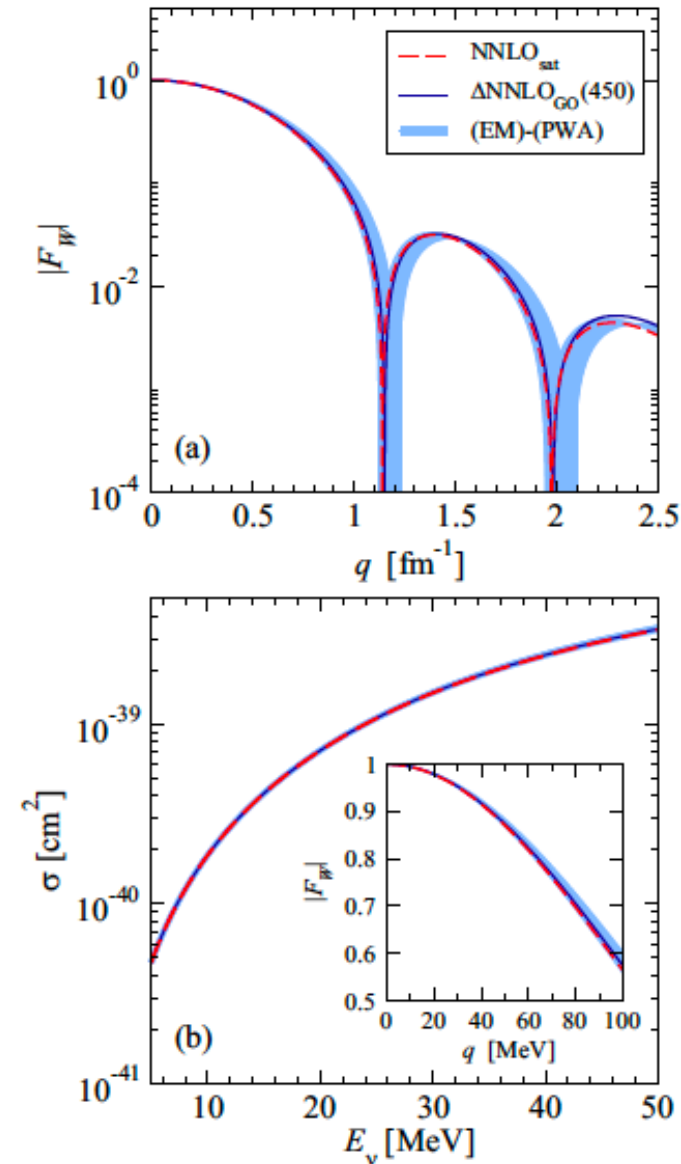
Lepton-nucleus interactions (Image credit: Jefferson Lab)

Progress in neutrino-nucleus scattering



Neutrino scattering on ^{12}C with one (green) and one plus two-body currents (blue) compared to MiniBooNE experimental data.

Lovato et al, Phys. Rev. X 10, 031068 (2020)

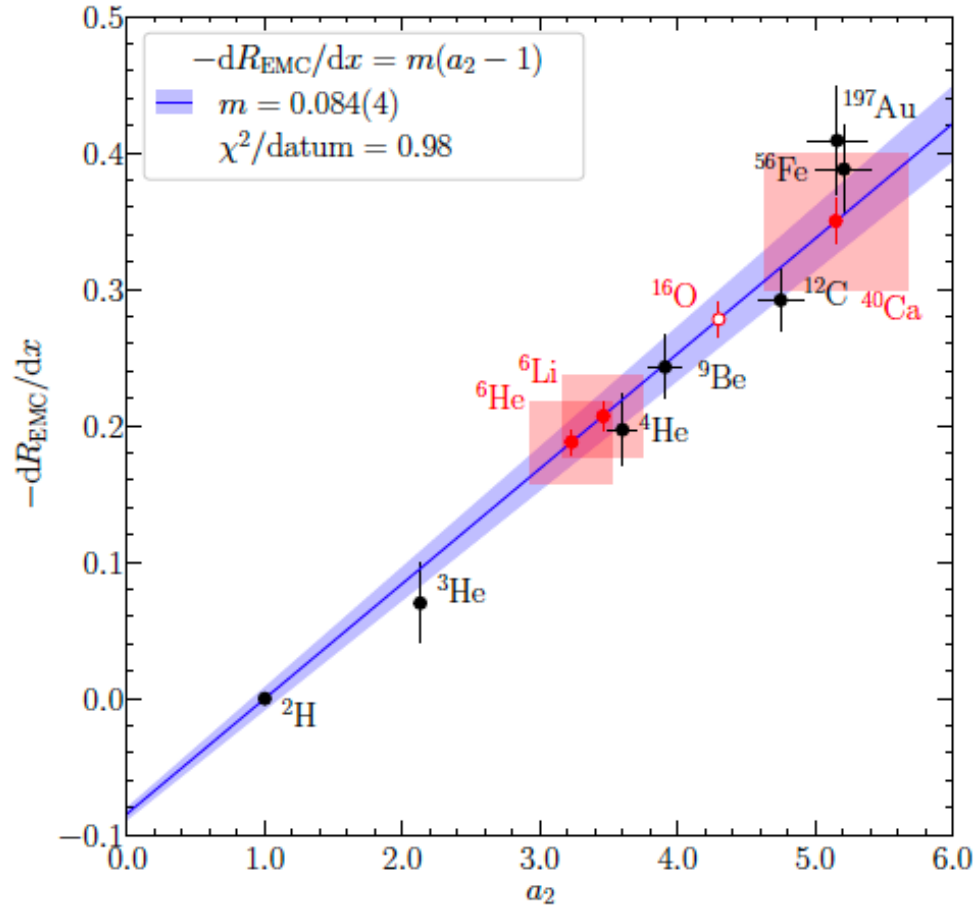


Top: ^{40}Ar weak form factor.

Bottom: Cross section for CE ν NS for ^{40}Ar

Payne et al., Phys. Rev. C 100, 061304(R) (2019)

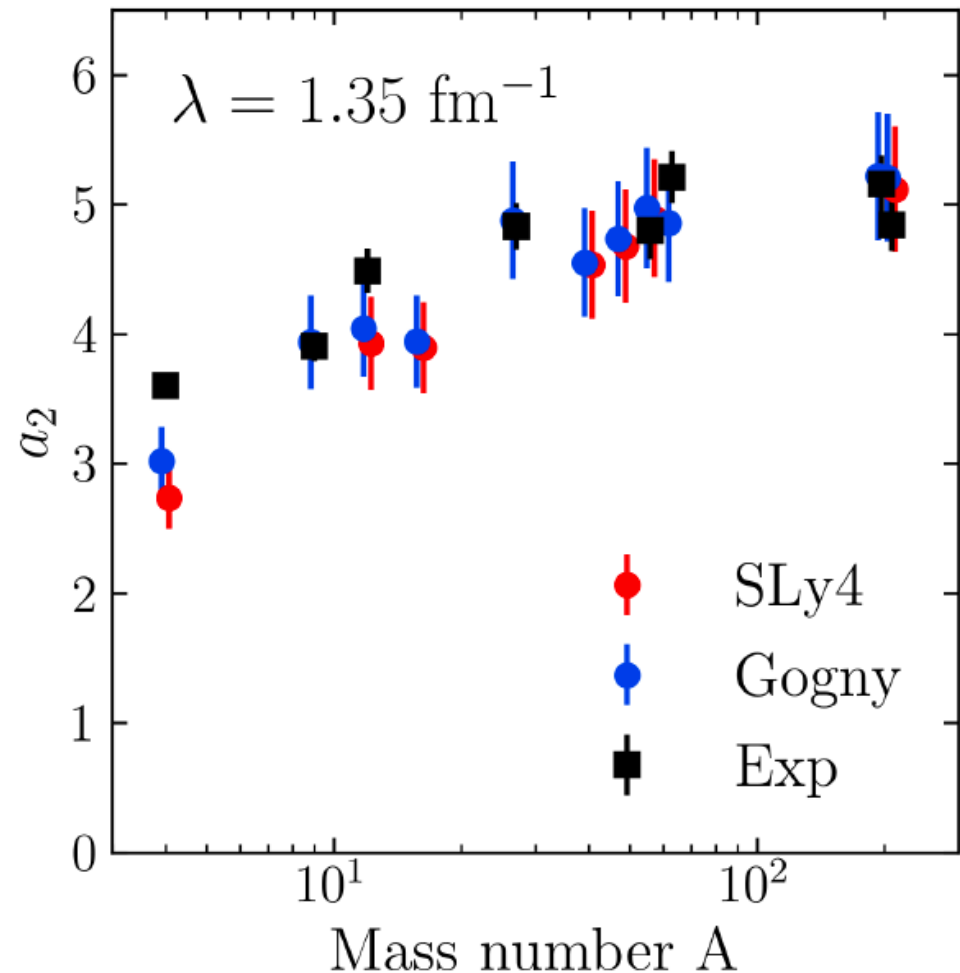
EMC effect and short-range correlations



Lynn, Lonardoni et al., J. Phys. G 47 (2020) 045109

Chen et al., Phys. Rev. Lett. 119, 262502 (2017)

Chen and Detmold, Phys Lett B 625, 165 (2005)



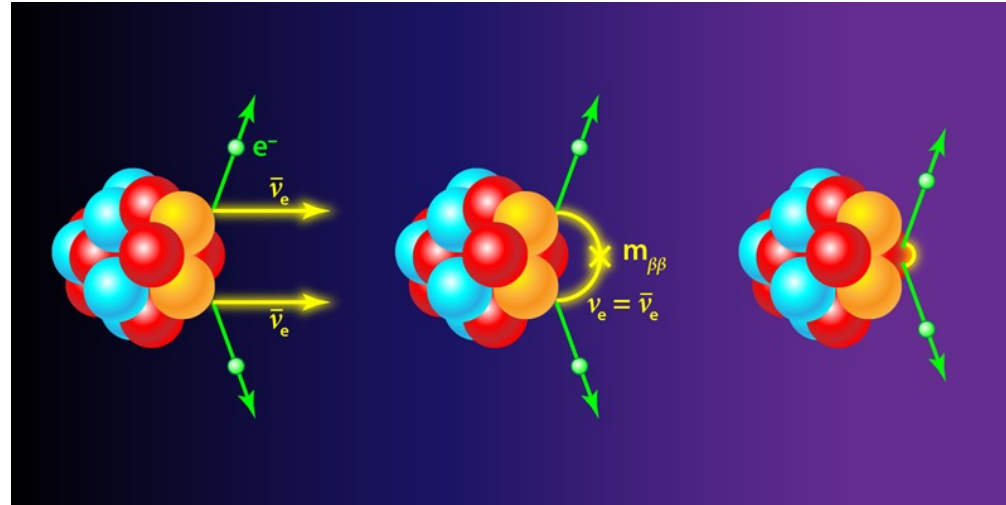
Tropiano, Bogner, Furnstahl,
Phys. Rev. C 104, 034311 (2021)

Much improved understanding between mean-field effects and short-range correlations

