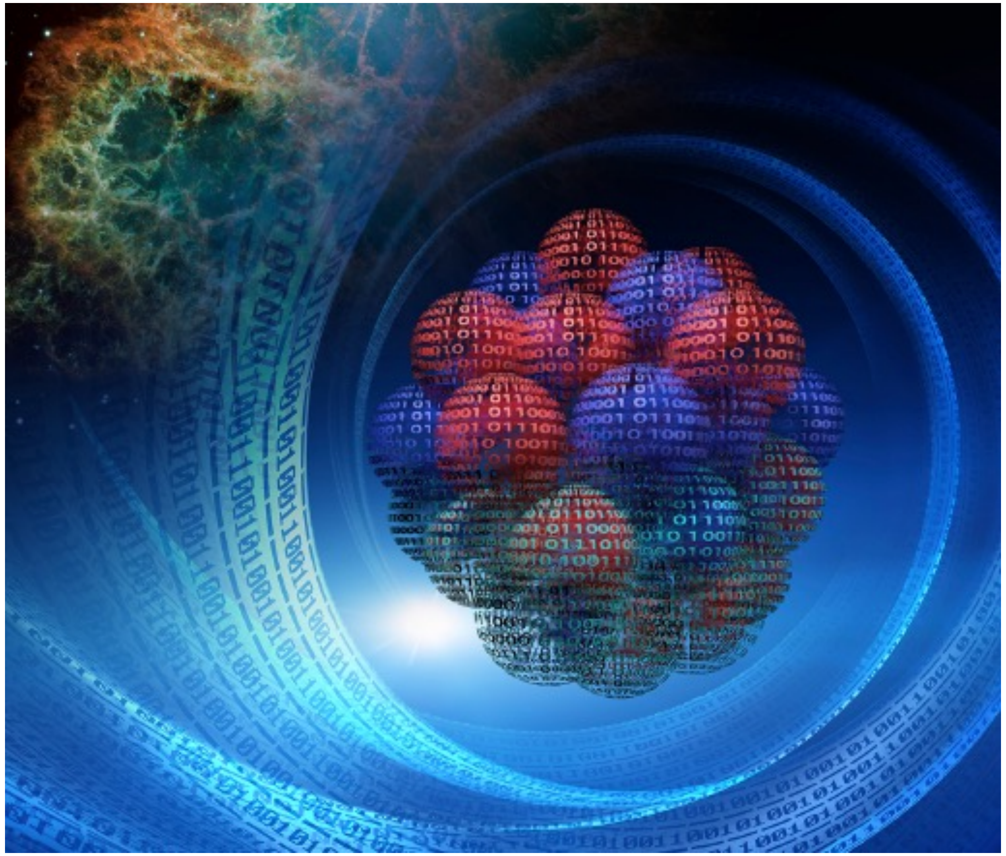
# Quantum many-body problems



Thomas Papenbrock (Thanks to many colleagues!)
University of Tennessee & Oak Ridge National Laboratory

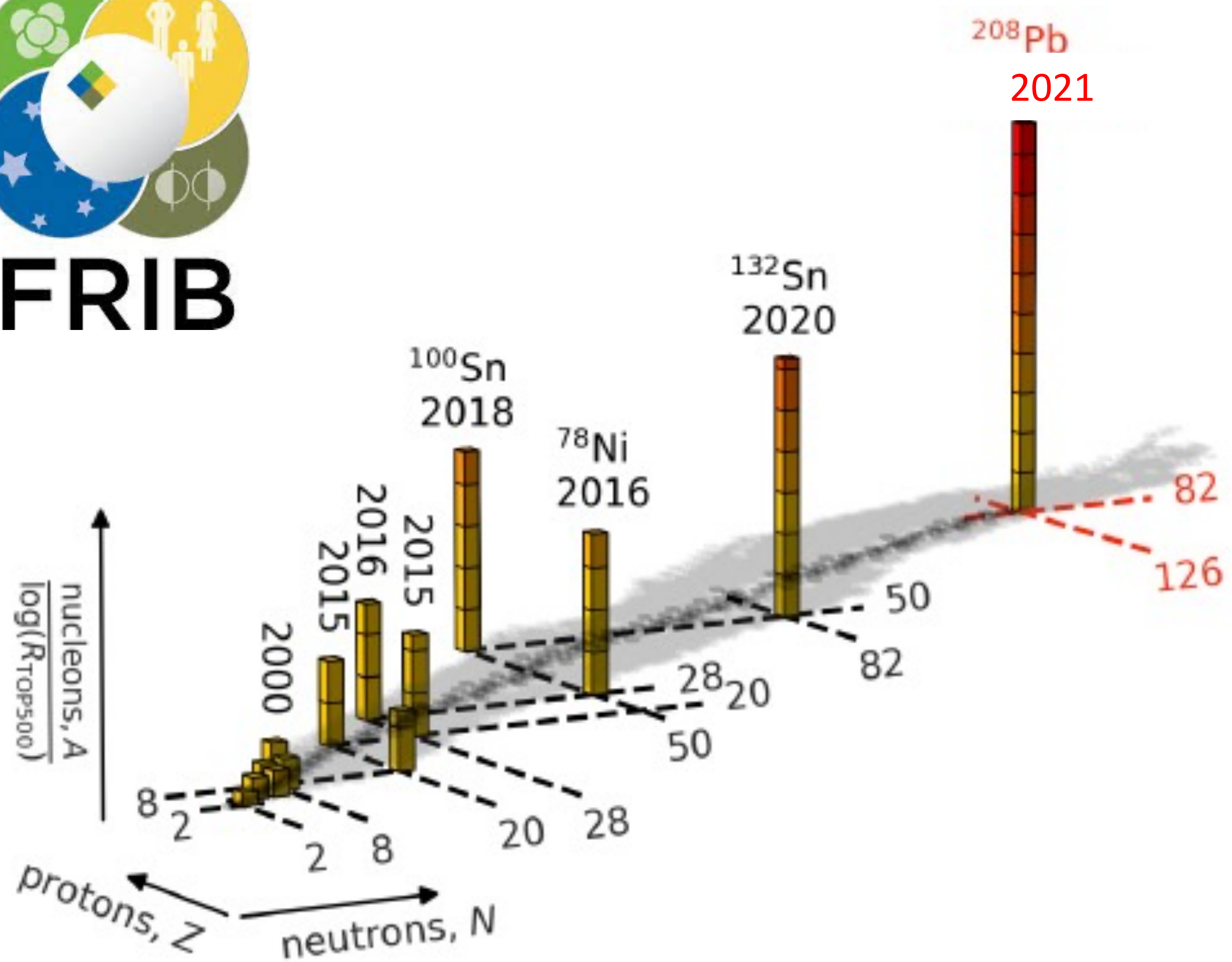
SciDAC
Scientific Discovery through Advanced Computing

Computational Nuclear Physics and AI/ML Workshop

Work supported by the US Department of Energy

NUCLEI
Nuclear Computational Low-Energy Initiative

# Progress in computing nuclei from EFT Hamiltonians

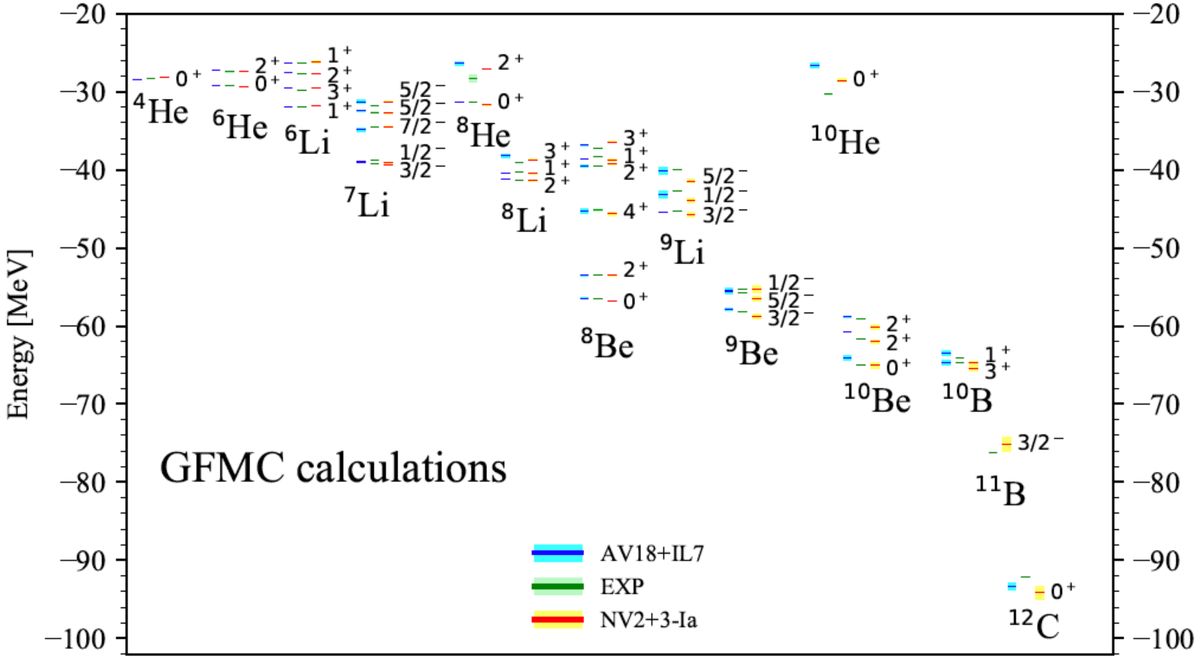



Tremendous progress

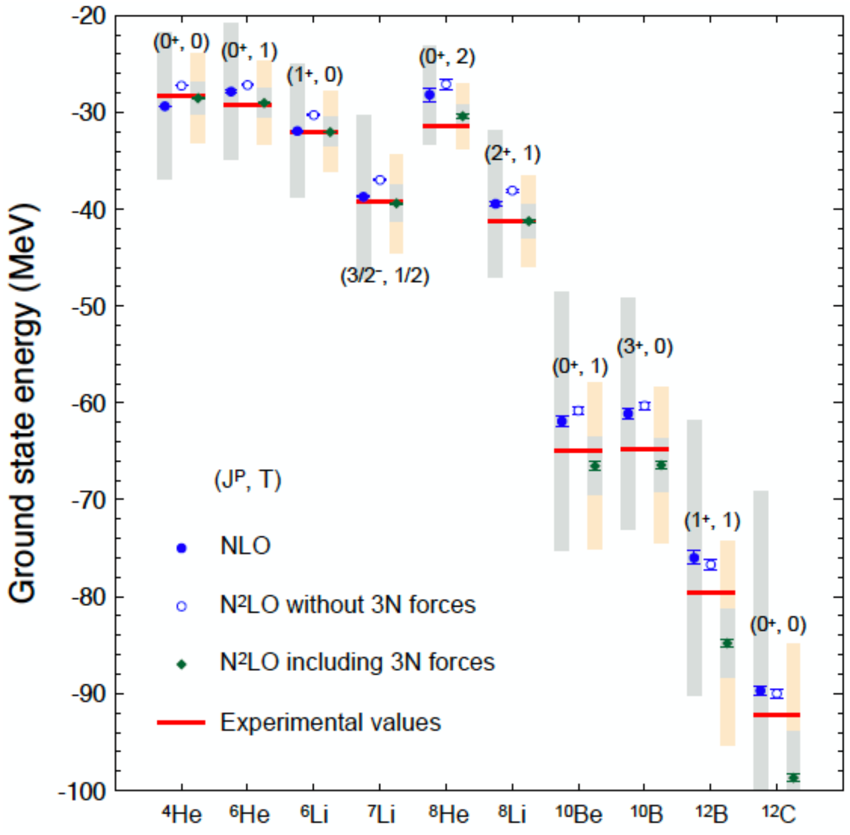
- Ideas from EFT and RG
- Methods that scale polynomially with mass number
- Ever-increasing computing power

