Scientific Report

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1. Accomplishments

The main goals of the project, can be summarized as follows:

i. Development of effective energy functionals that are appropriate for the description of heavy nuclei. Our goal is to improve the existing energy density (Skyrme) functionals to develop a force that will be used in calculations of fission dynamics. To this end, we use specialty Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) codes.
ii. Systematic self-consistent calculations of binding energies and fission barriers of actinide, pre-actinide, and trans-actinide nuclei using modern density functionals. This is followed by calculations of spontaneous fission lifetimes and mass and charge splits using dynamic adiabatic approaches.
iii. Investigate novel microscopic (non-adiabatic) methods to study the fission process. In particular, we are going to assess whether the imaginary time method and the generator coordinate method can be used in practical self-consistent calculations.
iv. Develop codes and technology that can be freely used by NNSA researchers and, generally, by the low-energy nuclear physics community.
v. Train junior scientists and students to apply nuclear many-body techniques to describe low-energy nuclear phenomena.

We are pleased to report substantial progress in the all areas of the program. One measure of this progress is publications and invited material. During the reported period, our research resulted in 8 publications (Section 2.A). We presented our research in 9 invited and contributed talks at international meetings, colloquia, and seminars (Section 2.B). The results obtained under this project have been crucial for identifying microscopic description of fission as the forefront scientific problem in the era of extreme computing.

Our group has been very active, in terms of presentations, publications, and organizational involvement, in publicizing the research covered by this grant. Specifically:

- We presented the status of microscopic fission theory at several meetings, including SSAA Annual Workshop and several conferences in the U.S., Europe, and Asia (see below).
- We established a fission project website, https://people.nscl.msu.edu/~witek/fission/fission.html, that popularizes our research.
- Our research that uses high performance computing to study, for the first time, spontaneous fission microscopically within a theoretical model using realistic collective mass was featured by DOE Office of Science as a August 2015 `Science Highlight' in an article entitled *Shape Matters when Modeling Nuclear Fission*.
- Our paper on *Twist-averaged boundary conditions for nuclear pasta Hartree-Fock calculations* was highlighted by Phys. Rev. C as Editors' Suggestion.
- We edited a special focus issue of the Journal of Physics G devoted to *Enhancing the interaction between nuclear experiment and theory through information and statistics*.
- The JPhys+ website of the Journal of Physics has featured an interview with W. Nazarewicz

about uncertainty quantification and the ISNET initiative.

- We edited a Special Issue of Buclear Physics A on *“Superheavy Elements”*.
- Our work on twisted-angle boundary conditions was featured by the Institute for Cyber-Enabled Research in ICER News.
- Our paper on Impact of Nuclear Mass Uncertainties on the r Process was highlighted by public media, including MSU Today, TU Darmstadt, Science Daily, and John Hopkins.
- In “*The Limits of the Nuclear Landscape*,” Nature 486, 509 (2012), we used nuclear density functional theory to calculate properties of nuclei at the quantum mechanical level based on densities and currents of protons and neutrons. In an effort to share this data with other research groups, the new website Massexplorer has been launched. Created by Dr. Erik Olsen, it contains mass table data obtained with six nuclear energy density functionals — representing nuclear interactions. The website also contains visualization tools that graph data so that trends can be studied more easily. Massexplorer is designed to be a work in progress and will be updated as more data relevant to fission become available.