Progress in computing electroweak decays



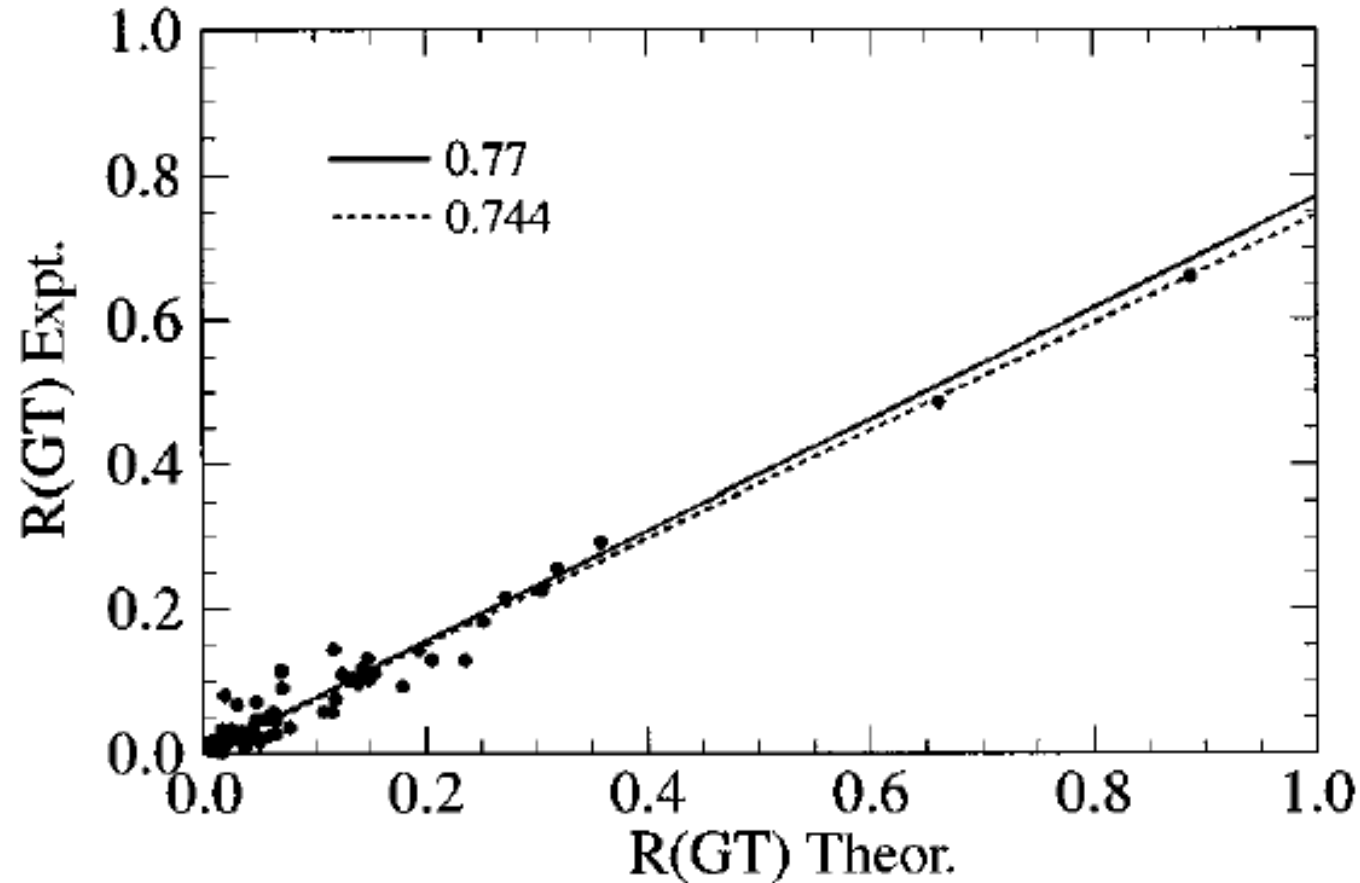
Role of two-body currents in beta decay
(Image credit: Andy Sproles/ORNL)



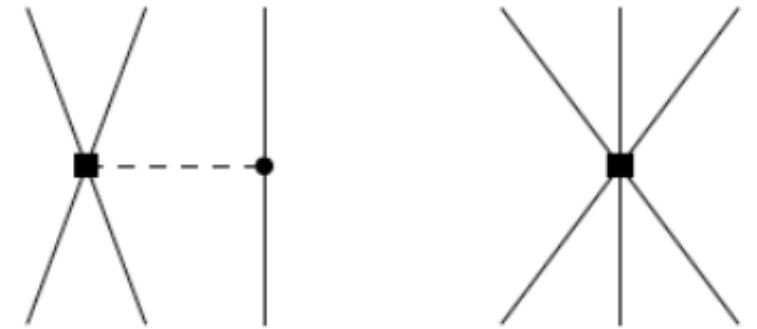
Double beta decay and neutrinoless double beta decays
(Image credit: APS Physics)

The puzzle of quenched β -decay rates

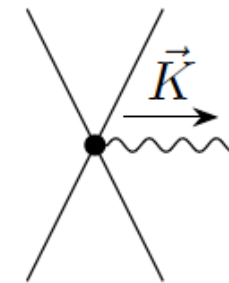
Computed β decays of nuclei are faster than what is expected from the β decay of the neutron



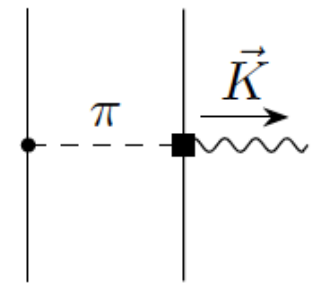
G. Martinez-Pinedo et al, PRC **53**, R2602 (1996)



EFT: Three-nucleon forces and two-body currents

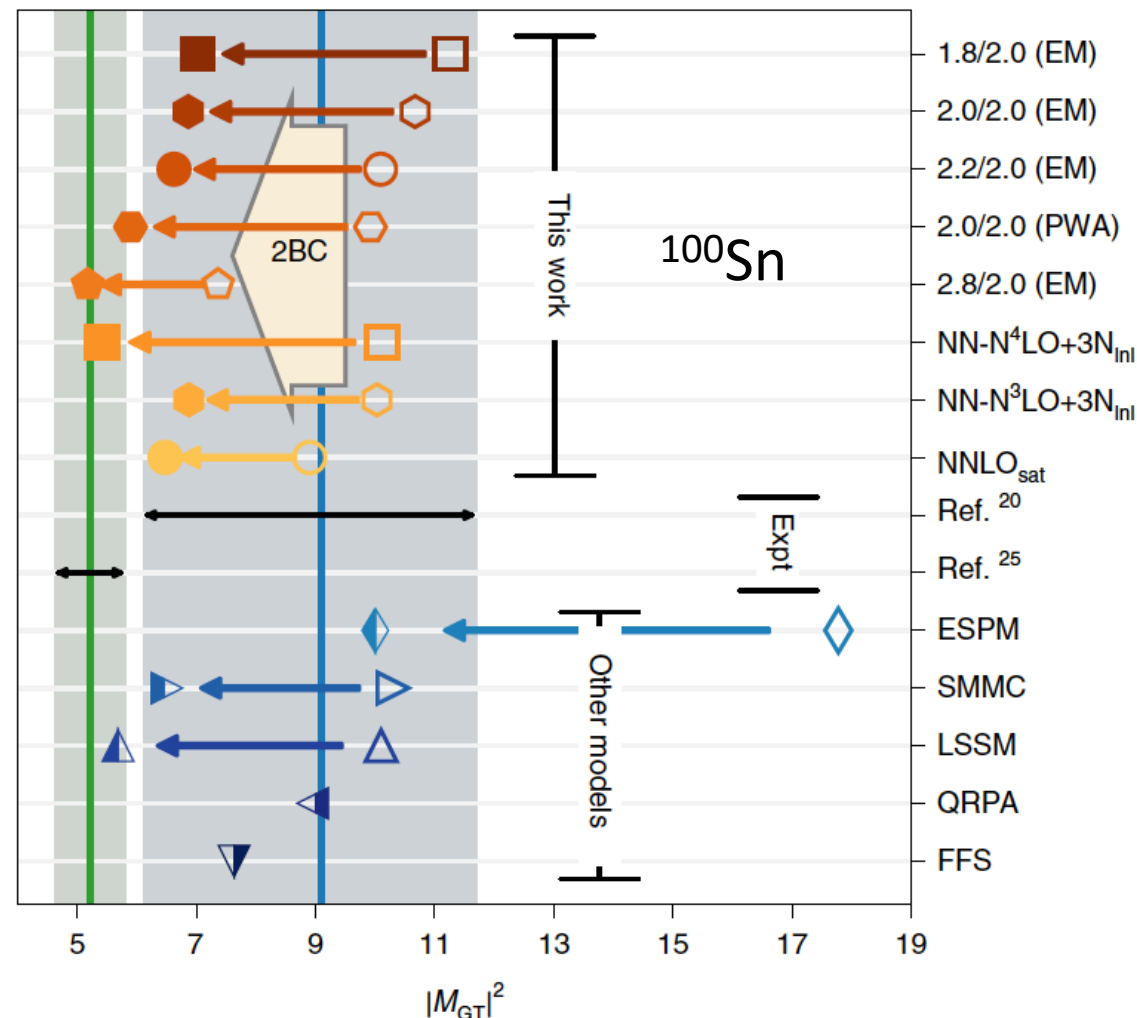
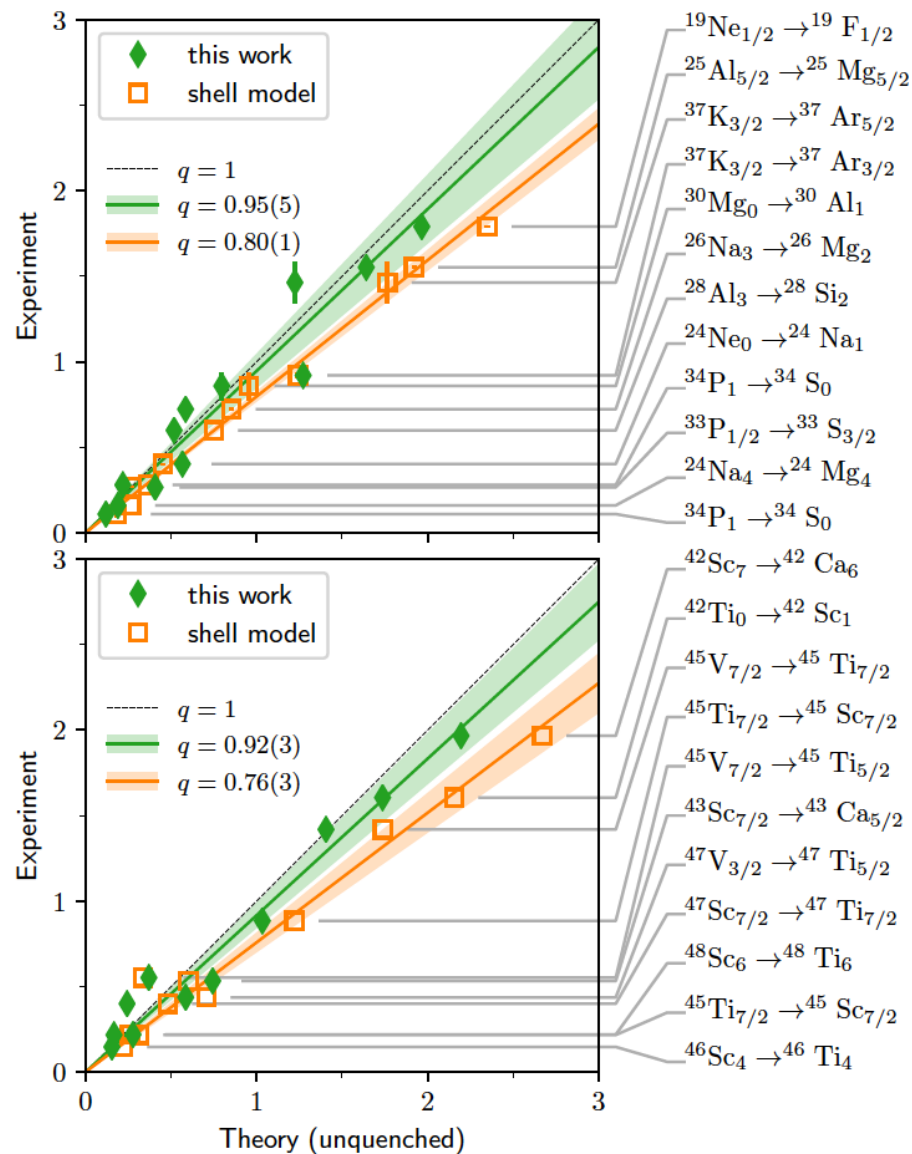