- 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, …

# Nuclear interactions and light nuclei




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



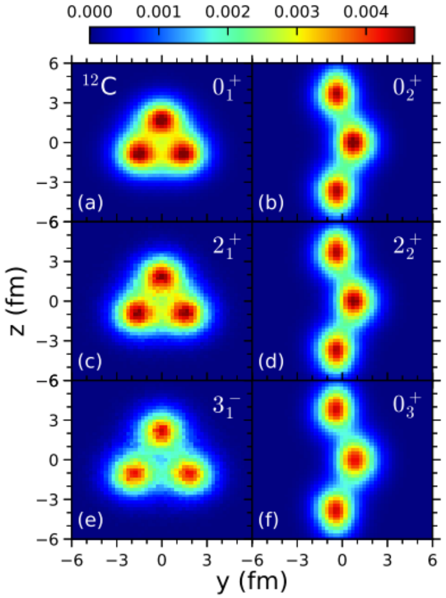

Ground-state energies of light nuclei from semi-local chiral EFT and compared to data.
Charge radii still a challenge for $A \sim 16$

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

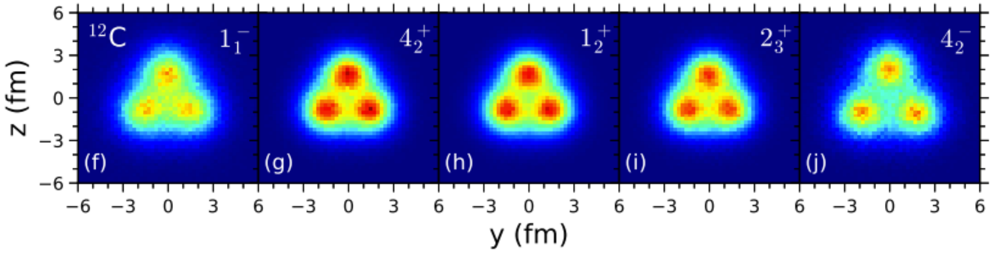
P. Maris et al, Phys. Rev. C 103, 054001 (2021)

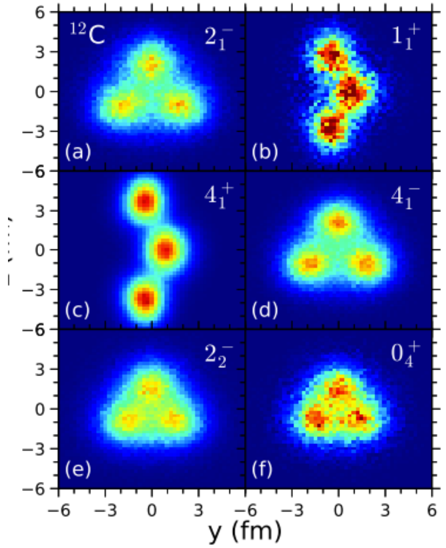
# Clustering in nuclei

## Lattice Effective Field Theory simulations of $^{12}C$



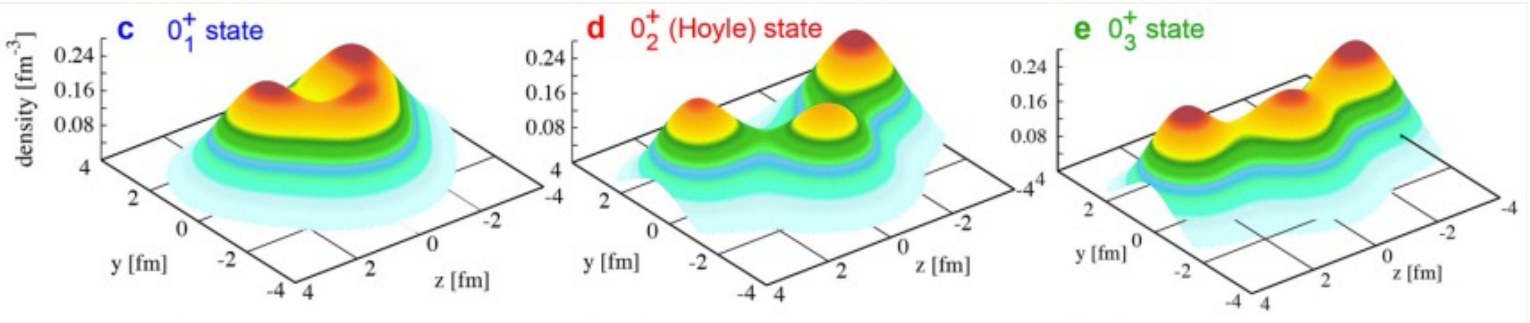

Epelbaum et at., Phys. Rev. Lett. 106, 192501 (2011)
Shen et al., arXiv:2202.13596 (2022)



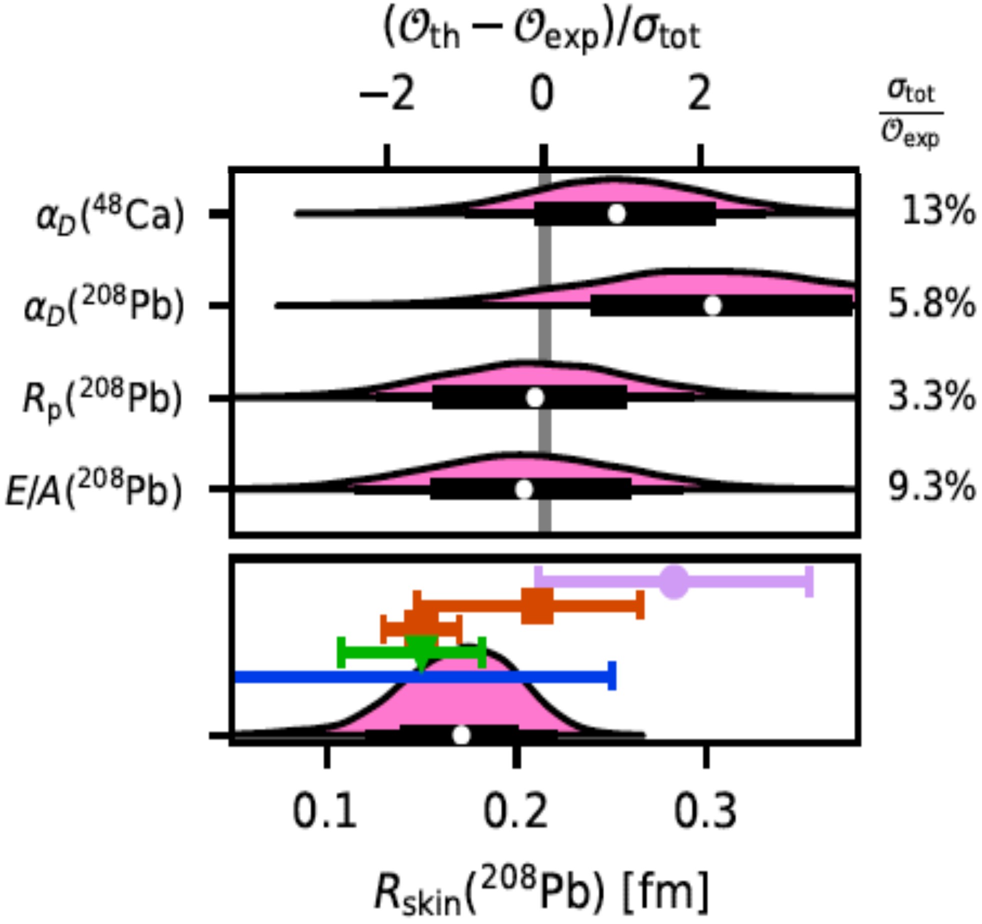




## Ab initio No-Core Monte Carlo Shell Model calculations of $^{12}C$

Otsuka et al., Nat. Comm. 13, 2234 (2022)



# Ab initio computation of the neutron skin in $^{208}$Pb




Top: Predicted probability distributions of the dipole polarizability ($\alpha_D$) in $^{48}$Ca and $^{208}$Pb, the point-proton radius ($R_p$), and the binding energy per nucleon ($E/A$) in $^{208}$Pb. Bottom: Predicted probability distribution of neutron skin ($R_{skin}$) in $^{208}$Pb compared to various extractions from experiments (CEBAF in purple)

Objectives

- First principles computation of the difference between the radii of neutron and proton distributions in $^{208}$Pb

Impact

- Confront recent extraction of neutron skin from parity-violating electron scattering at CEBAF with state-of-the-art theory
- Sample more than 100 million parameterizations of nuclear forces to find non-implausible set
- Quantify theoretical errors
- Ab initio computation of heavy nucleus $^{208}$Pb

Accomplishments

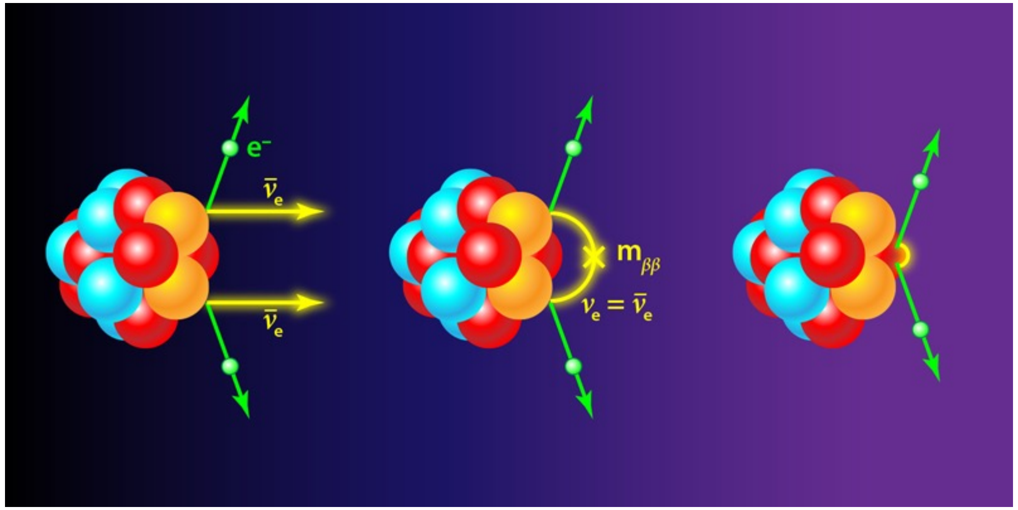
- Theory predicts a neutron skin that is in mild tension with less precise extraction from CEBAF experiment
- Baishan Hu et al., *Nat. Phys.* (2022); https://doi.org/10.1038/s41567-022-01715-8

# Challenges and opportunities in nuclear structure

- Accurate input: nuclear interactions and currents
- Accurate calculations of nuclear binding energies, charge radii, and saturation
- Clustering in light nuclei
- Calculations of resonance widths
- Accurate calculations of astrophysical capture reactions
- Precision of computations for heavy nuclei (energies, radii, transitions)
- Estimate systematic uncertainties
- Odd-mass and odd-odd nuclei

