Building the Atomic Nucleus from the Ground Up

Presented by
Computational Nuclear Structure and Reactions Collaboration

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An unprecedented theoretical effort

The *Universal Nuclear Energy Density Functional*

SciDAC Collaboration of nuclear theorists, applied mathematicians, and computer scientists is developing a comprehensive description of nuclei and their reactions that delivers maximum predictive power with quantified uncertainties.

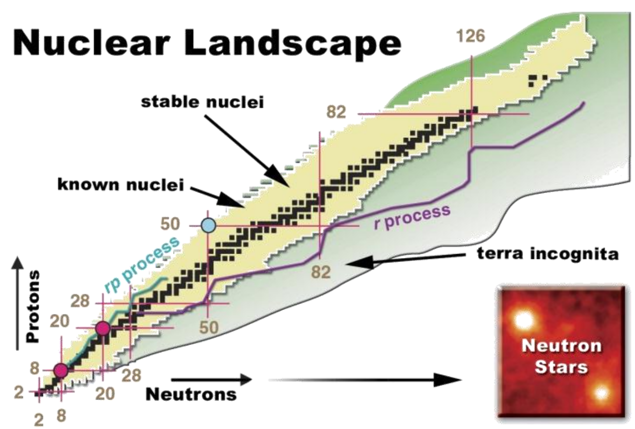
- **UNEDF**
  - Is a 5 year SciDAC collaboration under the auspices of the Office of Science ASCR and Nuclear Physics and NNSA
  - Involves over 50 researchers from 9 universities and 7 national laboratories and provides training to about 30 young researchers (postdocs and students) annually

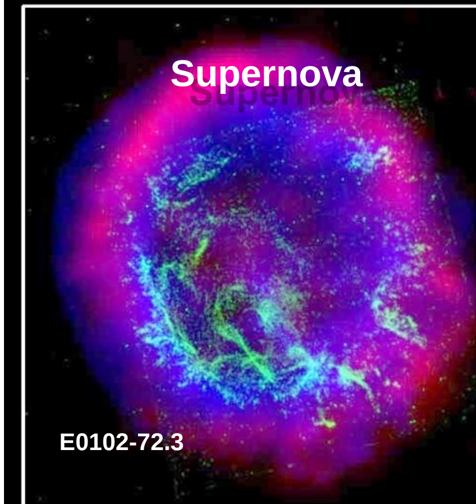
M. Stoitsov, H. Nam, W. Nazarewicz, A. Bulgac, G. Hagen, M. Kortelainen, J. C. Pei, K. J. Roche, N. Schunck, I. Thompson, J. P. Vary, S. M. Wild, *UNEDF: Advanced Scientific Computing Transforms the Low-Energy Nuclear Many-Body Problem*, SciDAC2011

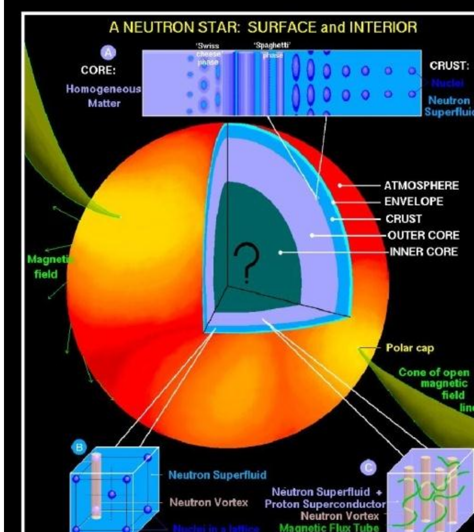
Describing nuclei we cannot measure

"Given a lump of nuclear material, what are its properties and how does it interact?"