Heavy meson
exchange
 c_D



Pion exchange
 c_3, c_4

Quenching of β -decay rates from chiral EFT



P. Gysbers *et al.*, Nature Physics (2019)

Challenges: Nuclear matrix element for neutrinoless $\beta\beta$ decay

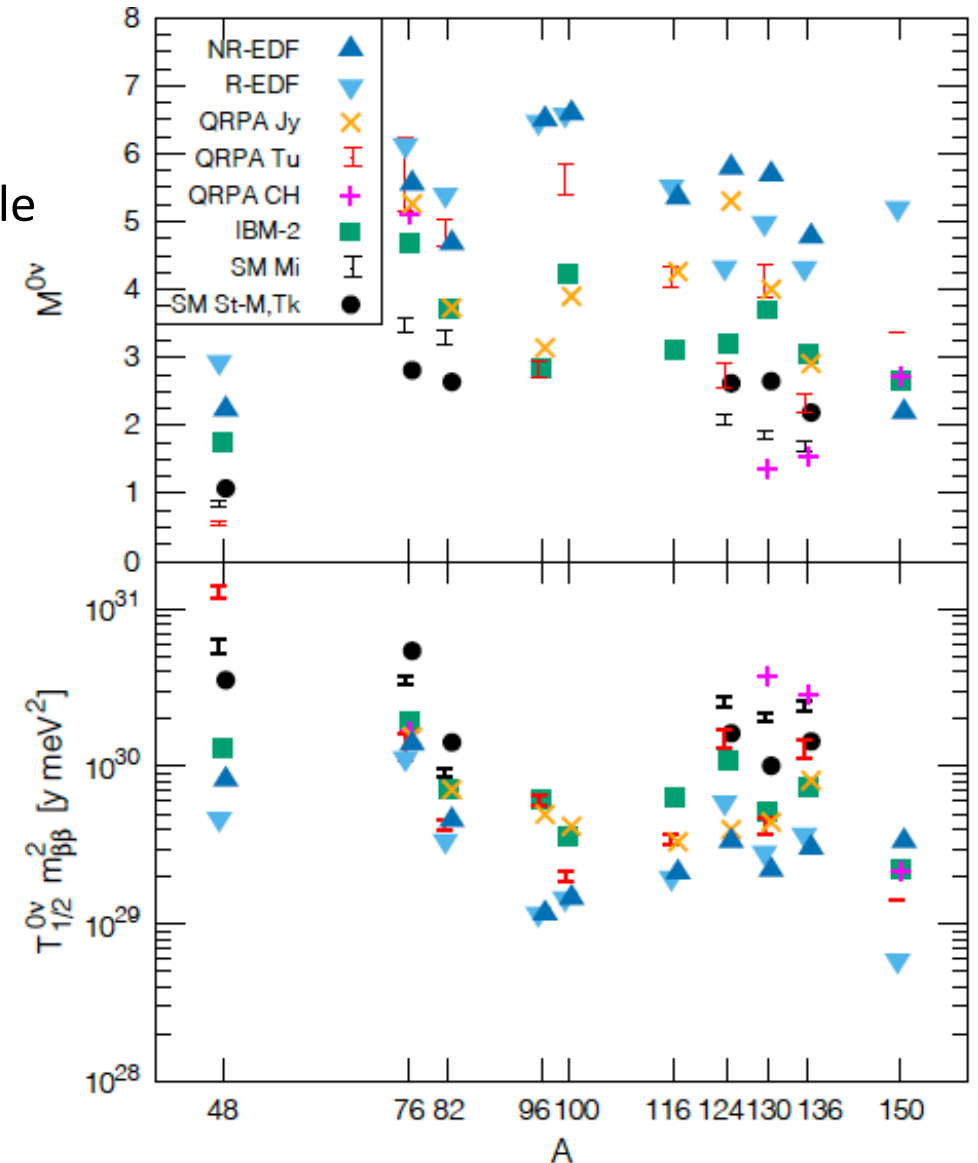
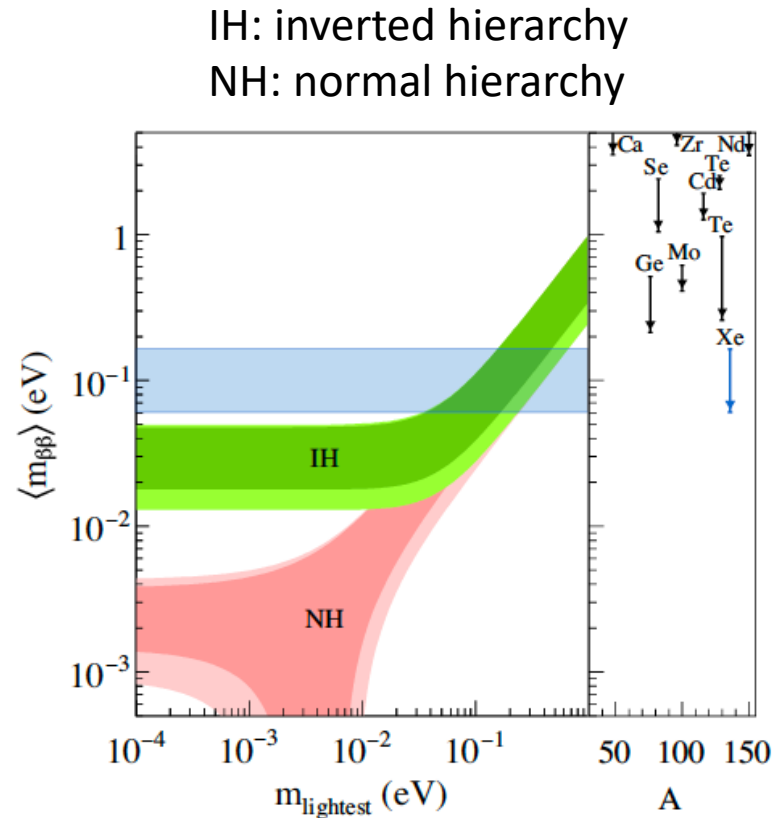
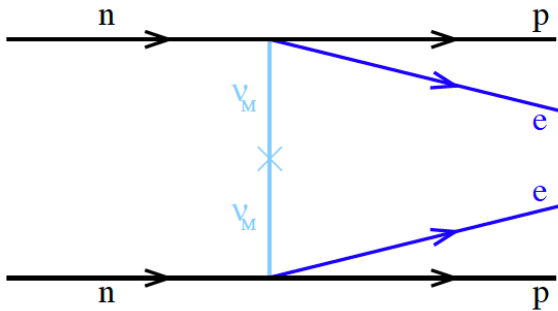
Hypothesis: The neutrino is a Majorana fermion

→ Search for neutrinoless $\beta\beta$ decay

Interest: Next-generation experiments will probe inverted hierarchy

Need: Nuclear matrix element to relate lifetime to neutrino mass scale

Light Majorana-neutrino exchange in $\beta\beta$ decay



Nuclear matrix element for neutrinoless double beta decay of ^{48}Ca

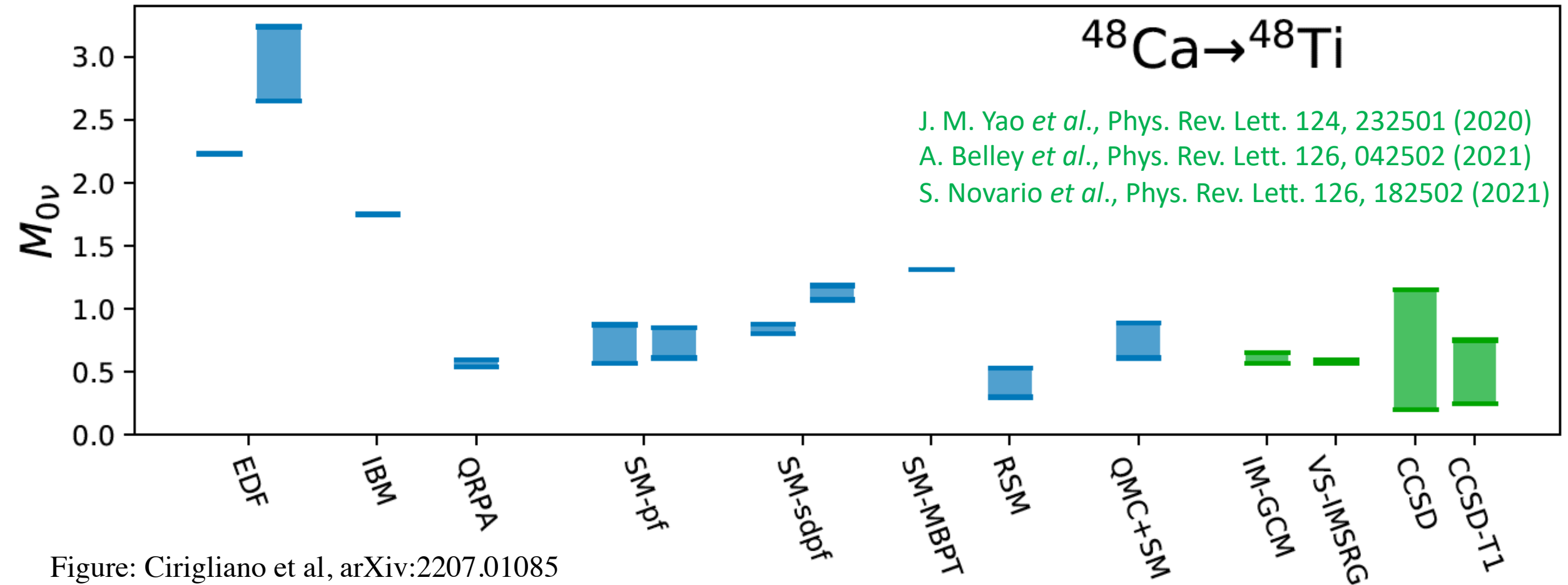


Figure: Cirigliano et al, arXiv:2207.01085

Unknown two-body contact needed for proper renormalization [Cirigliano et al, Phys. Rev. Lett. 120, 202001 (2018)]

- Lattice QCD?
- Cottingham method?