# Progress in computing electroweak decays


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



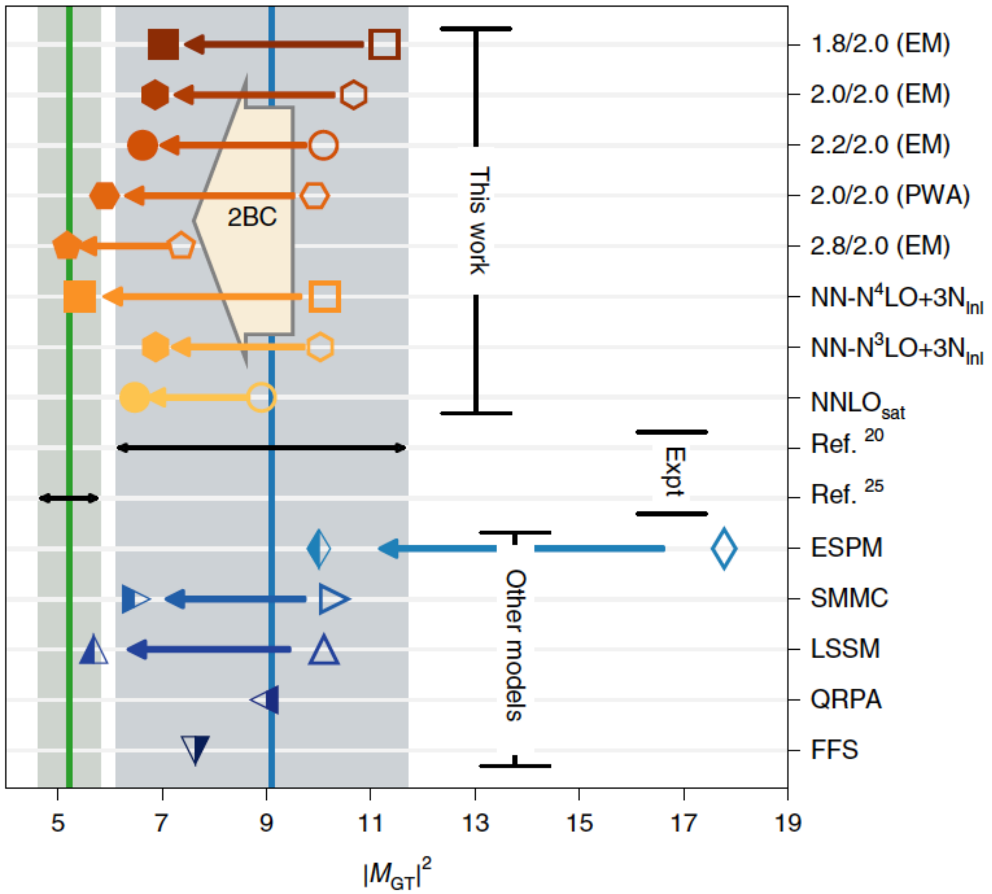

Double beta decay and neutrinoless double beta decays
(Image credit: APS Physics)

LEGEND
Large Enriched
Germanium Experiment
for Neutrinoless ββ Decay

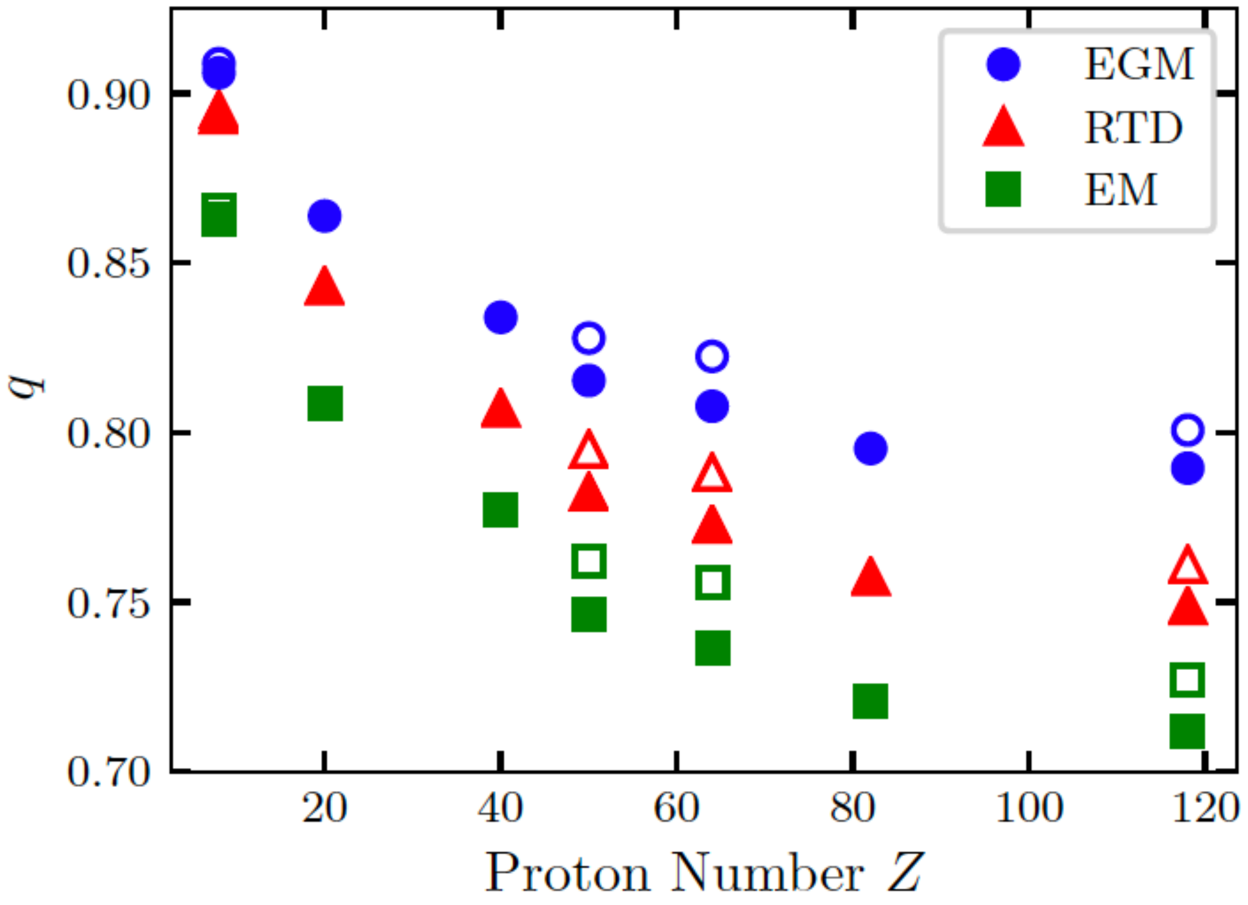
nEXO

CUPID

# Quenching of $\beta$-decay rates from chiral EFT




Gamow–Teller strength $|M_{GT}|^2$ for the β-decay of $^{100}$Sn calculated via ab initio methods compared to data, systematics, and other models. Open symbols: standard Gamow–Teller operator; filled symbols: two-body currents (2BC); partially filled symbols: phenomenological quenching factor.
P. Gysbers *et al.*, Nature Physics (2019)

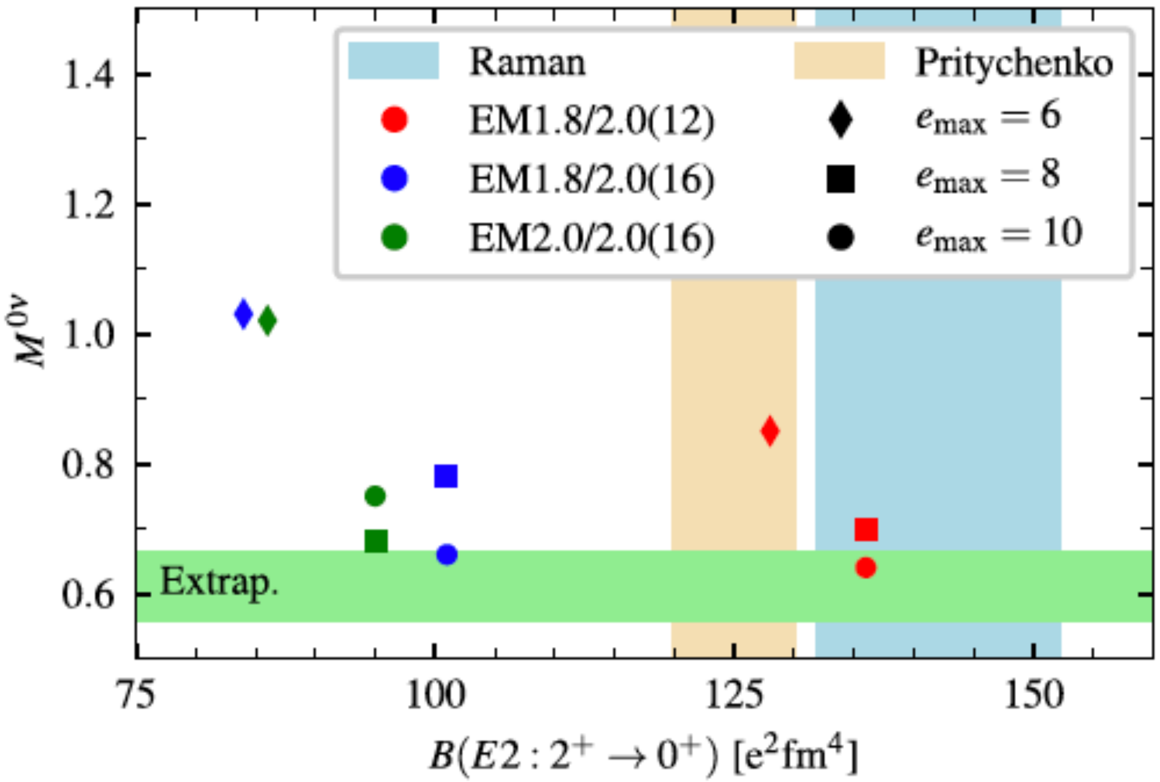



Quenching factor from two-body currents from three different parameterizations in chiral EFT for a number of isotopes with charge number Z, computed with energy-density functionals.

E. M. Ney, J. Engel, and N. Schunck
Phys. Rev. C 105, 034349 (2022)

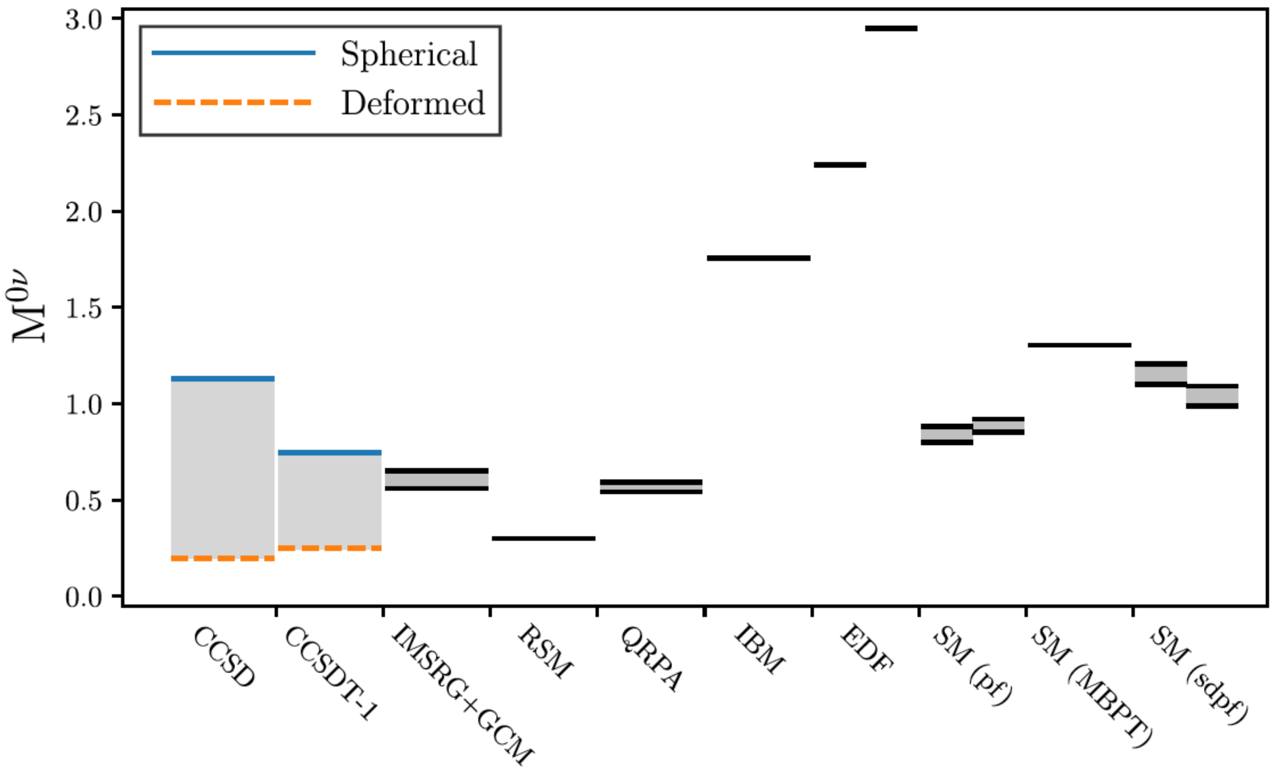
Light nuclei: G. B. King et al., Phys. Rev. C 102, 025501 (2020)

# Ab initio calculation of neutrinoless double beta decay in $^{48}$Ca




The nuclear matrix element for the neutrinoless double-beta decay of $^{48}$Ca versus the calculated B(E2) value in $^{48}$Ti, with different interactions and model-space parameters, computed via IMSRG.