- Half of all elements heavier than iron produced in r-process nucleosynthesis where limited (or no) experimental information exists
- Use experimental nuclear data to constrain theory
- Mission relevant to DOE-NP, NNSA
- Nuclear reaction information relevant to NNSA and AFCI

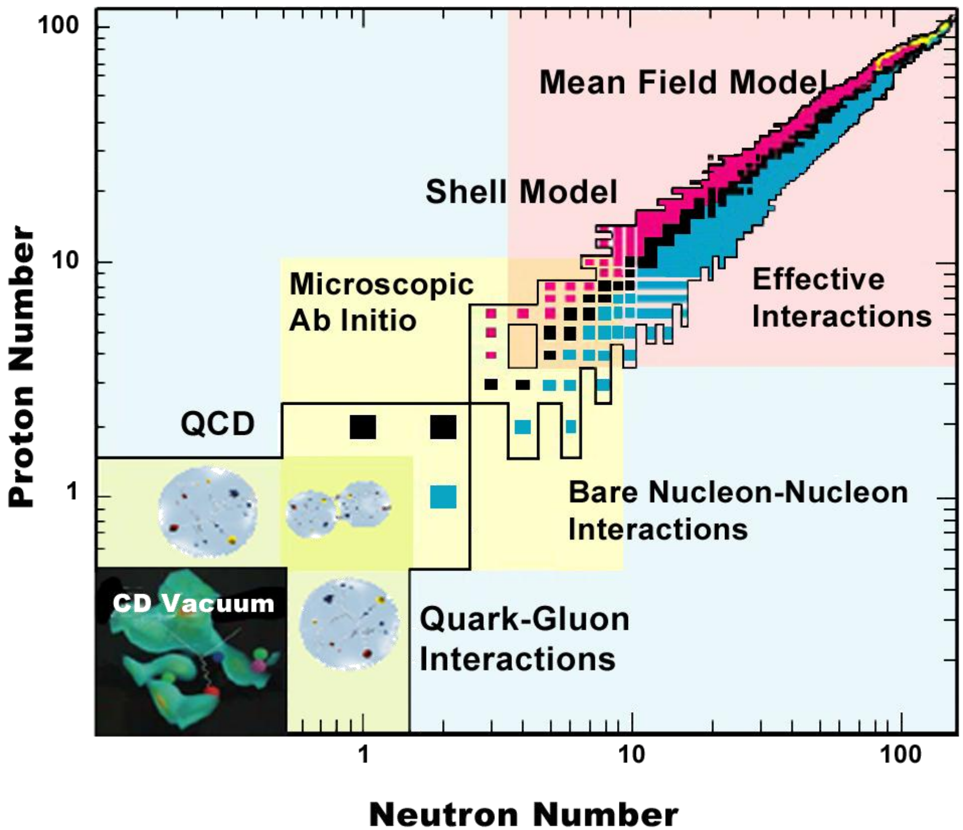






OAK RIDGE National Laboratory

Pushing the nuclear boundaries



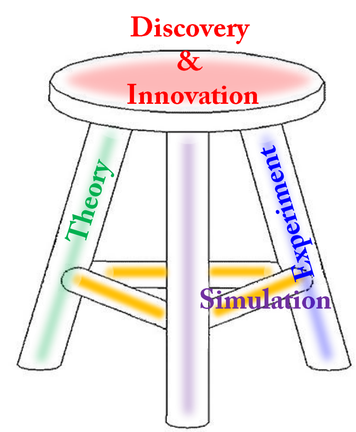
In All Regions

Mission relevant to

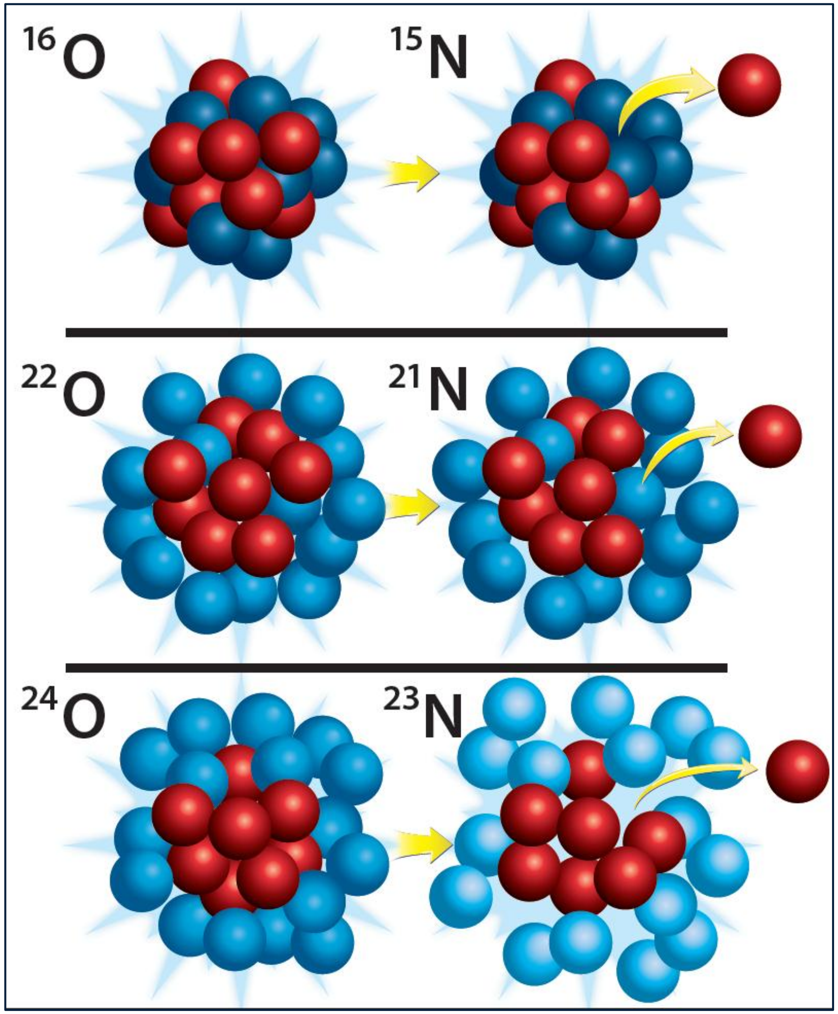
NNSA, SC/NP, Nuclear Energy, AFCI

The Oak Ridge Leadership Computing Facility

- Enables global nuclear Density Functional Theory (DFT) calculations
- Increases *ab initio* reach for selected nuclei up to mass 100



Probing the limits of nuclear stability



- The nuclear Coupled-Cluster method provides a way to study nuclei rich in neutrons or protons, the so-called "driplines," where adding just one more nucleon robs a nucleus of the stability it needs to stay intact