2. Products

A. Completed projects - Publications

1. *“Benchmarking Nuclear Fission Theory”,* G.F. Bertsch, W. Loveland, W. Nazarewicz, and P. Talou, J. Phys. G 42, 077001 (2015). We suggest a small set of fission observables to be used as test cases for validation of theoretical calculations. The purpose is to provide common data to facilitate the comparison of different fission theories and models. The proposed observables are chosen from fission barriers, spontaneous fission lifetimes, fission yield characteristics, and fission isomer excitation energies. Obviously the fission process is very complex and rich, and many more data exist beyond this very small sample. One should view these notes as a living document, which will need to be updated as more useful information becomes available, and as fidelity of fission theory improves.
2. *Complex-energy approach to sum rules within nuclear density functional theory*, N. Hinohara, M. Kortelainen, W. Nazarewicz, and E. Olsen, Phys. Rev. C 91, 044323 (2015). The linear response of the nucleus to an external field contains unique information about the effective interaction, correlations governing the behavior of the many-body system, and properties of its excited states. To characterize the response, it is useful to use its energy-weighted moments, or sum rules. By comparing computed sum rules with experimental values, the information content of the response can be utilized in the optimization process of the nuclear Hamiltonian or nuclear energy density functional (EDF). But the additional information comes at a price: compared to the ground state, computation of excited states is more demanding. To establish an efficient framework to compute energy-weighted sum rules of the response that is adaptable to the optimization of the nuclear EDF and large-scale surveys of collective strength, we have developed a new technique within the complex-energy finite-amplitude method (FAM) based on the quasiparticle random- phase approximation. The proposed sum-rule technique based on the complex-energy FAM is a tool of choice when optimizing effective interactions or energy

functionals. The method is very efficient and well-adaptable to parallel computing. The FAM formulation is especially useful when standard theorems based on commutation relations involving the nuclear Hamiltonian and external field cannot be used.

3. *"Twist-averaged boundary conditions for nuclear pasta Hartree-Fock calculations"*, B. Schuetrumpf and W. Nazarewicz, Phys. Rev. C 92, 045806 (2015) [Editor's Suggestion]. Nuclear pasta phases, present in the inner crust of neutron stars, are associated with nucleonic matter at subsaturation densities arranged in regular shapes. Those complex phases, residing in a layer which is approximately 100-m thick, impact many features of neutron stars. Theoretical quantum-mechanical simulations of nuclear pasta are usually carried out in finite three-dimensional boxes assuming periodic boundary conditions. The resulting solutions are affected by spurious finite-size effects. To remove spurious finite-size effects, it is convenient to employ twist-averaged boundary conditions (TABC) used in condensed matter, nuclear matter, and lattice quantum chromodynamics applications. In this work, we study the effectiveness of TABC in the context of pasta phase simulations within nuclear density functional theory. We demonstrated that by applying TABC reliable results can be obtained from calculations performed in relatively small volumes. By studying various contributions to the total energy, we gain insights into pasta phases in mid-density range. Future applications will include the TABC extension of the adaptive multiresolution 3D Hartree-Fock solver and Hartree-Fock-Bogoliubov TABC applications to superfluid pasta phases and complex nucleonic topologies as in fission.
4. *"Special Issue on Superheavy Elements"*, Edited by Ch. E. Düllmann, R.-D. Herzberg, W. Nazarewicz and Y. Oganessian, Nucl. Phys. A 944, 1-690 (2015). Reflecting the breadth of research opportunities in the field of superheavy element research, this special issue covers the range of topics in a comprehensive way, including synthesis of superheavy isotopes, nuclear structure, atomic shell structure, and chemical properties. The contributions detail the status of the field and lay out perspectives for the future. The prospects are bright: new isotopes are awaiting discovery, completing the landscape of superheavy nuclei and bridging the currently existing gap between nuclei synthesized in cold fusion reactions and those from ^{48}Ca induced fusion reactions. The possibility that the limits of nuclear structure studies can be pushed even further in mass and charge has greatly motivated a number of new facilities. Advances in experimental techniques will allow studies on isotopes produced significantly be-low the 1pb level. Chemical studies progressing to elements never studied to date are already being prepared. Ultra-fast chemistry setups are under development and it will be fascinating to see them at work, elucidating the influence of relativistic effects on superheavy elements. The richness of chemical systems available for transactinides will expand further, giving access to new chemical systems, giving more information on the architecture of the periodic table.
5. *"Properties of nuclei in the nobelium region studied within the covariant, Skyrme, and Gogny energy density functionals",* J. Dobaczewski, A.V. Afanasjev, M. Bender, L.M. Robledo and Yue Shi, Nucl. Phys. A 944, 388 (2015). We calculated properties of the ground and excited states of nuclei in the nobelium region for proton and neutron numbers of $92 \leq Z \leq 104$ and $144 \leq N \leq 156$, respectively. We used three different energy-density-functional (EDF) approaches, based on covariant, Skyrme, and Gogny functionals, each with two different parameter sets. A comparative analysis of the results obtained for quasiparticle spectra, odd–even and two-particle mass staggering, and moments of inertia allows us to identify single-particle and shell effects that

are characteristic to these different models and to illustrate possible systematic uncertainties related to using the EDF modeling.