J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, H. Hergert, [Phys. Rev. Lett. 124, 232501 (2020)]



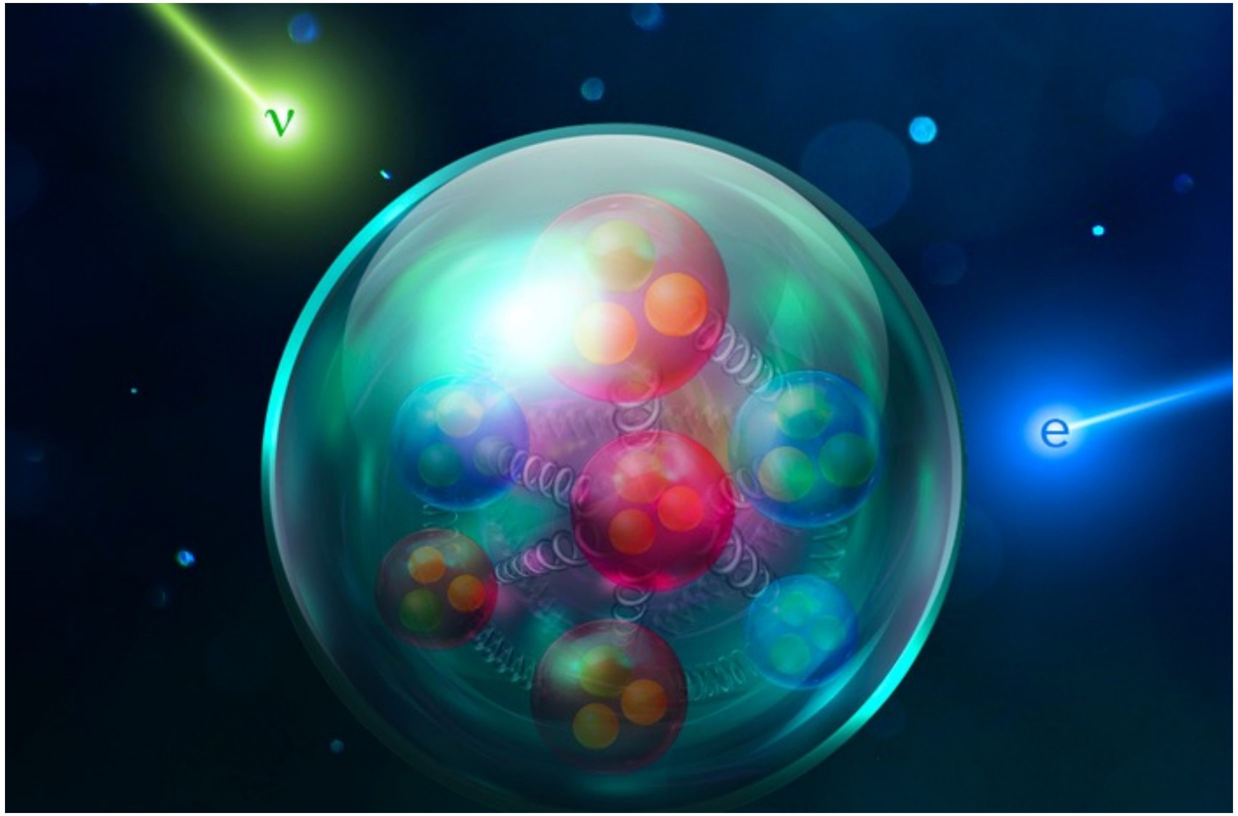

*Nuclear matrix element for neutrinoless double beta decay of $^{48}$Ca computed with coupled-clusters (first two results from the left) and compared to previous computations. The uncertainty bands reflect the effects of deformations in the final nucleus.*

S. Novario *et al.*, Phys. Rev. Lett. 126, 182502 (2021)
https://doi.org/10.1103/PhysRevLett.126.182502

# Challenges in computing neutrinoless double beta decay

- Estimate and eventually quantify uncertainties
- Link correlations of nuclear matrix element to other observables
- Accurately compute ground states of initial and final nuclei in $^{76}Ge$, $^{100}Mo$, Xe, and Te
- Different structures of initial and final nuclei complicate computation of matrix elements
- Explore impact of higher-rank currents
- Unknown strength of the two-body contact: Cottingham method / LQCD

# Progress in lepton-nucleus scattering



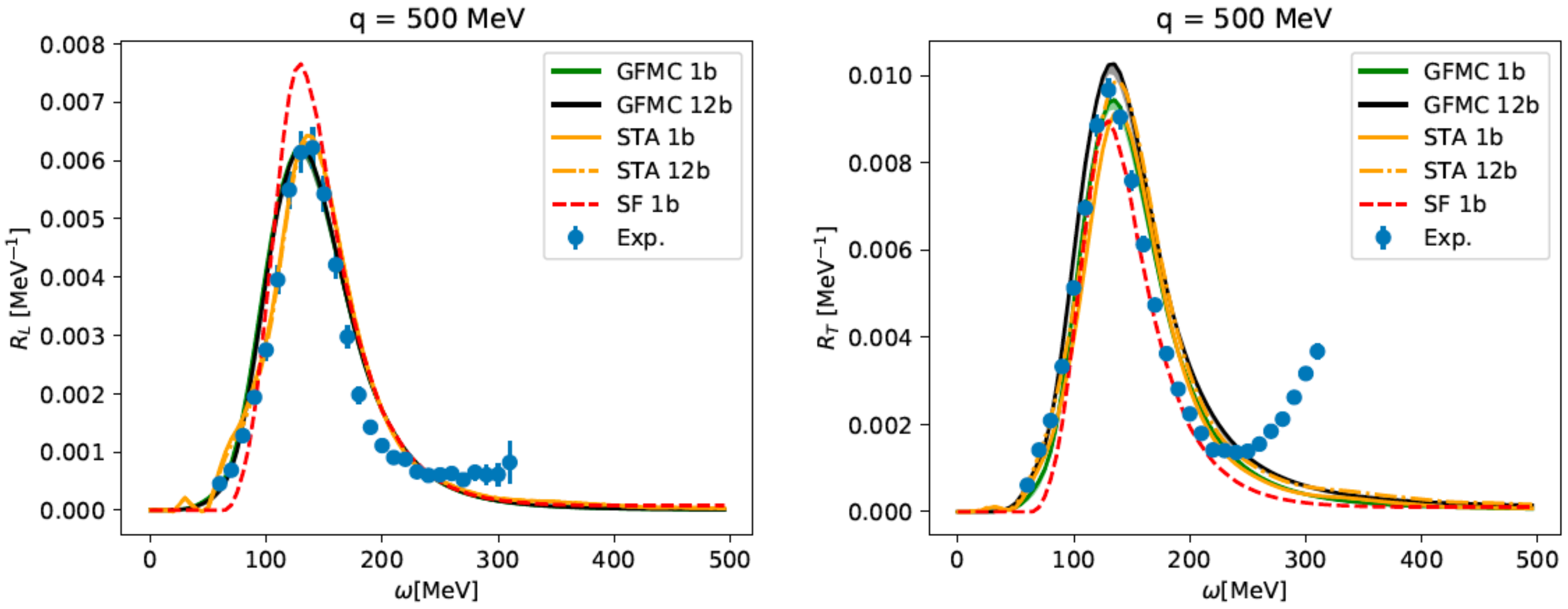

Lepton-nucleus interactions (Image credit: Jefferson Lab)

Jefferson Lab

DUNE DEEP UNDERGROUND NEUTRINO EXPERIMENT

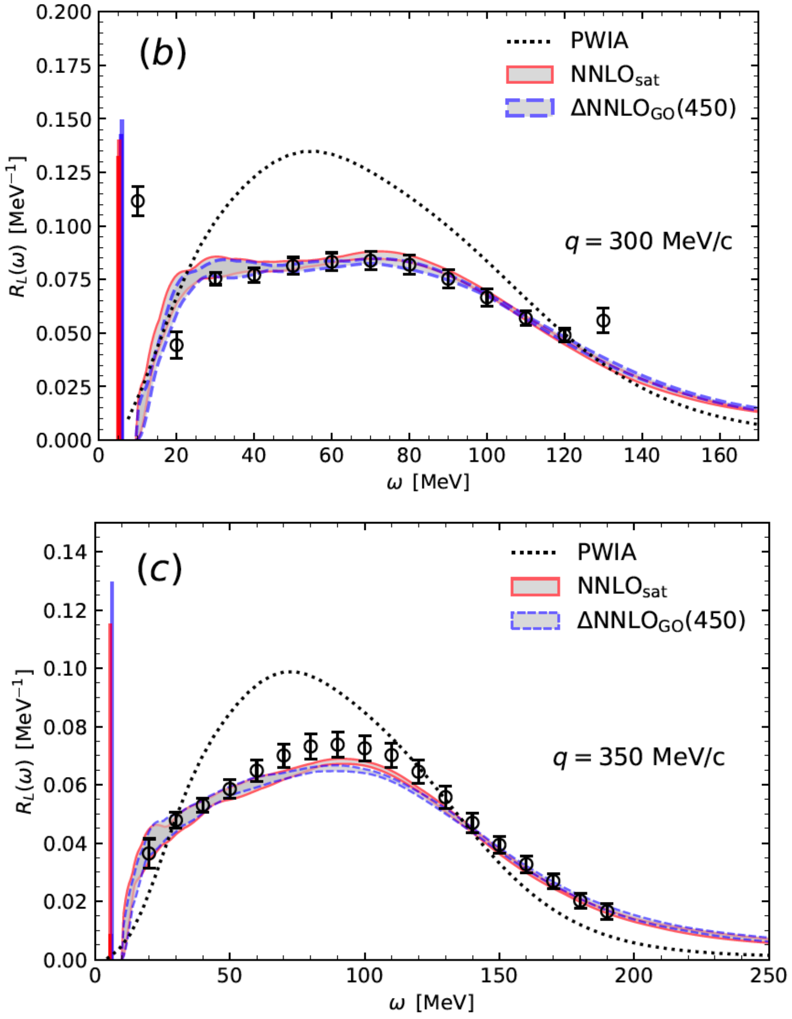
COHERENT SNS

# Progress in electron-nucleus scattering




Longitudinal and transverse response function of electron-$^{3}$He scattering. The role of two-body currents is strong for the transverse response.