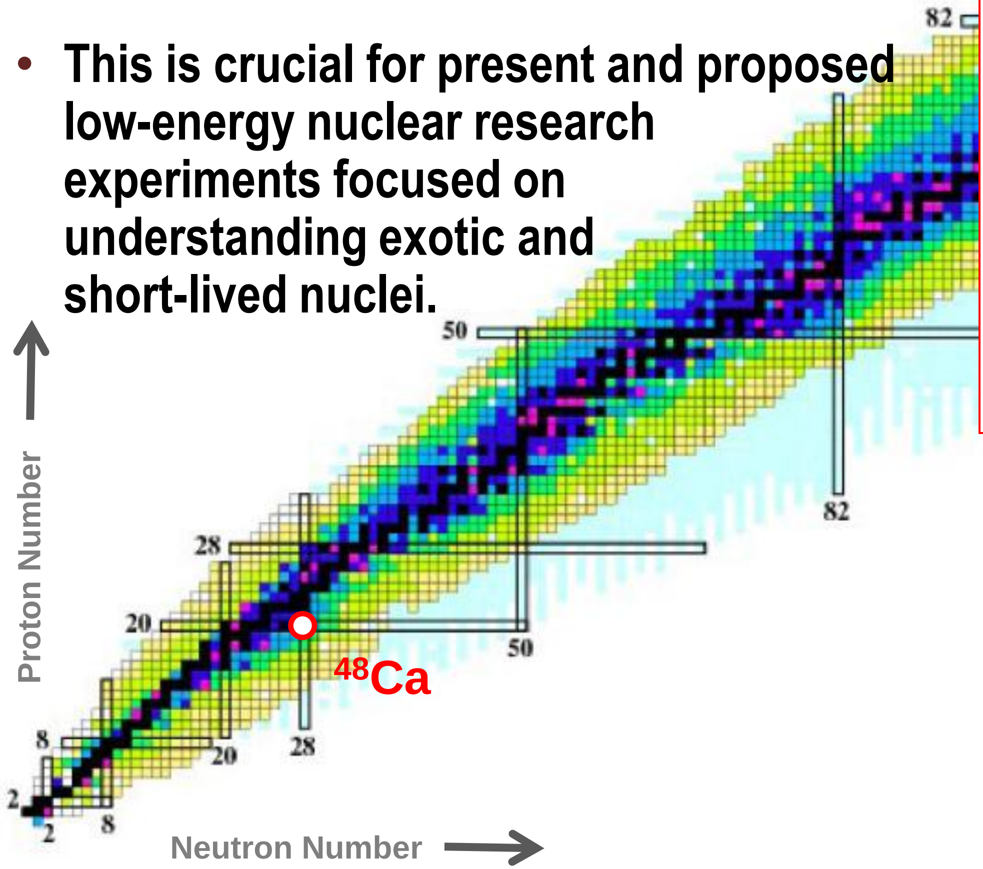
Proton knockout from Oxygen-16, Oxygen-22 and Oxygen-24. The thickness of the arrow showing the removed proton reflects the spectroscopic factor for this process, or in other words how "free" the protons can be considered in neutron rich oxygen isotopes.

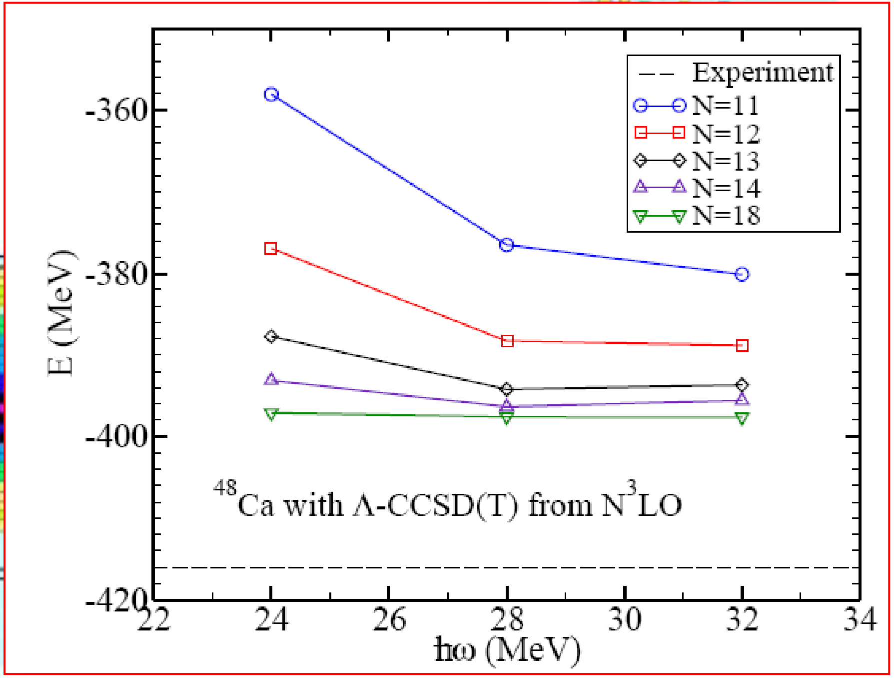
Illustration by Andy Sproles, Oak Ridge National Laboratory

