Prospects for Breakthroughs in Low-Energy Nuclear Theory Witold Nazarewicz (FRIB/MSU)

First Tsukuba-CCS-RIKEN joint workshop on microscopic theories of nuclear structure and dynamics, December 12-16, 2016

Menu

- Prospects
- Creating unfair advantage





The Nuclear Landscape and the Big Questions

- Where did the atoms and atomic nuclei come from?
- How are the nuclei of atoms made and organized?
- What are the fundamental particles and forces at work inside atomic nuclei?
- What are practical and scientific uses of nuclei?





Guiding principle: the scientific method...



J. Phys. G 43, 044002 (2016)



Optimizing the cycle







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Rooting nuclei in QCD





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Nuclei from the first principles





Linking few-body with many-body









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Revision of nuclear structure textbook knowledge



E (MeV)

- ^{24,25,26}O: open quantum systems
- A dineutron in ²⁶O? The lifetime could be as large as 10⁻¹² s.
- Is (doubly-magic) ²⁸O unbound? If so, how much?

Unification of structure and reactions



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Large Amplitude Collective Motion

exceedingly difficult, many fundamental questions remain unsettled





Time-dependent density-functional description of nuclear dynamics

Takashi Nakatsukasa, Kenichi Matsuyanagi, Masayuki Matsuo, and Kazuhiro Yabana Rev. Mod. Phys. **88**, 045004 (2016) – Published 9 November 2016 "Many excitation modes of atomic nuclei and their reactions can be described as time-dependent processes, in which nuclei oscillate, rotate, collide, and split. A theoretical framework to describe nuclear dynamics at low energy is the time-dependent density functional theory. This reviews the foundations and extensions of this theory and its applications to nuclear collective motion, including giant resonances, heavy-ion collisions, and shape coexistence. Conceptual differences between nuclear and electronic applications are also discussed."



N. Hinohara et al, Phys. Rev. Lett. 116, 152502 (2016).



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What are the limits of atoms and nuclei?





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Quest for understanding the neutron-rich matter on Earth and in the Cosmos

Bounds on EOS



Exciting multi-disciplinary science



Crustal structures



EOS with hyperons



Data







Creating unfair advantage: the whole is greater than the sum of its parts

Sociology of the field is changing: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math





... and let us not forget about education and training!



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Uncertainty quantification

http://iopscience.iop.org/journal/0954-3899/page/ISNET

- Regression analysis
- Bayesian inference
- Extrapolations
- Model mixing
- Information content of new measurements



PRC 89, 054314 (2014)

HUGE PROSPECT Bivariate posterior distributions of energy density functionals from Bayesian analysis PRL 114, 122501 (2015) 8 Energy (MeV)

UNEDF1

UNEDF1_{CPT}
90% confidence
50 100 150
Quadrupole moment Q₂₀ (b)



In many cases, nuclear modeling MUST involve massive extrapolations...



PROSPECT

Uncertainty quantification Getting critical measurements



"It is exceedingly difficult to make predictions, particularly about the future" (Niels Bohr)

Looking into the crystal ball: year 2030 and beyond

- We will understand the QCD origin of nuclear forces. We will develop the predictive ab-initio description of light and medium-mass nuclei and their reactions, including electroweak probes. We will construct the spectroscopic-quality energy density functional that will extrapolate in mass, isospin, and angular momentum. We will develop the comprehensive reaction theory consistent with nuclear structure. We will have a comprehensive description of weak transitions in nuclei and utilize them in multi-dimensional stellar evolution simulations.
- We will know if very long-lived superheavy elements existen nature. We will understand the mechanism of clustering and other aspects of open many-body systems. We will know whether proton-neutron superfluidity exists in finite nuclei. We will know the nuclear equation of state for normal and neutron matter from 0.1 to twice the saturation density.
- We will have a quantitative microscopic model of fission that will provide the missing data for nuclear security, astrophysics, and energy research. We will predict important fusion reaction rates important for fusion vesearch and nuclear forensics. We will improve the sensitivity of EDM searches in atoms by one to two orders of magnitude over current limits. over current limits.



MATERIALS SCIENCE

Making the most of materials computations

Databases of theoretical structures and properties of materials can speed real-world discovery

By Kristian S. Thygesen and Karsten W. Jacobsen Science 354, 180 (2016)

For more than a century, materials scientists have accumulated experimental data on the structures of chemical compounds and the thermal, electronic, and mechanical properties that they exhibit. These data have been a cornerstone in the development, selection, and design of materials. In the past decade, experimental data have been augmented by an explosion of computational data from quantum-mechanical calculations, which can be obtained more quickly and in some cases with comparable accuracy.

The computational databases supplement the experimental ones mainly by providing additional systematic information about materials, but they also provide information about the properties of materials that do not occur naturally or that have never been synthesized in a laboratory.

Materials data and discovery

DFT calculations in the NoMaD repository (in millions)

The number of DFT calculations in the NoMaD repository from December 2014 to September 2016. The large jumps in October/November 2015 and February 2016 arose from inclusion of data from the AFLOWLIB and OQMD repositories, respectively.



Computational materials scientists apply a range of different codes that all solve the same fundamental equations of DFT but apply diverse numerical approaches. In a large community effort, it was recently shown that in simple situations, like the calculation of the equation of state of elemental crystals, agreement between different codes can be established.

Computational databases mainly contain entries for bulk solids in simple crystal structures, primarily because calculation times grow quickly with the number of atoms N in the unit cell (typically as N to a power between 2 and 3). However, many materials properties are determined by defects, such as vacancies, atoms in interstitial sites, or impurities, or by grain boundaries or surfaces. For many applications, the simple materials described in the databases are not directly relevant, and more complex structures and materials must be included.



Some nuclei are more important than others

Over the last decade, tremendous progress has been made in techniques to produce and describe designer nuclei, rare atomic nuclei with characteristics adjusted to specific research needs and applications



PREDICTION CONCEPT FABRICATION





⁶⁰Ca

Nuclei Matter

Our current understanding of nuclei has benefited from technological improvements in experimental equipment and accelerators that have expanded the range of available isotopes and allowed individual experiments to be performed with only a small number of atoms. Concurrent advances in theoretical approaches and computational science have led to a more detailed understanding and pointed toward which nuclei and what phenomena to study, creating conditions for major advances.

Profound intersections

- Astrophysics
- Fundamental Symmetries
- Complex systems
- Computing

THE FUTURE IS EXCITING

How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

- Energy (fission, reactions, decays...)
- Security (stewardship, forensics, detection...)
- Isotopes (medicine, industry, defense, applied research...)
- Industry (radiation, ion implantation...)

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