L. Andreoli, et al., arXiv:2108.10824 (2021)

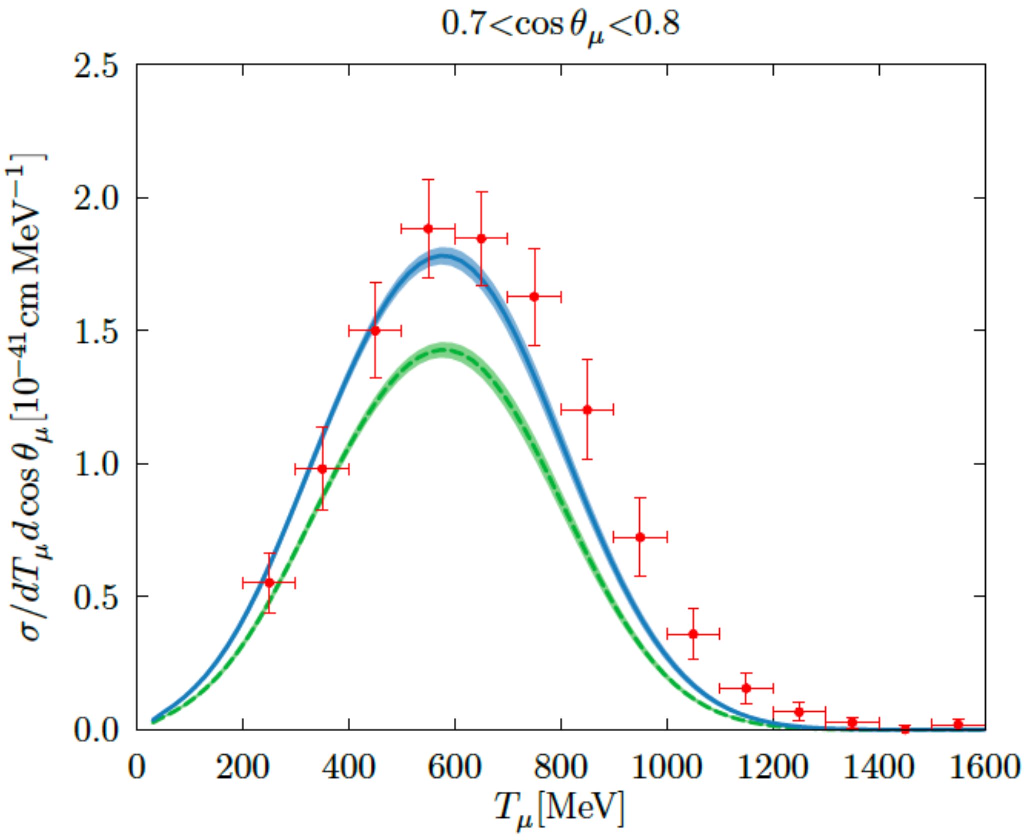



Longitudinal response of electron-$^{40}$Ca scattering (1-body currents only).

J. E. Sobczyk et al.,
Phys. Rev. Lett. 127, 072501 (2021)

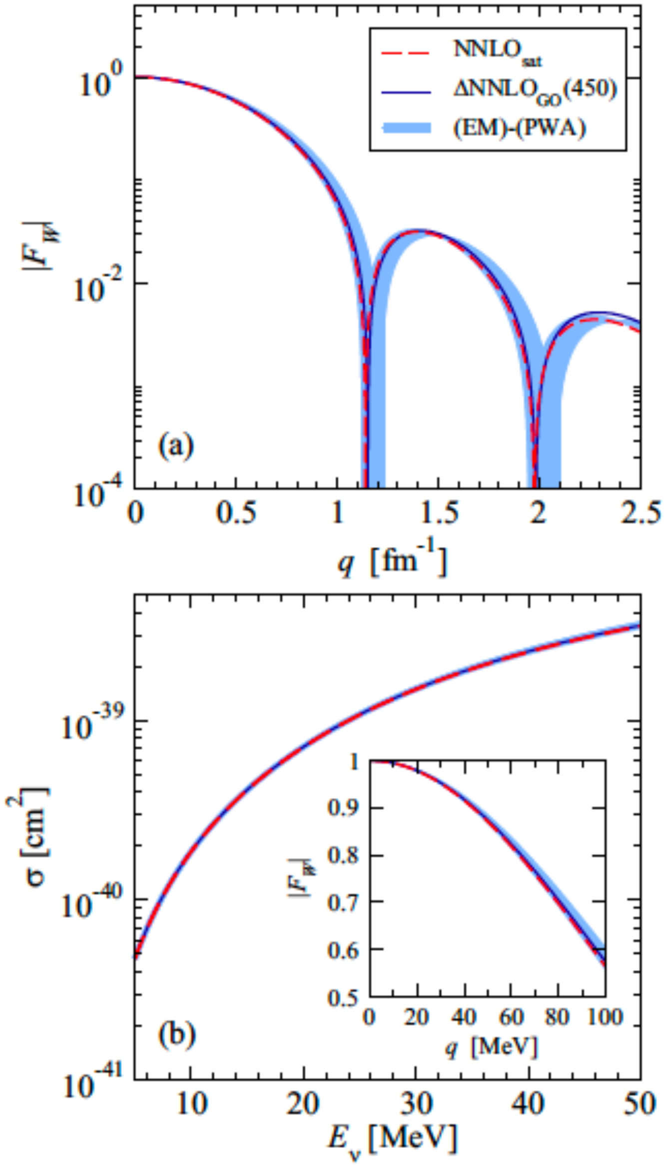
e$^-$ – $^{12}$C scattering: Lovato et al, Phys. Rev. Lett. 117, 082501 (2016)

# 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$\nu$NS for $^{40}Ar$

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

# Challenges in computing lepton-nucleus scattering

- Full computations in $^{16}O$ and $^{40}Ar$ as relevant detector materials
  - Inclusion of two-body currents
  - Uncertainty quantification
- Three-body short-range correlations

# Progress: heavy nuclei, fission

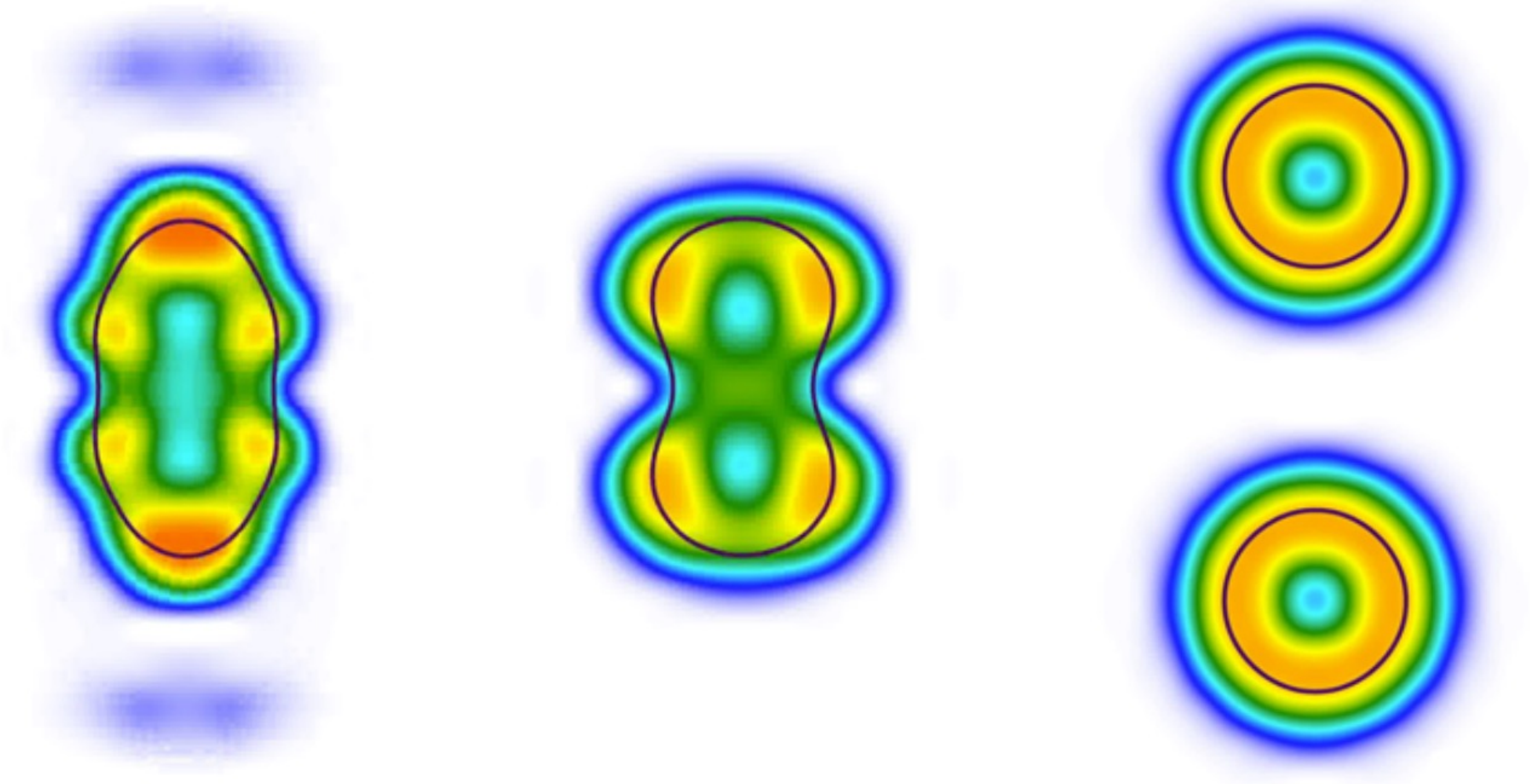


Image credit: Schuehtrumpf & Nazarewicz

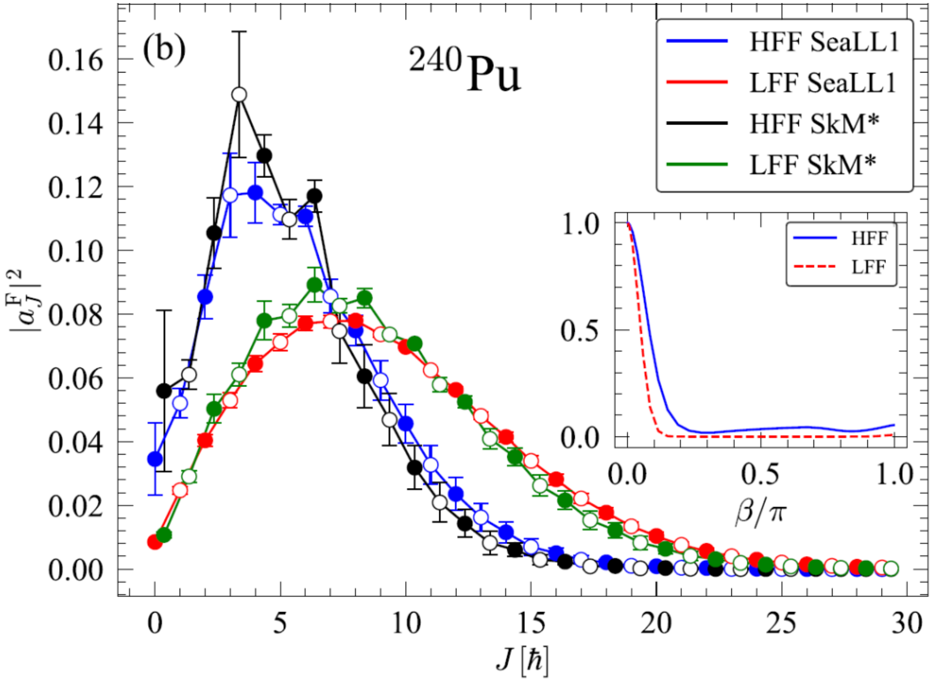
# Angular momentum distribution of fission fragments

Objectives

- The particles emitted by the fission fragments carry angular momentum
- Density functional theory with an extension of angular momentum projection predicts the spin distribution of fission fragments