Ø. Jensen, G. Hagen, M. Hjorth-Jensen, B. Alex Brown, A. Gade , *Quenching of spectroscopic factors for proton removal in oxygen isotopes*, Phys. Rev. Lett. 107, 032501 (2011)

Investigating the nuclear force in medium mass nuclei

- The nuclear Coupled-Cluster method is a microscopic approach for the study of medium-mass nuclei.
- This is crucial for present and proposed low-energy nuclear research experiments focused on understanding exotic and short-lived nuclei.

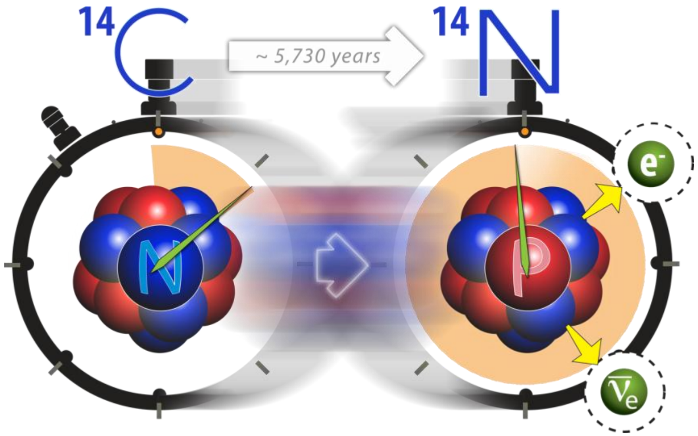




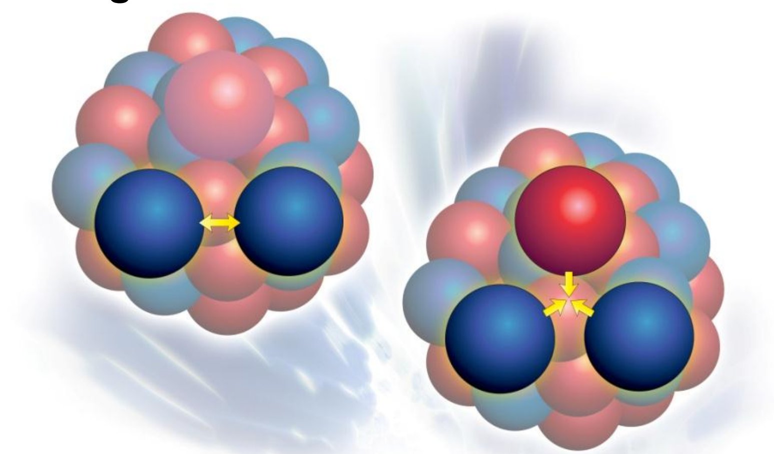
Coupled-cluster calculations for calcium isotopes suggest the need for three-nucleon forces (3NF) and that the 3NFs will exhibit an interesting isospin dependence.

G. Hagen, T. Papenbrock, D.J. Dean, M. Hjorth-Jensen, *Ab initio coupled-cluster approach to nuclear structure with modern nucleon-nucleon interactions*, Phys. Rev. C 82, 034330 (2010)

Understanding the origin of the anamolous long lifetime of ^{14}C



- **The No-Core Shell Model approach provides detailed ab initio (*first principles*) studies of light nuclei to understand the strong nuclear force**



An accurate picture of the carbon-14 nucleus must consider the interactions among protons and neutrons both in pairs (known as the two-body force, left) and in threes (known as the three-body force, right).
Illustration by Andy Sproles, Oak Ridge National Laboratory