Progress: nuclear matter equation of state

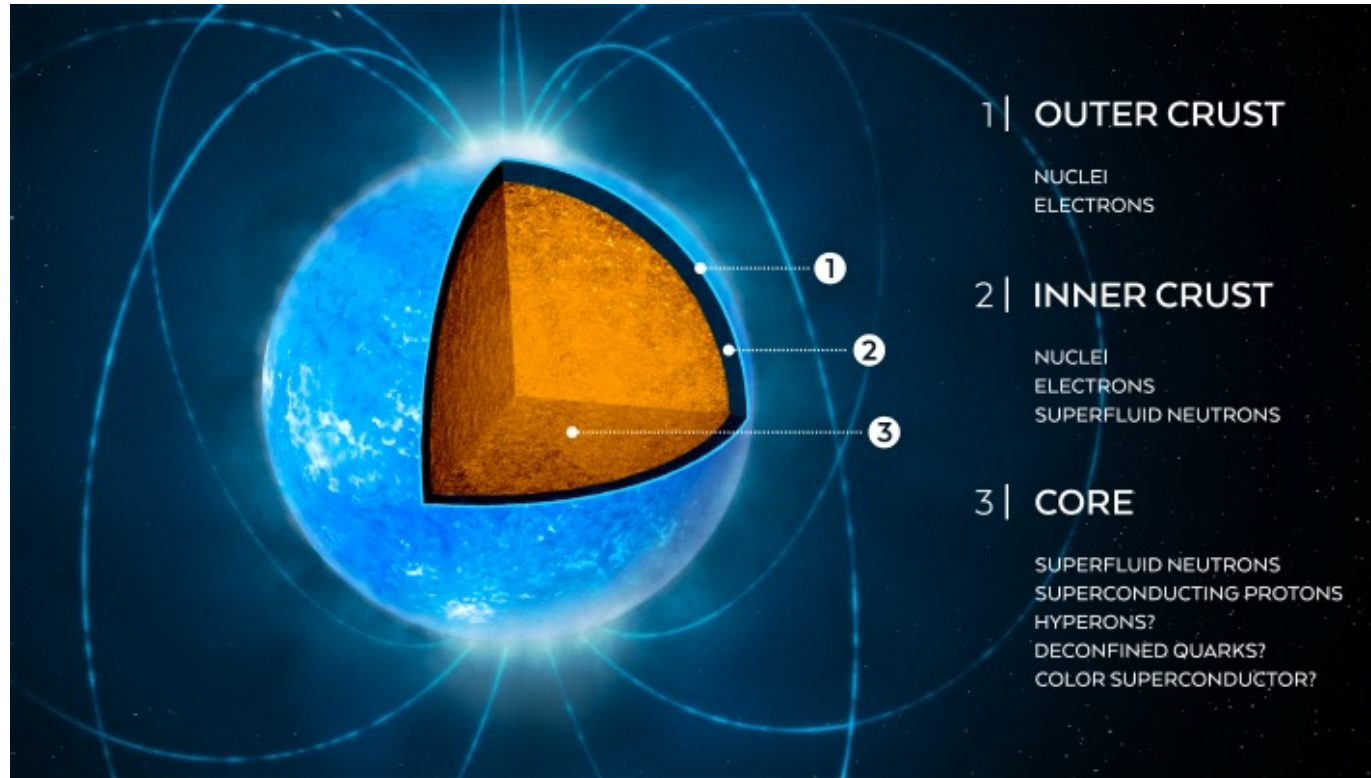
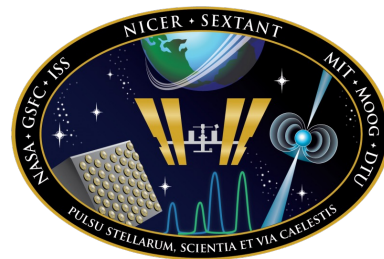


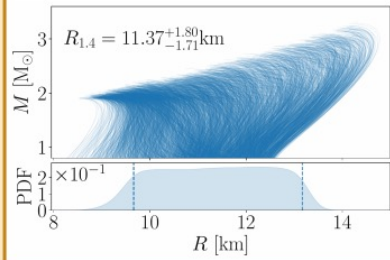
Image credit: Watts et al., Rev. Mod. Phys. 88 021001 (2016)



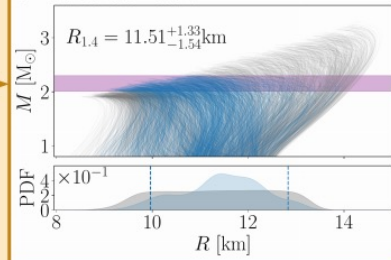
Multimessenger constraints on the neutron-star equation of state

Prior construction

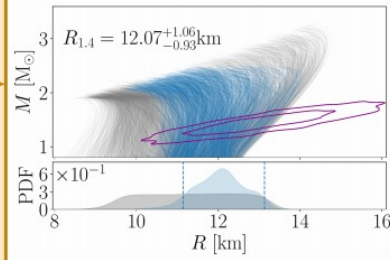
(A) Chiral effective field theory:
EOS derived with the chiral EFT framework



(B) Maximum Mass Constraints:
PSR J0740+6620/ PSR J0348+4032/ PSR J1614-2230 and GW170817/AT2017gfo remnant classification

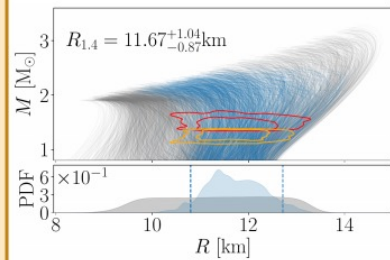


(C) NICER:
PSR J0030+0451

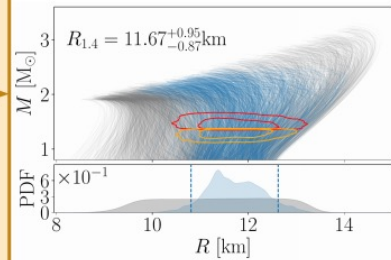


Parameter estimation

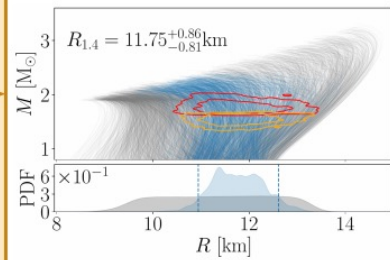
(D) GW170817:
reanalysis with IMRPhenomPv2_NRTidalv2



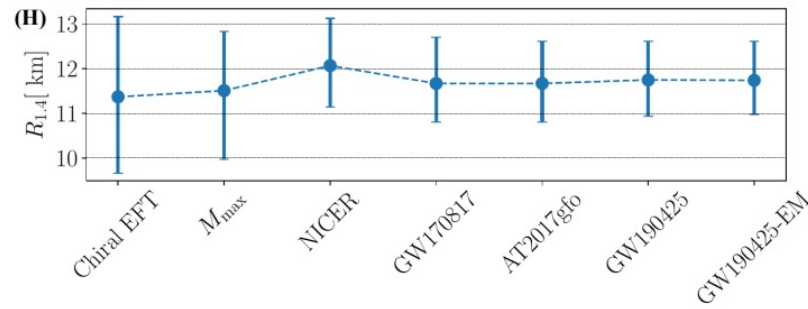
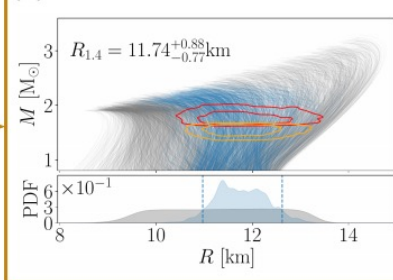
(E) AT2017gfo:
analysis of the observed lightcurves



(F) GW190425:
reanalysis with IMRPhenomPv2_NRTidalv2



(G) No EM detection for GW190425:



EOS constrained by QMC calculations combined with neutron-star (NS) data from gravitational-wave and electromagnetic observations of NS mergers, mass measurements, and NICER.

Statistical analysis of all available data from NSs and NS mergers provides the most stringent constraints on the radius of a typical $1.4 M_{\text{sol}}$ NS

$$R_{1.4} = 11.75^{+0.86}_{-0.81} \text{ km}$$

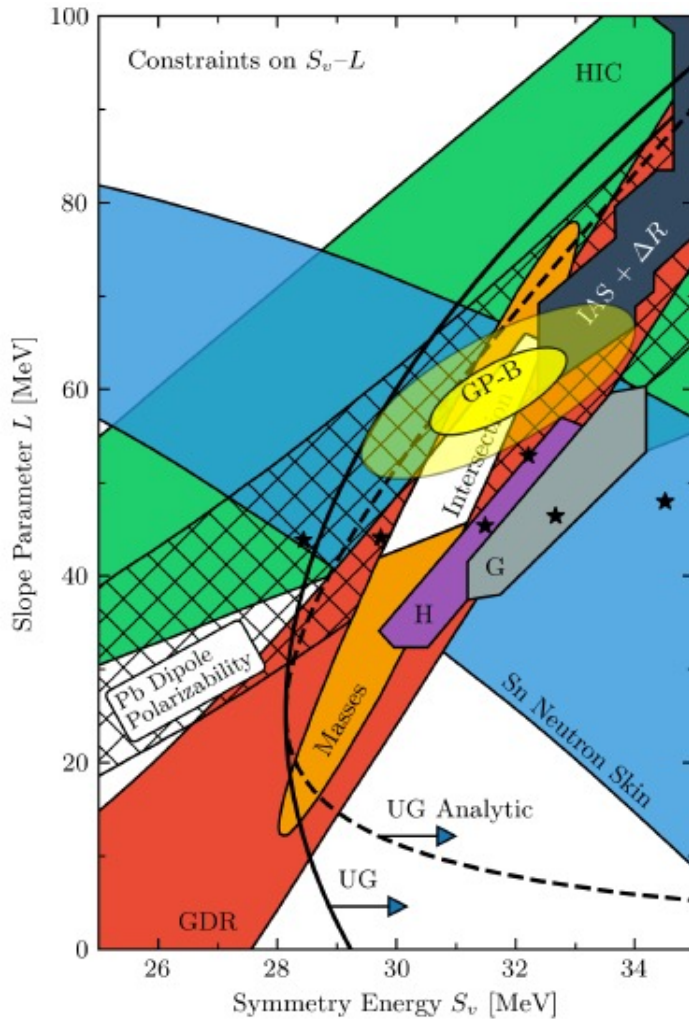
Evolution of neutron-star mass-radius relation as more astrophysical data is included. Insets show the radius posterior of a typical $1.4 M_{\text{sol}}$ neutron star.