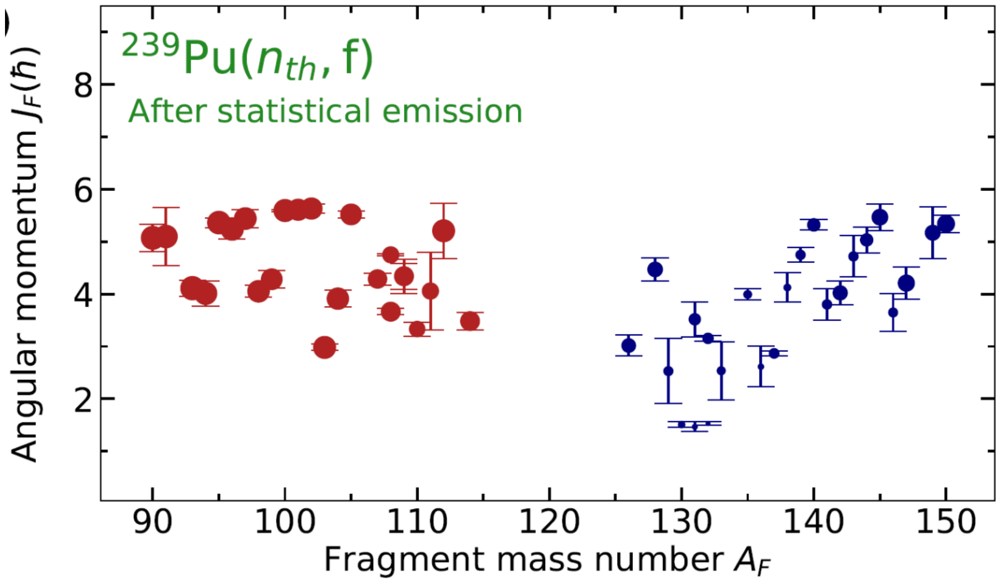
Impact

- The spins of the fission fragments are uncorrelated and shell effects at scission are essential to reproduce experimental average spins J
- The results significantly improve phenomenological models used to simulate the fission spectrum for applications




**Left**: Spin distribution of light (LFF) and heavy (HFF) fission fragment in 240Pu computed from TDDFT with several energy functionals

**Right**: Average spin of the fragments as a function of their mass after statistical emission of photons





A. Bulgac, I. Abdurhamann, S. Jin, K. Kodbey, N. Schunck, I. Stetcu, Phys. Rev. Lett. **126**, 142502 (2021)

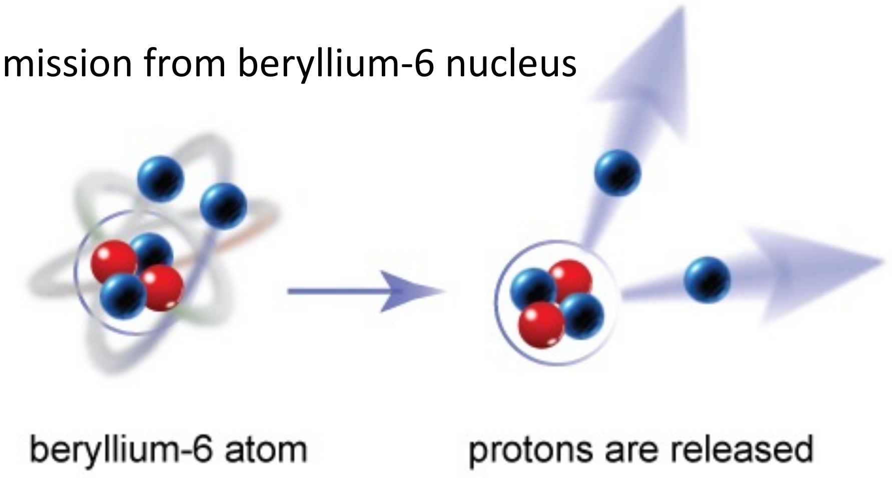
P. Marevic, N. Schunck, J. Randrup, R. Vogt, Phys. Rev. C. **104**, L021601 (2021)

# Fermion pair dynamics in open quantum systems

## Objectives

- Three-body decay is a rare decay mode observed in a handful of unbound rare isotopes.
- We developed a realistic time-dependent framework that allows for a full control of the nuclear structure inside the nucleus, where nucleonic pairs are formed, and the dynamics of escaping nucleons.
- Using this new approach, we study the angular and energy correlations between emitted nucleons in a 3-body decay.

Two-proton emission from beryllium-6 nucleus




Density evolution for the two-proton decay of the ground state of beryllium-6 for different strengths of pairing interaction $V_{pp}$.

## Impact

- To study the mechanism of two-nucleon decay, theoretical models must fully control the behavior of the decaying system at large distances and long propagation times. To this end, we developed a realistic time-dependent framework that allows for precise three- body solutions asymptotically.
- By comparing the dynamics of two-proton and two-neutron decays, we demonstrated that while the two-proton emission is largely affected by the electrostatic repulsion, some fingerprints of nucleonic pairing remain.
- Our results indicate that the anticipated high-resolution data on energy and angular nucleon-nucleon correlations from FRIB will provide unique insights into the structure of proton and neutron pairs in rare isotopes.

S. M. Wang and W. Nazarewicz, Phys. Rev. Lett 126, 142501 (2021)

# Challenges in fission studies

- Develop/Calibrate modern energy-density functionals with quantified uncertainties
- Link energy density functionals to chiral physics
- Identify the essential ingredients in fission theory
- Develop comprehensive approach to fission observables

Bender et al., “Future of fission theory,” J. Phys. G: Nucl. Part. Phys. 47 (2020) 113002

# Progress: nuclear matter equation of state

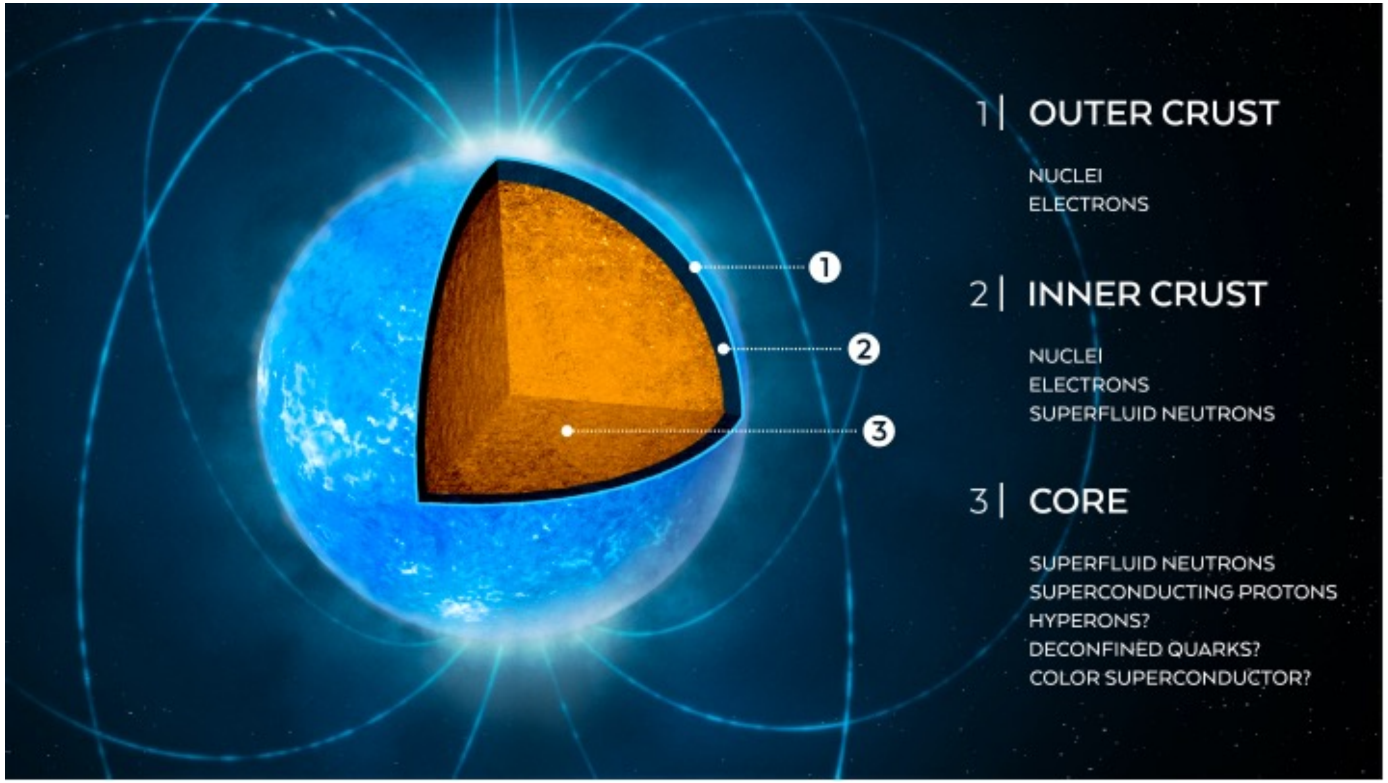



Image credit: Watts et al., Rev. Mod. Phys. 88 021001 (2016)

LIGO

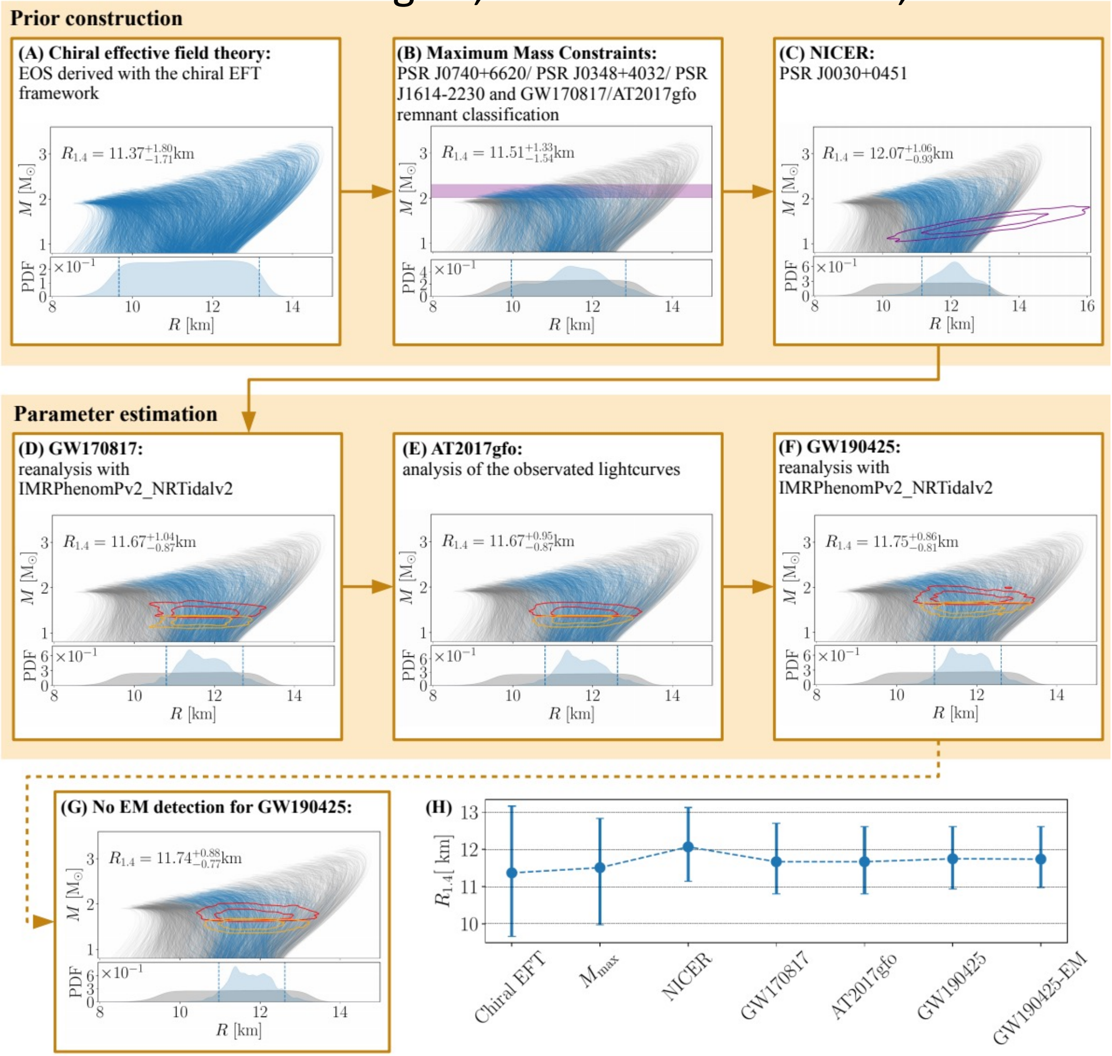
FRIB

NICER • SEXTANT

# Multimessenger constraints on the neutron-star equation of state and the Hubble constant

## Objectives

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




## Impact

- The robust statistical analysis of all available data from NSs and NS mergers provides the most stringent constraints on the radius of a typical 1.4 $M_{sol}$ NS:

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

- Our analysis also allows us to measure the expansion rate of the Universe described by the Hubble constant $H_0$. Previous determination using type I-a supernovae or the Cosmic Microwave Background (CMB) disagree, know as Hubble tension. Our findings agree with the CMB:

$$H_0 = 66.2^{+4.4}_{-4.2}\text{km Mpc}^{-1}s^{-1}$$

- We also use our framework to address the recent NS merger GW190814, whose nature cannot be determined from observations alone. We find that this system likely was a binary black-hole merger.