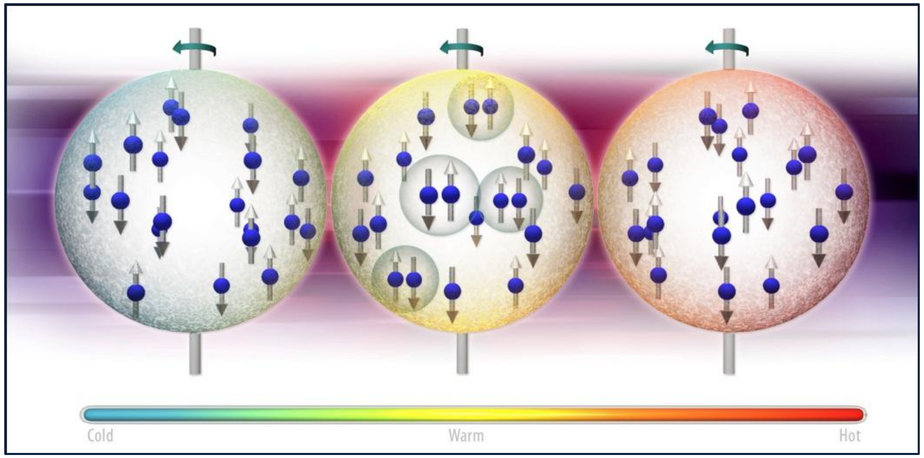
Carbon-14, with six protons and eight neutrons, is the isotope behind carbon dating, allowing researchers to determine the age of plant- or animal-based relics going back as far as 60,000 years.

Previous studies dramatically underestimate the isotope's half-life, which is around 5,700 years.

P. Maris, J.P. Vary, P. Navratil, W.E. Ormand, H. Nam, D.J. Dean, *Origin of the anomalous long lifetime of ^{14}C*, Phys. Rev. Lett. 105, 202502 (2011)

The curious case of Germanium-72

- **The Shell Model Monte Carlo method shows the first realistic description of an elusive phenomenon of successive pairing phase transitions in nuclei**



As a rapidly rotating gemanium-72 nucleus gets hotter, pairing among the protons and neutrons within the nucleus tends to decrease steadily. At one critical temperature, however, the pairing spikes back up, as represented in the center illustration. This odd behavior marks a phase transition within the germanium-72 nucleus.

Illustration by Andy Sproles, Oak Ridge National Laboratory

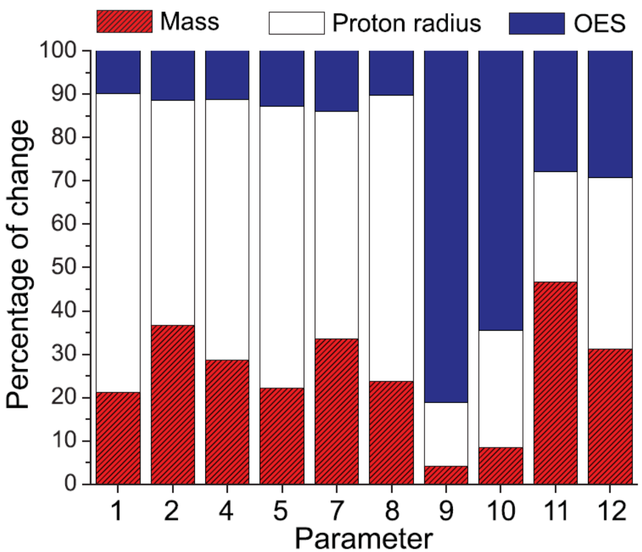
"The competition between superconductivity, rapid rotation, and temperature is a fascinating topic that can be studied in diverse physical systems, including tiny atomic nuclei and macroscopic-scale ferromagnets,"

Witold Nazarewicz
University of Tennessee–Knoxville
Poland's Warsaw University,
Scientific Director of ORNL's Holifield Radioactive Ion Beam Facility.