C. Capano, I. Tews, et al., Nat. Astron. **4**, 625 (2020)

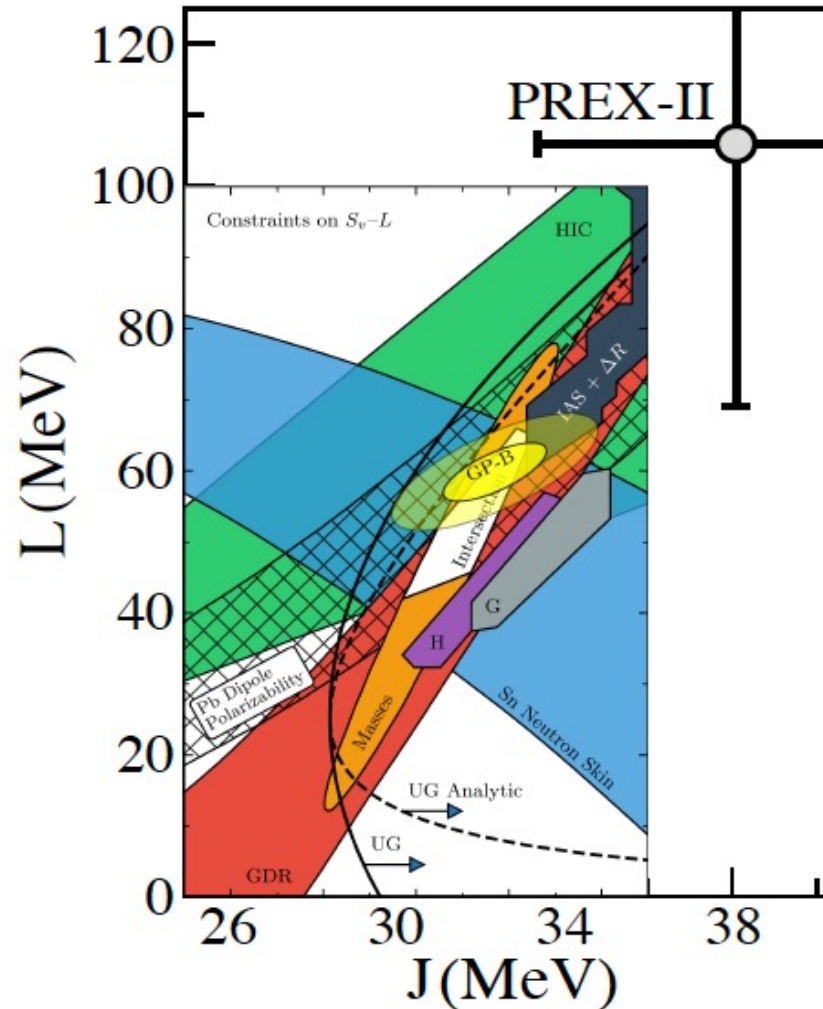
T. Dietrich et al., Science **370**, Iss. 6523, 1450 (2020)

I. Tews et al., Astrophys. J. Lett. **908**, L1 (2021)

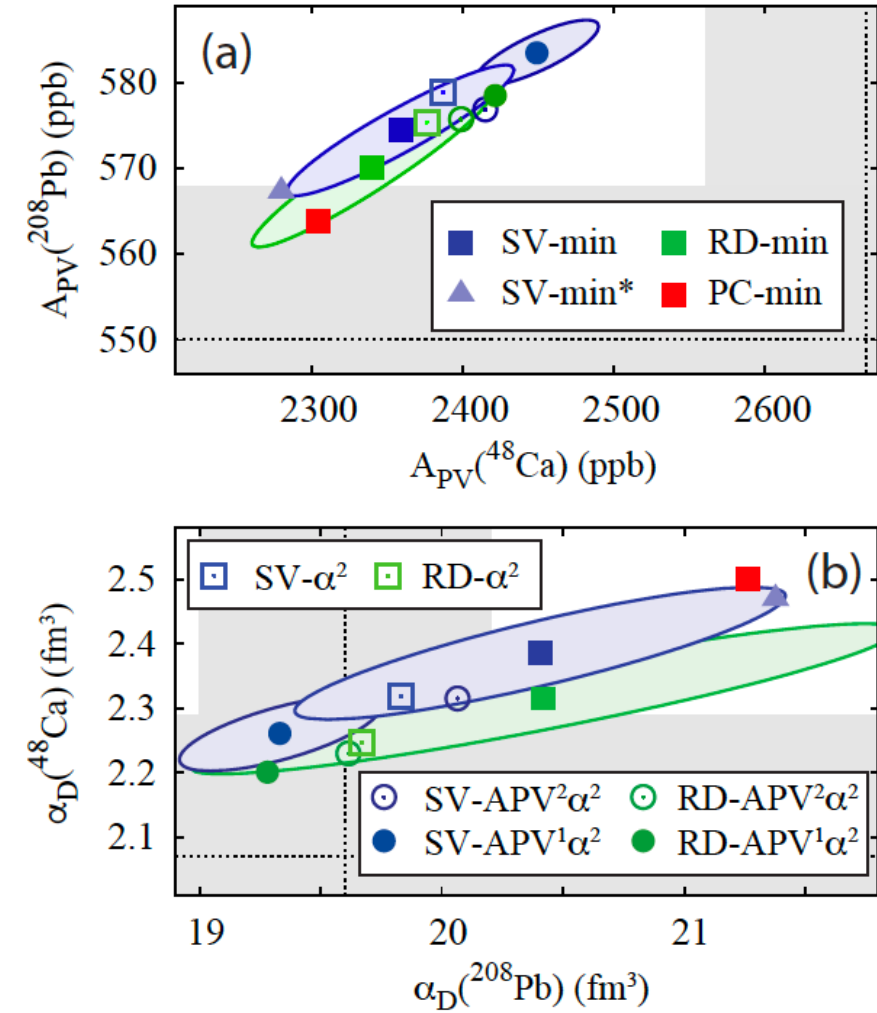
Nuclear equation of state near saturation



Drischler et al., Phys. Rev. Lett. 125, 202702 (2020)
 Drischler, Hebeler & Schwenk, Phys. Rev. Lett. (2019)



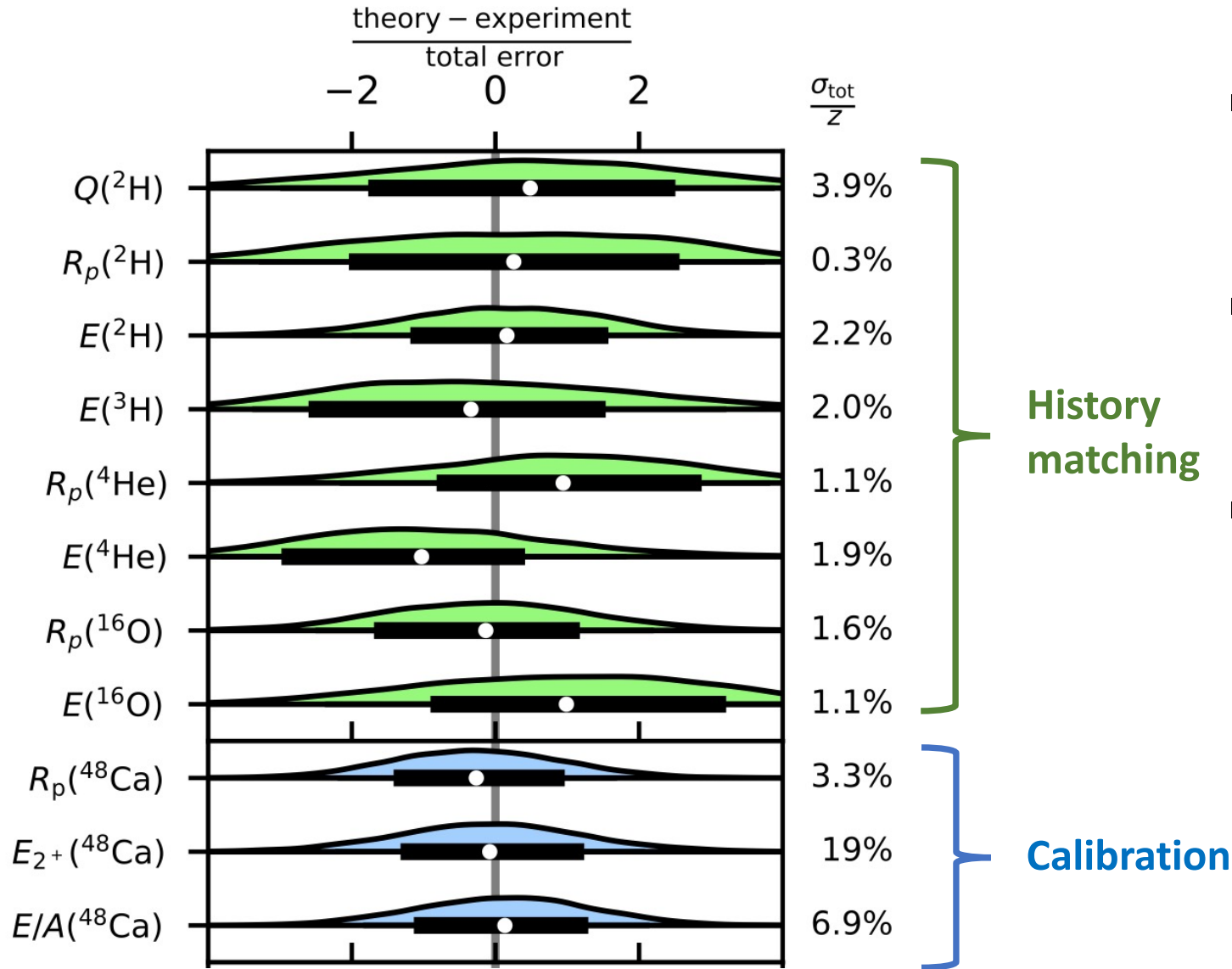
Reed, Fattoyev, Horowitz, Piekarewicz,
 Phys. Rev. Lett. 126, 172503 (2021)



Reinhardt, Roca-Meza, Nazarewicz, arXiv:2206.03134

Some tension between the interpretation of the PREX result and nuclear structure knowledge