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

# Challenges in nuclear matter

- Link EOS from chiral physics to higher densities / more microscopic calculations
- Mapping the phase diagram of nuclear matter versus isospin, density, and temperature

# Progress: applications of machine learning & emulators

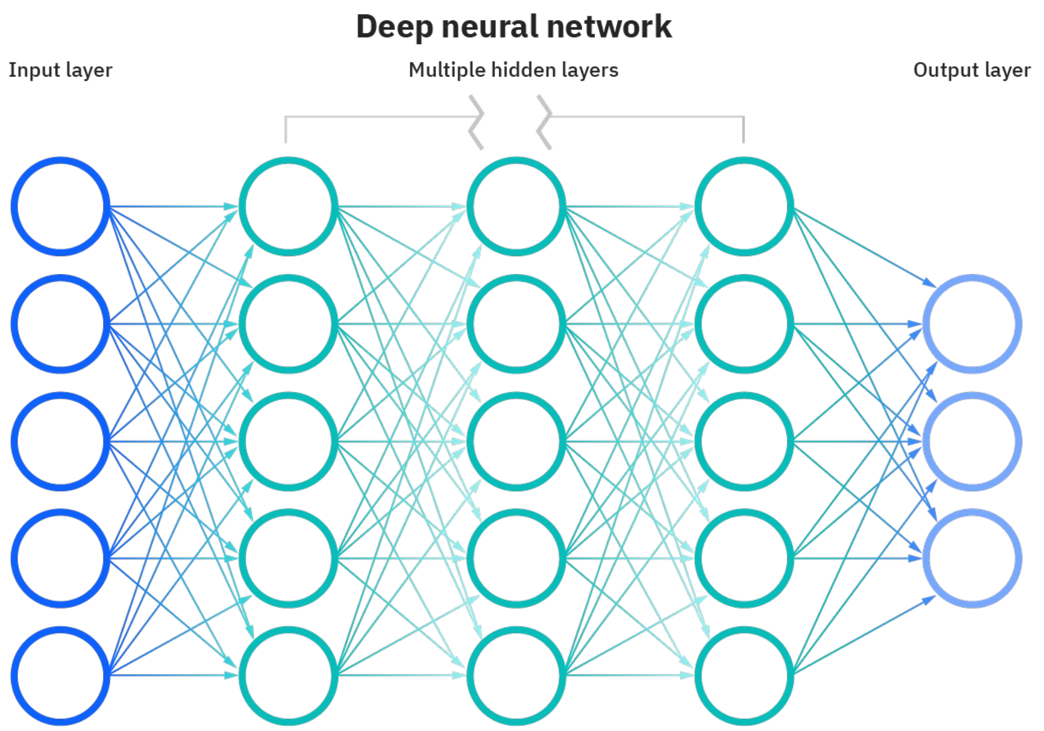



Image credit: IBM

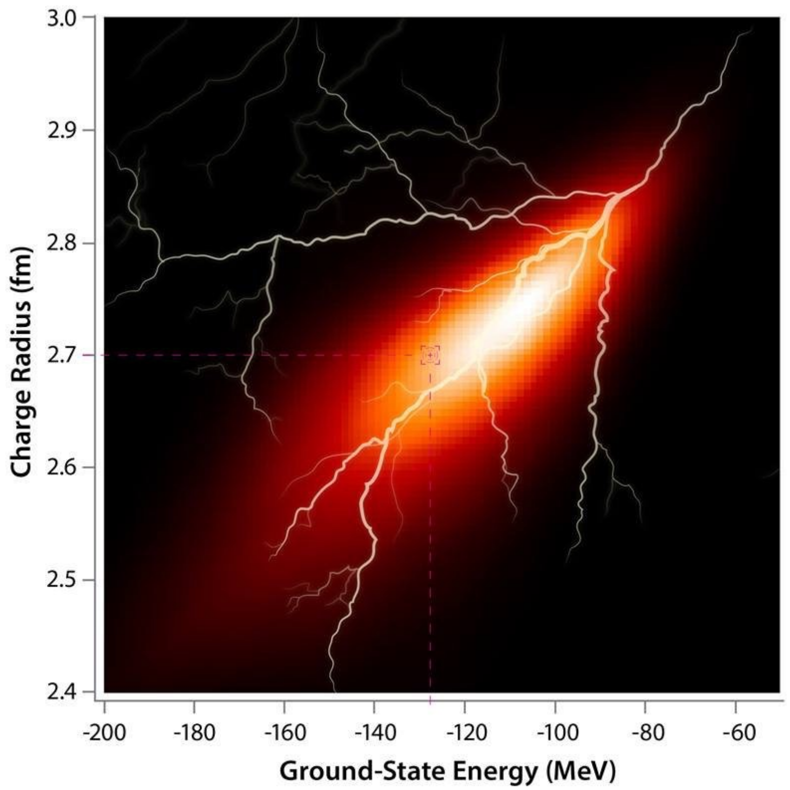
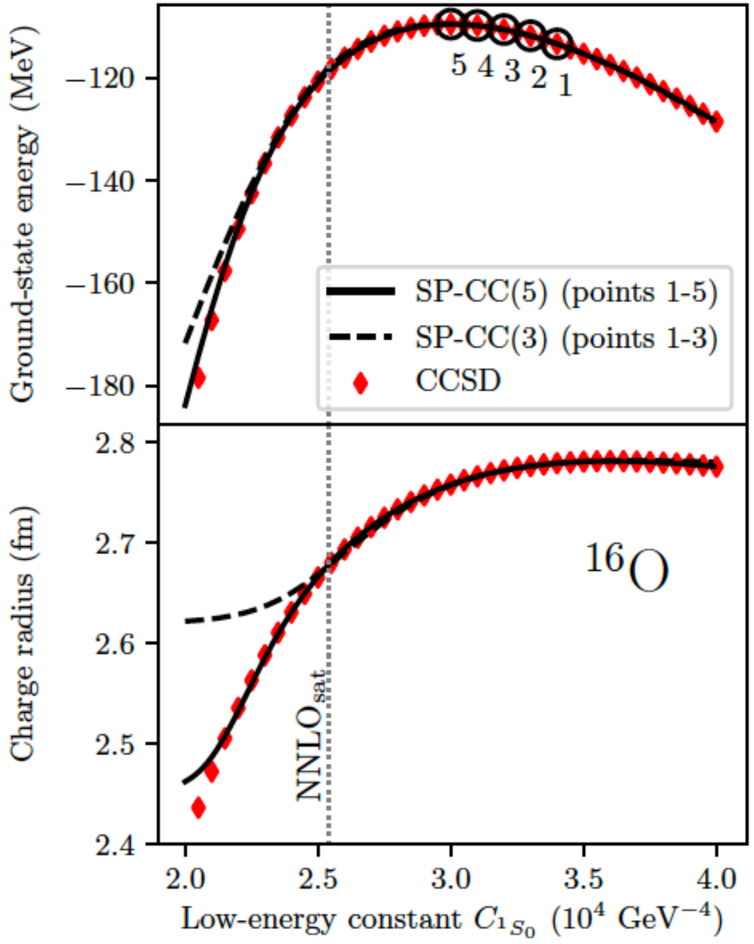
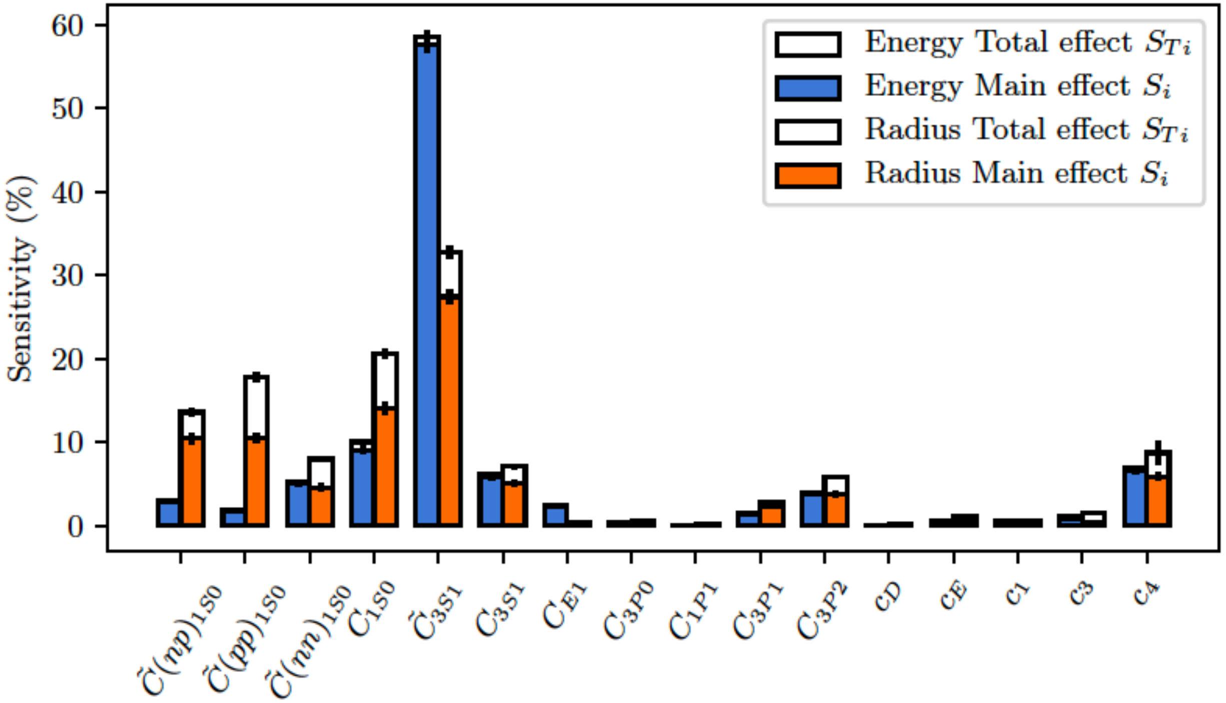



Image credit: Andy Sproles (ORNL)

# Progress: Emulators for fast computations



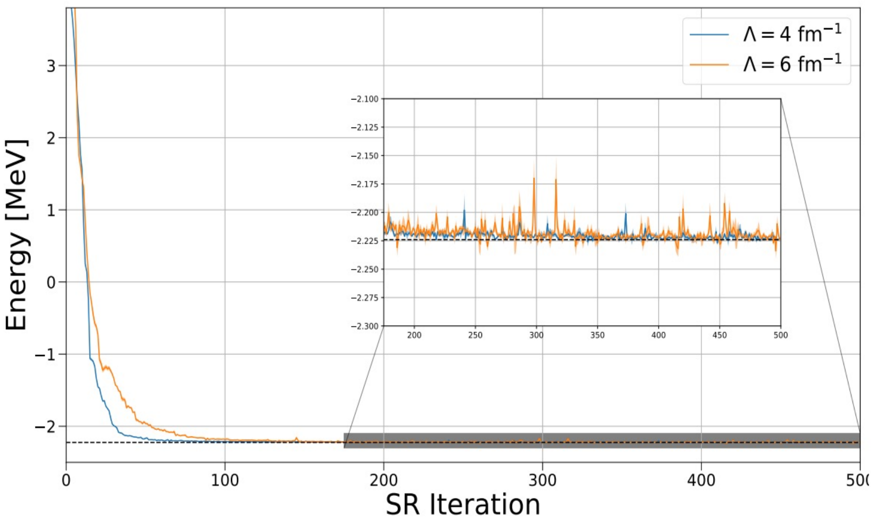




Main and total effects (in %) for the ground-state energy (left bar) and charge radius (right bar) in $^{16}$O, grouped per LEC. A larger sensitivity value implies that the corresponding LEC is more critical for explaining the variance in the model output.