D.J. Dean, K. Langanke, H. Nam, W. Nazarewicz, *Reentrance Phenomenon in Heated Rotating Nuclei in the Shell Model Monte Carlo Approach*, Phys. Rev. Lett. 105, 212504 (2010)

Advanced algorithms define new generation Energy Density Functional

"Density Functional Theory (DFT), a tool of choice for complex nuclei, is built on theorems showing the existence of universal energy functionals for many-body systems, which include, in principle, *all* many-body correlations."



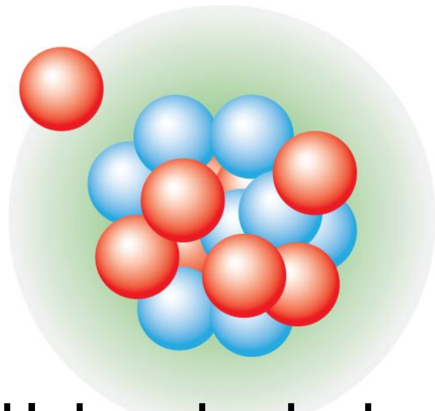
Sensitivity of the parameters of UNEDF0 to different data types entering *χ2.*

- All energy functionals rely on parameters that must be directly fitted to experimental data
- The new model-based, derivative-free optimization algorithm is significantly better than standard optimization methods in terms of reliability, speed, accuracy, and precision
- The resulting parameter set UNEDF0 results in good agreement with experimental masses, radii, and deformations and seems to be free of finite-size instabilities

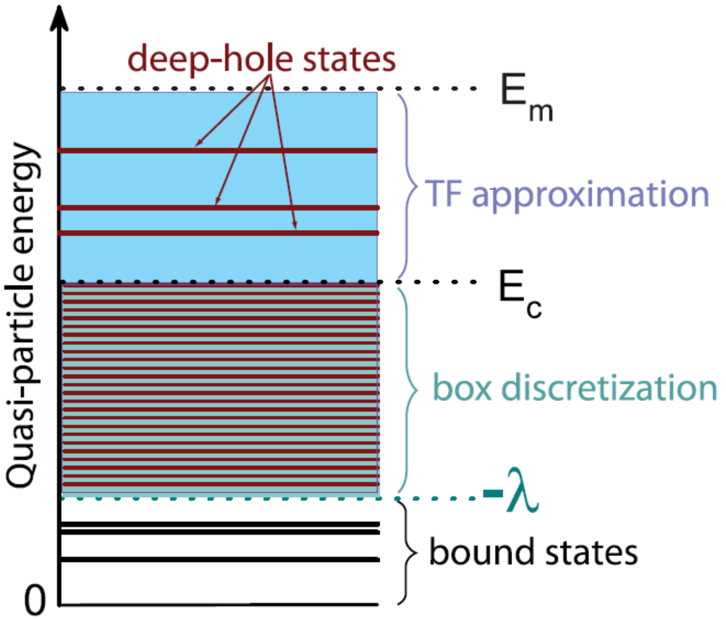
M. Kortelainen, T. Lesinski, J. More, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, *Nuclear Energy Density Optimization*
Phys. Rev. C 82, 024313 (2010)

Understanding weakly bound nuclei

- **At low excitation energies, well-bound nuclei can be considered as closed quantum systems**



- **Weakly bound and unbound nuclei are open quantum systems that are strongly coupled to the environment of scattering and decay channels**
- **The Hartree-Fock-Bogoliubov (HFB) equations of nuclear DFT properly take into account the scattering continuum**



In the hybrid HFB strategy, the quasiparticle continuum *is divided into the low-energy continuum (treated with the box discretization), and* the high-energy continuum, *which consists of* a non-resonant continuum (treated with the Thomas-Fermi approximation) and several deep-hole states.

J. C. Pei, W. Nazarewicz, A. T. Kruppa,
Quasi-particle continuum and resonances in the Hartree-Fock-Bogoliubov Theory,
Phys. Rev. C 84, 024311 (2011)

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Pei, Nazarewicz, Kruppa, *Phys. Rev. C 84, 024311* (2011)