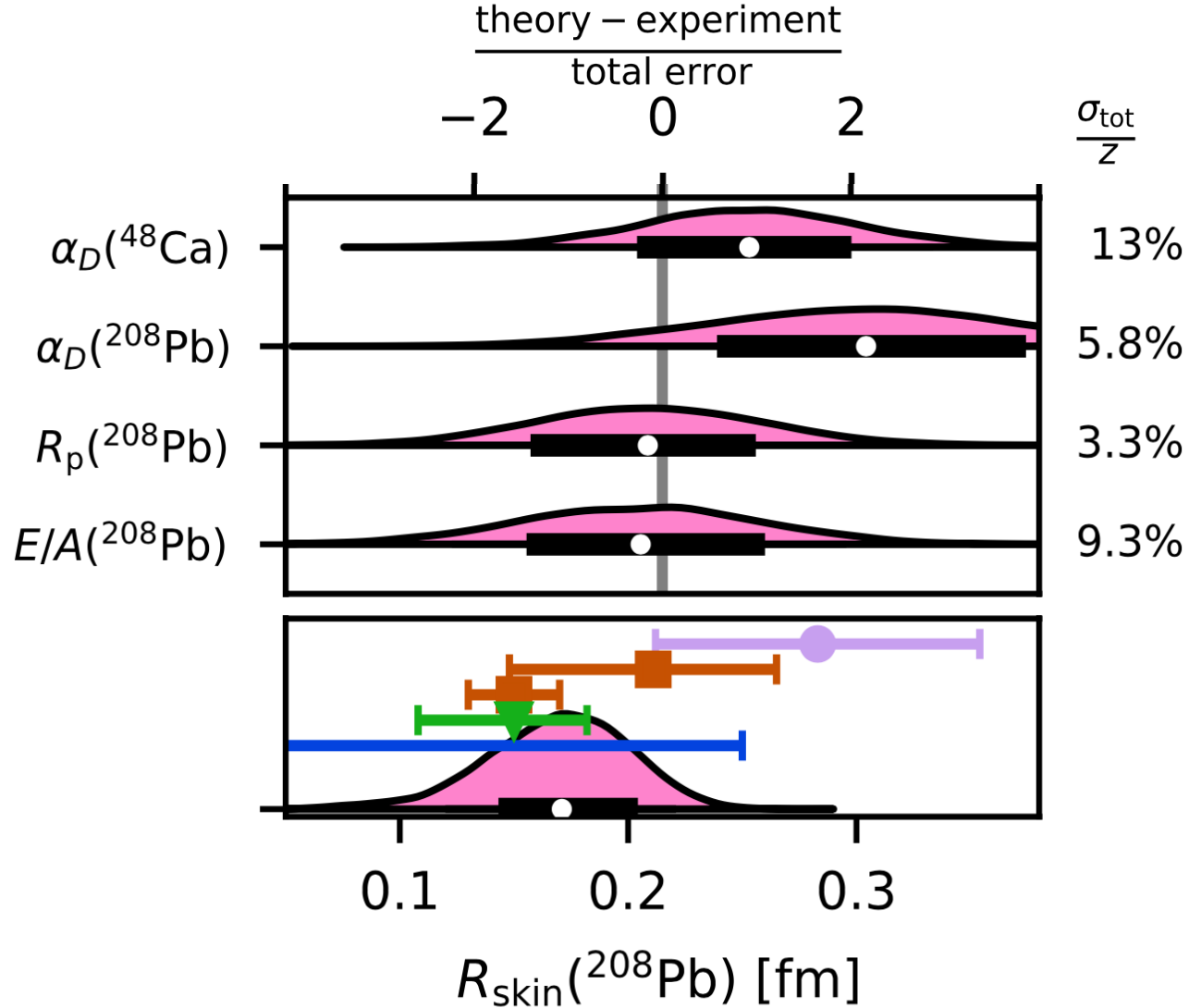
Neutron skin of ^{208}Pb



- Emulators allows for billions of ab-initio simulations of selected nuclei
- Opens up new ways for making predictions and addressing uncertainties
- History matching – identify parameters of the model that give results consistent with data

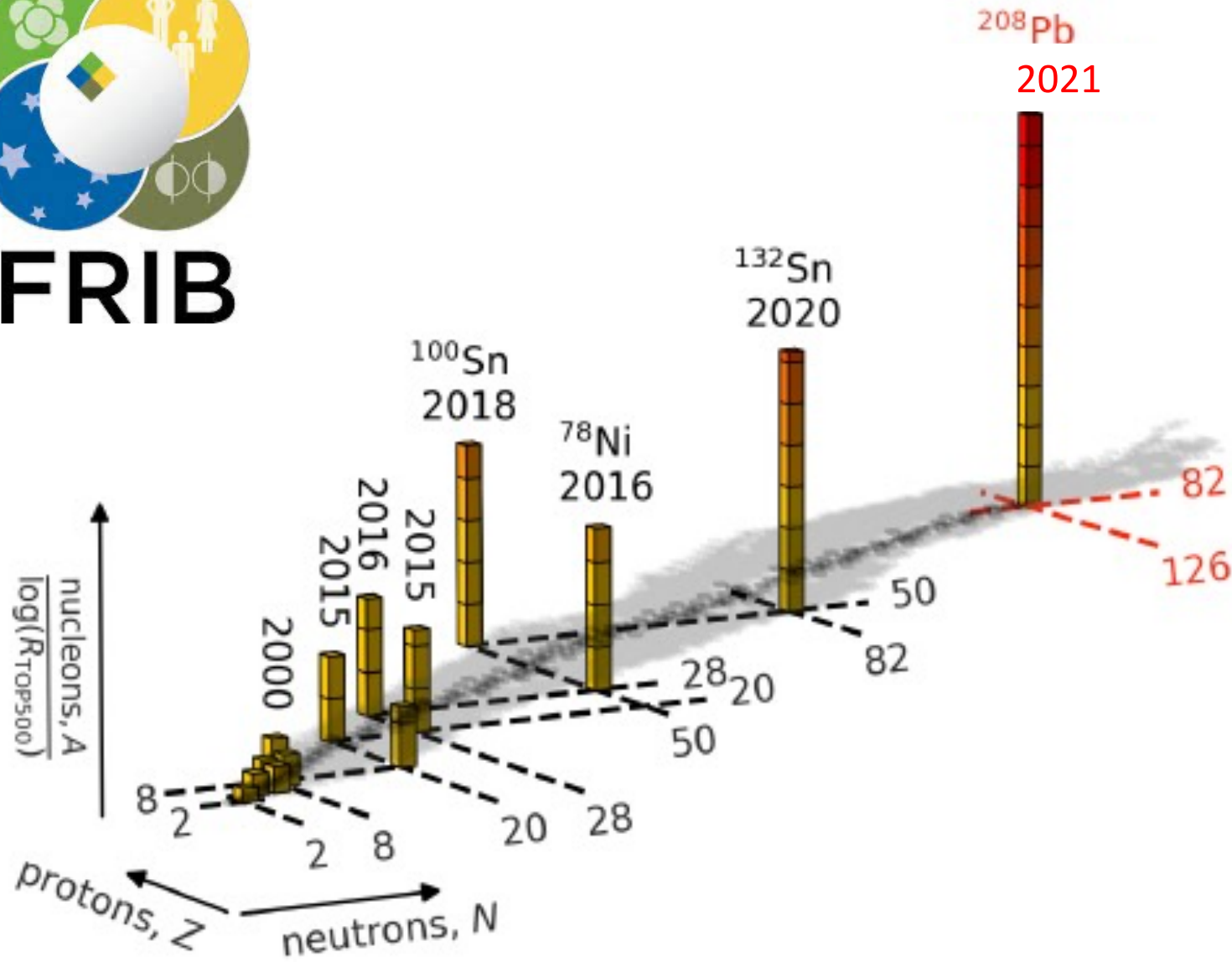
Explored 10^9 different parametrizations and found 34 non-implausible interactions
Calibration on ^{48}Ca yields weighted samples for which we can use for quantified predictions of ^{208}Pb

Neutron skin of ^{208}Pb



- Posterior predictive distribution for the neutron skin in ^{208}Pb (experiments: electroweak (purple), hadronic (red), electromagnetic (green), and gravitational waves (blue) probes)
- $R_{\text{skin}}(^{208}\text{Pb}) = 0.14 - 0.20$ fm (68% credible interval) exhibits a mild tension with the value extracted from the less precise PREX experiments

Progress in computing nuclei from EFT Hamiltonians



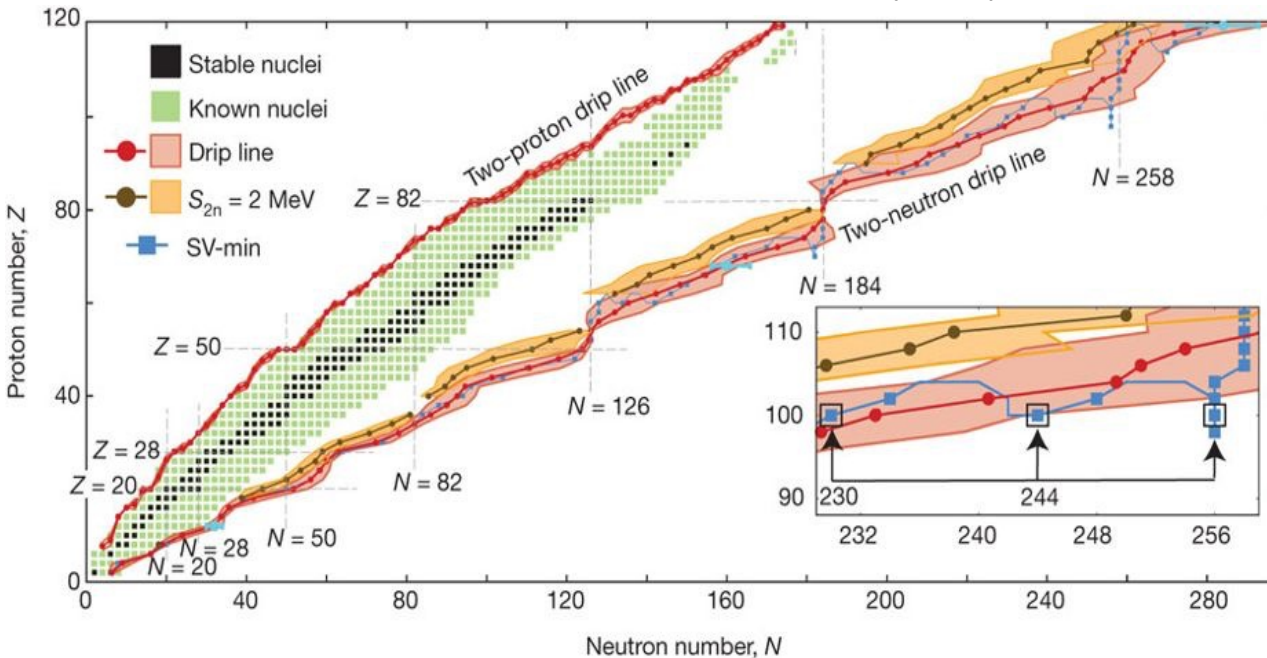
Tremendous progress

- Ideas from EFT and RG
- Methods that scale polynomially with mass number
- Ever-increasing computing power
- Light nuclei often very hard to compute because of their complex structure / extreme clustering
- Mean-field states enable computations of many heavier nuclei at polynomial cost
- Challenges: shape coexistence, clustering, weak binding, ...

Limits of the nuclear landscape ...