Emulator results for $^{16}$O, using three (dashed line) or five (full line) subspace vectors, for different values of the parameter $C_{1S0}$ and compared to exact results (red diamonds).

Ekström & Hagen, Phys. Rev. Lett. 123, 252501 (2019)
Dillon Frame et al., Phys. Rev. Lett. 121, 032501 (2018)

# *Variational Monte Carlo calculations with artificial neural-network correlators*




Convergence of the stochastic-reconfiguration training algorithm

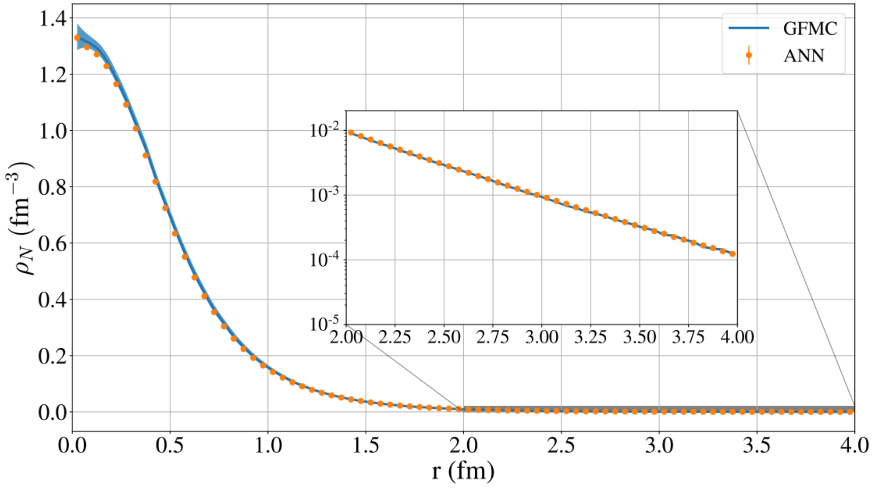



Figure: point-nucleon density of $^3$H from the ANN and GFMC calculations;

## *Objectives*

- Devise accurate nuclear wave functions for quantum Monte Carlo calculations that do not scale exponentially with the number of nucleons;
- Generalize artificial-neural network representations used in condensed-matter systems to account for the spin-isospin dependence of the nuclear force;

## *Impact*

- We used an artificial neural network to represent a nuclear correlation operator that takes as input the spatial and spin-isospin coordinates of the nucleons;
- We devised a stochastic reconfiguration algorithm to train the ANN;
- Using a LO pionless-EFT Hamiltonian, we showed that the ANN outperforms conventional Jastrow ansatz and accurately reproduces the nuclear density, including its long tail;

## *Publication*

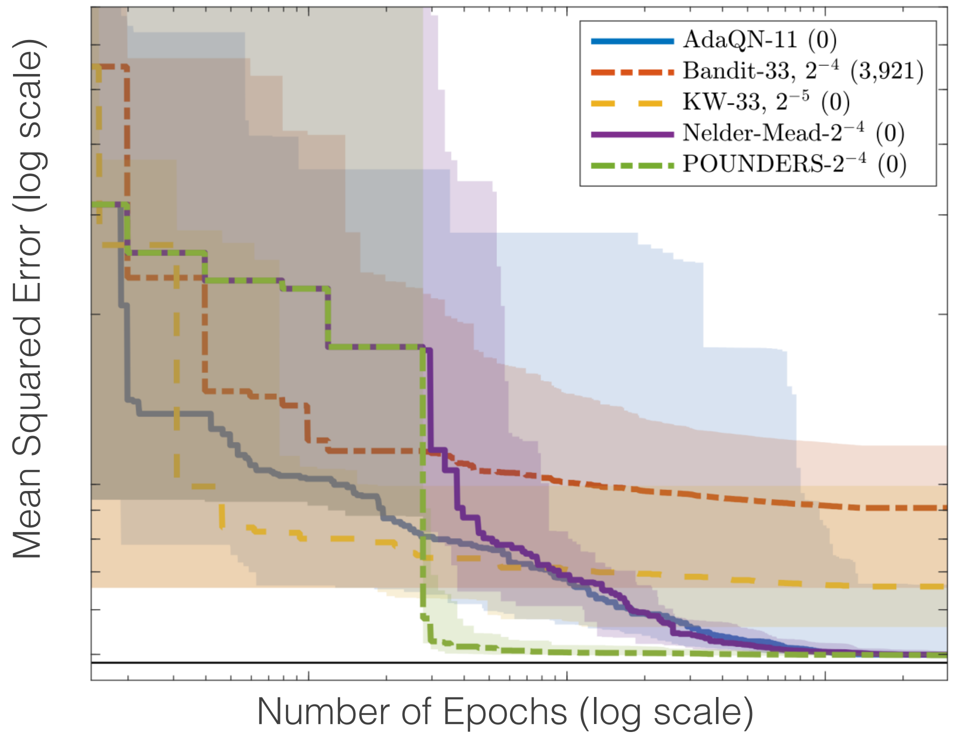
Adams, Carleo, Lovato, Rocco, arXiv:2007.14282 (PRL in press)

# Benchmarking Optimization & Supervised Machine Learning Methods

## Objectives

Understand potential of machine learning (ML) algorithms for calibrating computationally expensive energy density functionals using parallel computing resources given:

- Available training/experimental data (100s) much smaller than flagship ML uses (millions+).
- Derivatives are not available.




## Impact

- Reveals that targeted optimization methods typically outperform zeroth-order ML methods when little data are available for training computationally expensive nuclear physics models.
- Provides actionable guidelines and directions for future research for leveraging parallel physics simulations in an energy-efficient manner.
- Excellent results when applied to calibration of Fayans energy density functionals.

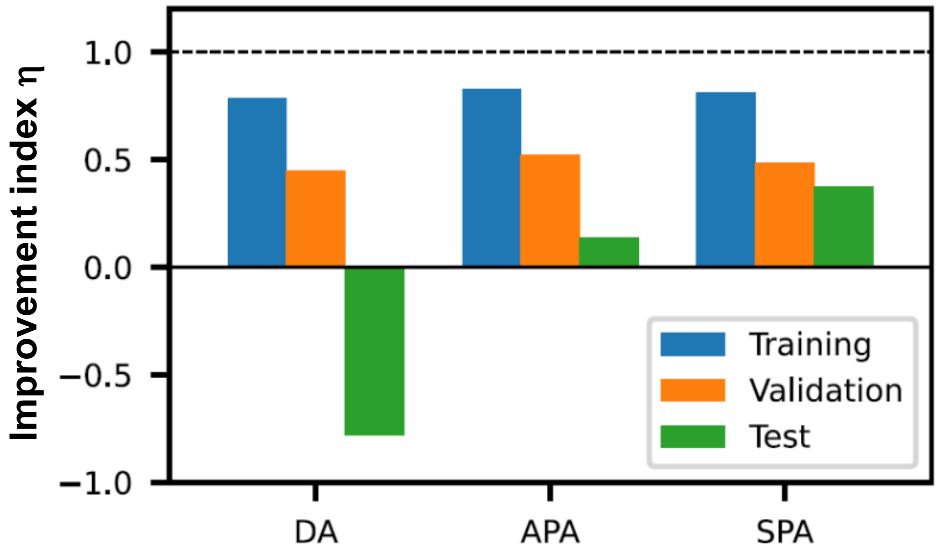
Bollapragada et al., [J. Phys. G 48 024001 (2021)]

Performance of best-tuned variants on an instance of calibrating the Fayans energy density functional. Solid lines indicate median performance ; transparent bands indicate 25th through 75th quantile performance. Best solutions are found in the allotted budget by POUNDERS; randomized methods achieve early reductions.

# Thou Shalt Not Extrapolate: Quantifying the Unknown

Objectives

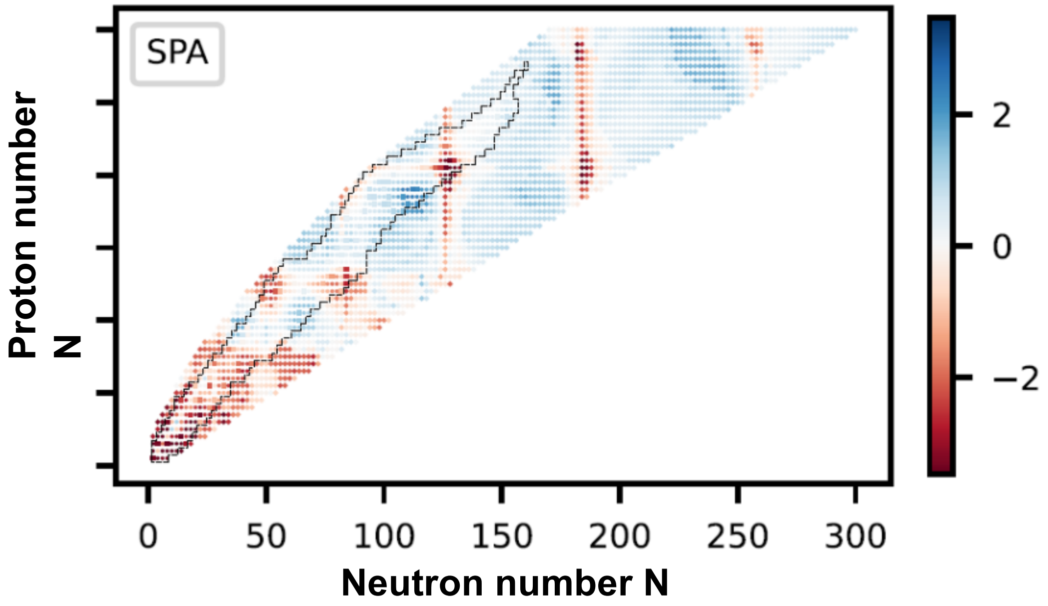
- Predictions of nuclear properties far from stability are based on theoretical models that must be corrected for systematic bias
- We developed a feature-learning novel method to compute reliable estimates of the model bias even in nuclei where experimental information is not available




Positive (negative) values of the improvement index indicate the model bias correction has improved (degraded) predictions. Without feature selection (DA), fitting the model bias can degrade predictions while with selected-feature learning (SPA), predictions are systematically better

Impact

- We proved that simple estimates of the model bias based only on proton and neutron numbers are unstable and lead to uncontrolled extrapolation errors
- Our feature learning approach gives robust estimates of model bias and is potentially generalizable to other observables and models




With feature learning, the model bias has learned the characteristic patterns of closed shells even outside the fitting range.

Navarro Perez & Schunck, Phys. Lett. B 833, 137336 (2022)

# Opportunities in ML

- Building emulators for heavy nuclei
- Bayesian ML with GP for propagation of theoretical uncertainties
- Complex function representations (variational ansatz, inversion of response functions, model-space extrapolations …)
- …

# 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, …