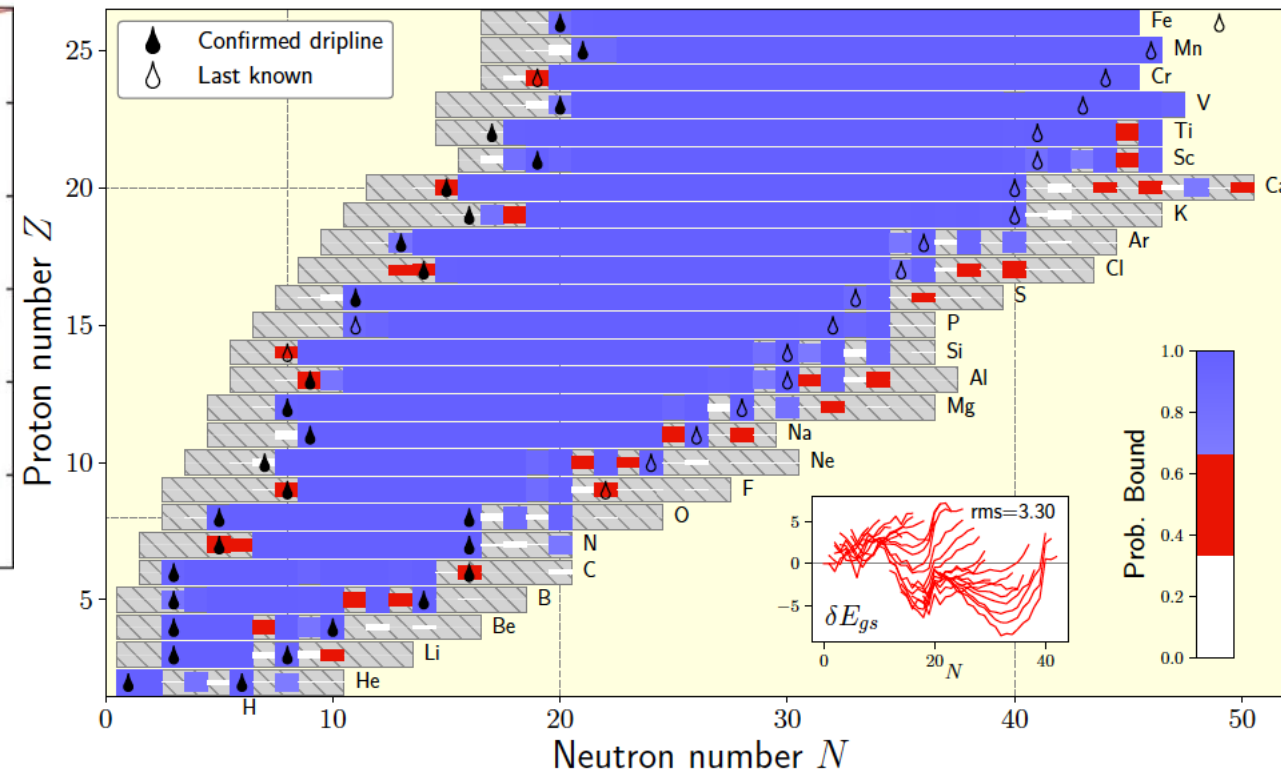
... come within the limits of Hamiltonian-based methods

Nuclear DFT: Erler et al, Nature (2012)



$6,900 \pm 500_{\text{sys}}$ nuclei with $Z \leq 120$

EFT Hamiltonian: Holt, Stroberg, Schwenk & Simonis (2019)



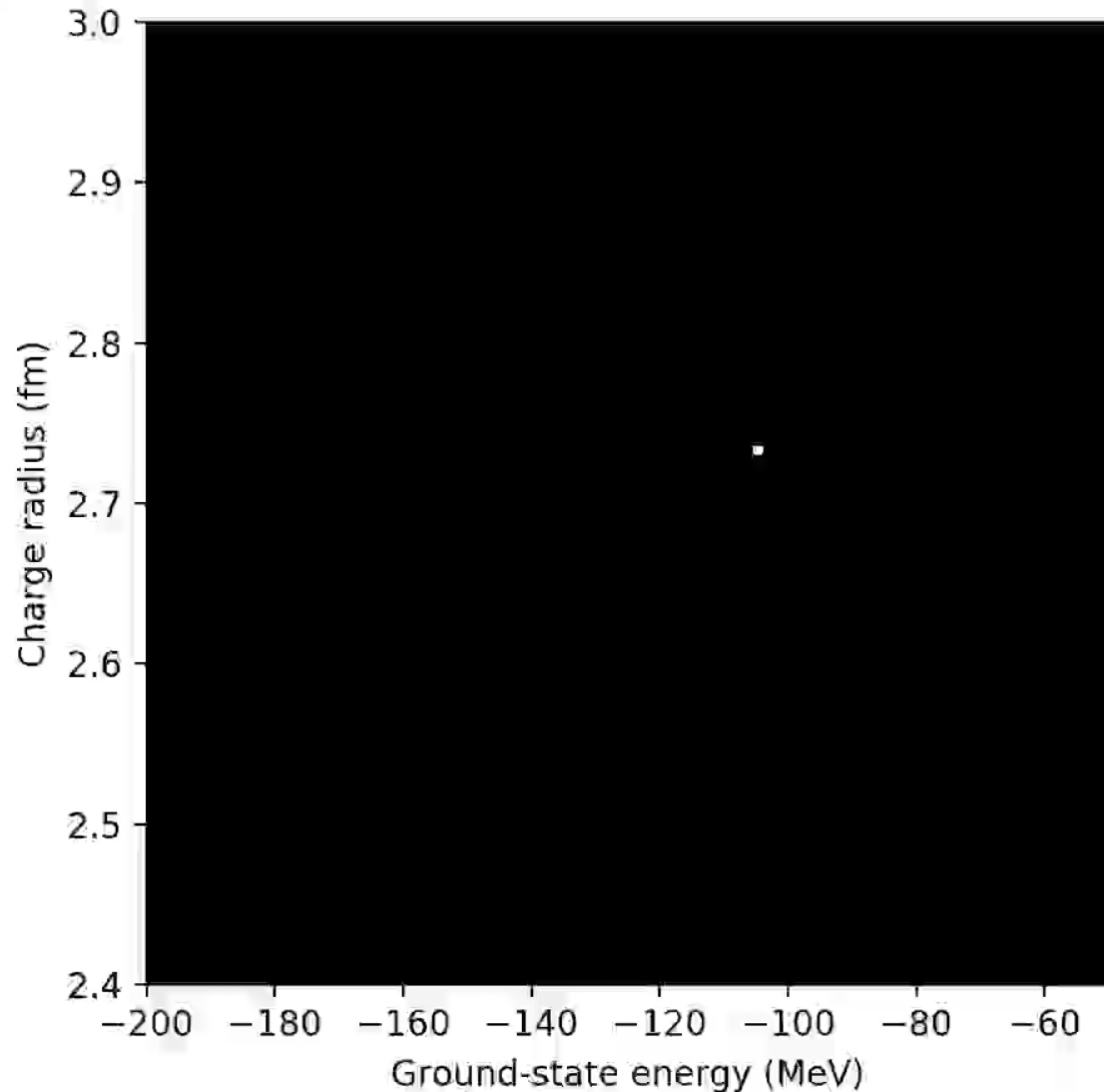
- Computing power continues to grow exponentially with time
- Combine with methods that scale polynomially with mass number

[Dickhoff & Barbieri; Dean & Hjorth-Jensen; Hagen, Jansen & TP; Tsukiyama, Bogner, Hergert & Schwenk; Elhatisari, Epelbaum, Lee, Lähde, Lu, Meissner; Soma & Duguet; Holt & Stroberg...]

Frontier: Emulators

(~5 mins: ~ 10^5 energy/radius calculations of ^{16}O)

[x1] SP-CC(64) evaluation 1 Time = 0 s

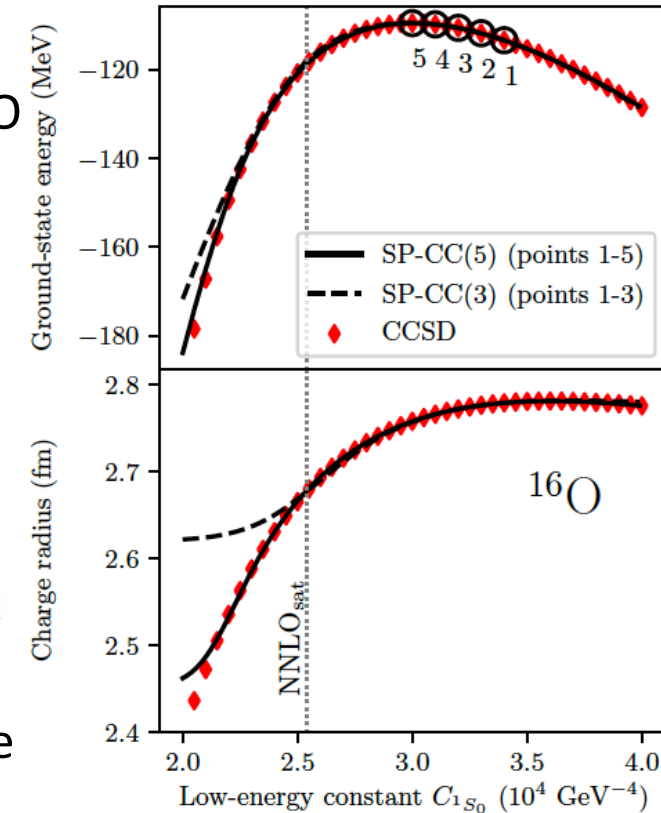


Emulators for ground-state energy and charge radius of ^{16}O for different values of interaction parameters, based on eigenvector continuation [Frame et al., Phys. Rev. Lett. 121, 032501 (2018)]

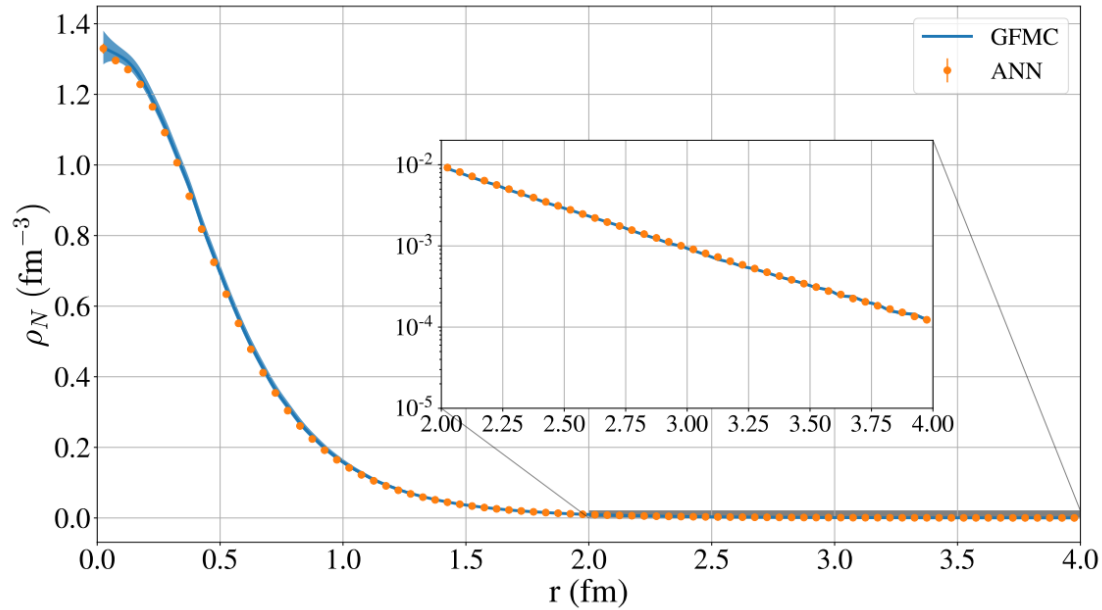
$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\text{LECS}}=16} \alpha_i h_i$$

Accuracy: roughly the pixel size

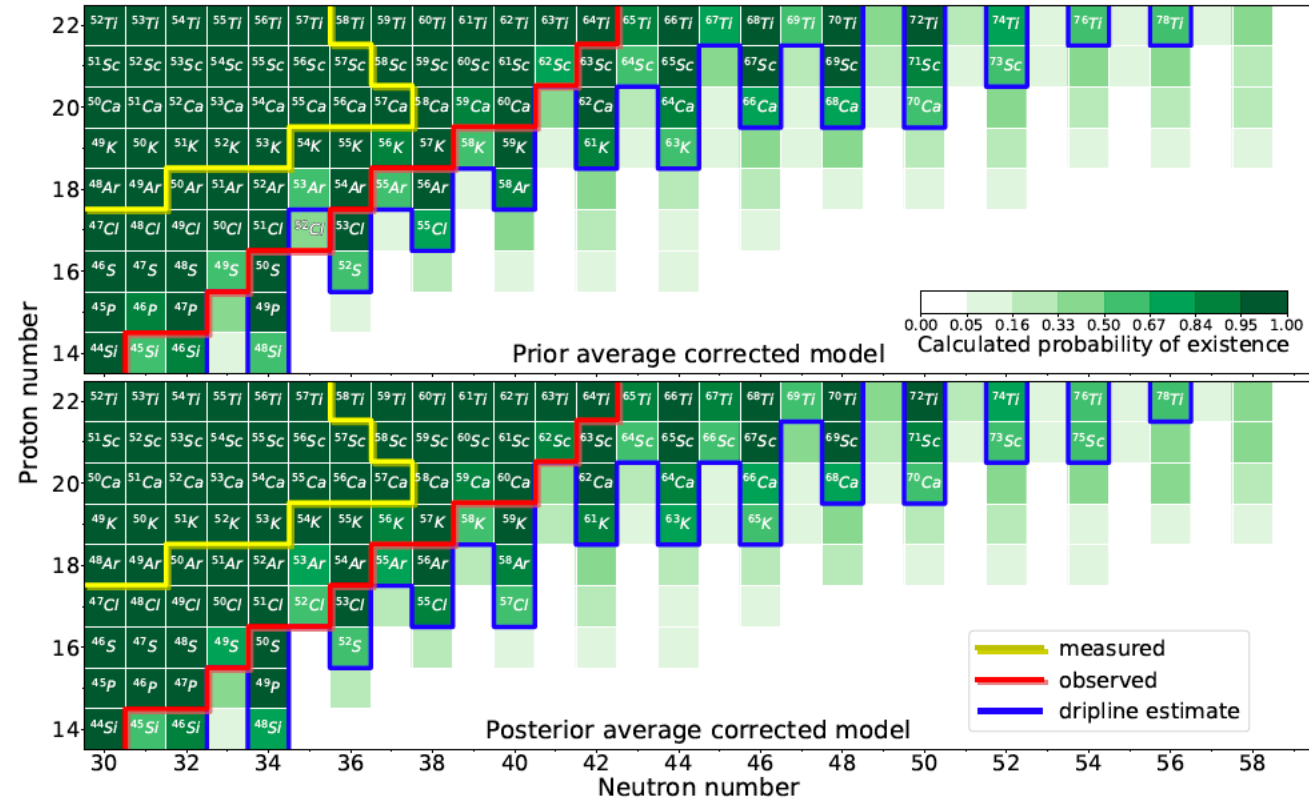
Speedup: 20 years of single node computations can be replaced by a 1 hour run on a laptop [Ekström & Hagen, Phys. Rev. Lett. 123, 252501 (2019)]



Frontier: Machine learning applications

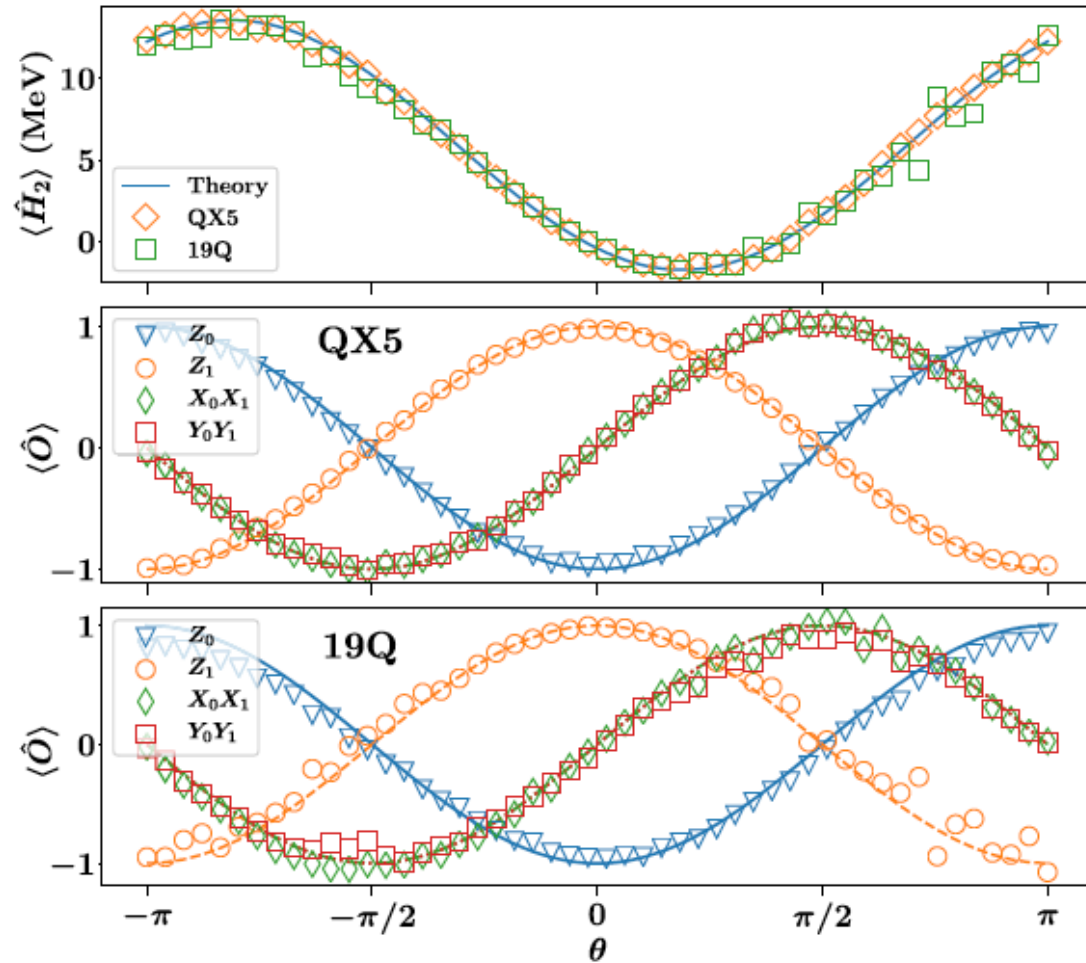


Point-nucleon density of ^3H from the ANN and GFMC
Adams, Carleo, Lovato, Rocco, arXiv:2007.14282

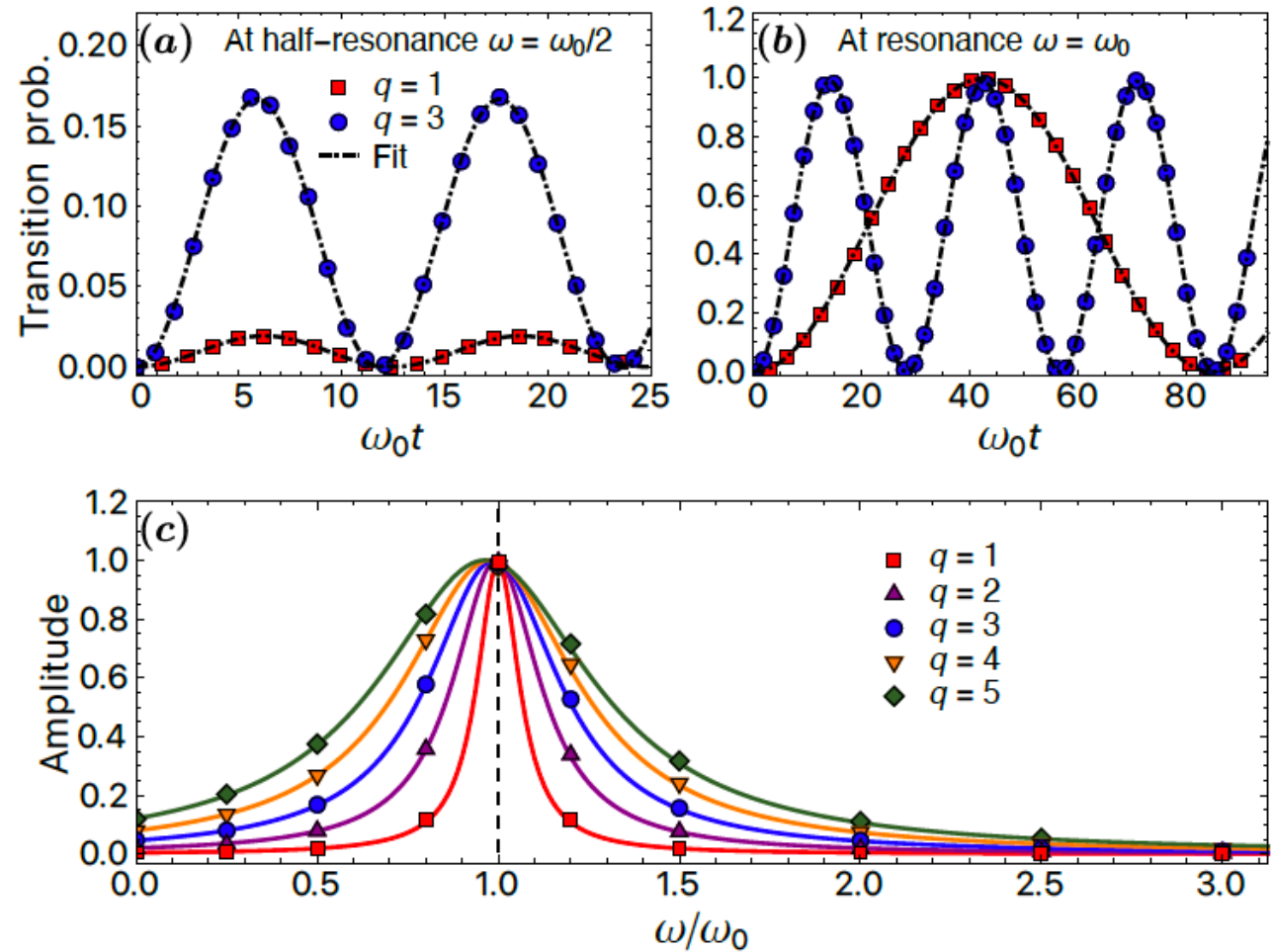


Bayesian model averaging constrains limits of nuclear binding
Neufcourt et al., Phys. Rev. Lett. 122, 062502 (2019)

Frontier: Quantum computing of atomic nuclei



Quantum computation of the deuteron
[Dumitrescu et al (2018)]



Radiative processes on a quantum computer
[Bedaque et al, arXiv:2209.09962]

Summary

- Computations of nuclei with EFT Hamiltonians become now available for heavy nuclei
 - Challenges: nuclear saturation, collective phenomena & clustering, EOS at higher densities, temperature dependence, ...
- Much progress for electroweak transitions and response functions
 - Challenges: role of two-body currents, neutrinoless double beta decay, ...
- Much progress in computing heavy rare isotopes and fission processes
 - Challenges: higher precision within quantified uncertainties, links to chiral EFT, ...
- We have entered a precision era: field moves towards quantified uncertainties
 - Opportunities: emulators, machine learning, history matching, quantum computing...