6. *"Microscopic modeling of mass and charge distributions in the spontaneous fission of ^{240}Pu",* J. Sadhukhan, W. Nazarewicz, and N. Schunck, Phys. Rev. C 93, 011304(R) (2016). In this paper, we outlined a methodology to calculate microscopically mass and charge distributions of spontaneous fission yields. We combined the multi-dimensional minimization of collective action for fission with stochastic Langevin dynamics to track the relevant fission paths from the ground-state configuration up to scission. The nuclear potential energy and collective inertia governing the tunneling motion were obtained with nuclear density functional theory in the collective space of shape deformations and pairing. We obtained a quantitative agreement with experimental data and find that both the charge and mass distributions in the spontaneous fission of ^{240}Pu are sensitive both to the dissipation in collective motion and to adiabatic characteristics.
7. *"Impact of Nuclear Mass Uncertainties on the r Process,"* D. Martin, A. Arcones, W. Nazarewicz, and E. Olsen, Phys. Rev. Lett. 116, 121101 (2016). Nuclear masses play a fundamental role in understanding how the heaviest elements in the Universe are created in the r process. In this work, we predicted r-process nucleosynthesis yields using neutron capture and photodissociation rates that are based on the nuclear density functional theory. Using six Skyrme energy density functionals based on different optimization protocols, we determined for the first time systematic uncertainty bands—related to mass modeling—for r-process abundances in realistic astrophysical scenarios. We find that features of the underlying microphysics make an imprint on abundances especially in the vicinity of neutron shell closures: Abundance peaks and troughs are reflected in trends of neutron separation energy. Further advances in the nuclear theory, such as modeling of fission yields of neutron-rich nuclei, will help in the understanding of astrophysical conditions in extreme r-process sites.
8. "Time-dependent density functional theory with twist-averaged boundary conditions," B. Schuetrumpf, W. Nazarewicz, and P.-G. Reinhard, Phys. Rev. C 93, 054304 (2016). Time-dependent density functional theory is widely used to describe excitations of many-fermion systems. In its many applications, 3D coordinate-space representation is used, and infinite-domain calculations are limited to a finite volume represented by a box. For finite quantum systems (atoms, molecules, nuclei), the commonly used periodic or reflecting boundary conditions introduce spurious quantization of the continuum states and artificial reflections from boundary; hence, an incorrect treatment of evaporated particles. These artifacts can be practically cured by introducing absorbing boundary conditions (ABC) through an absorbing potential in a certain boundary region sufficiently far from the described system. But also the calculations of infinite matter (crystal electrons, quantum fluids, neutron star crust) suffer artifacts from a finite computational box. In this regime, twist- averaged boundary conditions (TABC) have been used successfully to diminish the finite-volume effects. In this work, we extended TABC to time-dependent framework and applied it to resolve the box artifacts for finite quantum systems using as test case small- and large-amplitude nuclear vibrations. We demonstrated that by using such a method, one can reduce finite volume effects drastically without adding any additional parameters. While they are almost equivalent in the linear regime, TABC and ABC differ in the nonlinear regime in their treatment of evaporated particles.

B. Presentations

1. “Quantum Nuclear Pasta Calculations with Twisted Angular Boundary Conditions,” B. Schuetrumpf, 2015 Fall Meeting of the APS Division of Nuclear Physics, Oct. 28–31, 2015, Santa Fe, New Mexico
2. “Computational nuclear structure in the eve of exascale,” W. Nazarewicz, Symposium on Quarks to Universe in Computational Science (QUCS 2015), Nara, Japan, Nov. 4-8, 2015.
3. “Concluding Remarks,” W. Nazarewicz, Information and statistics in nuclear experiment and theory ISNET-3, ECT*, Trento, Italy, Nov. 16-20, 2015.
4. “Microscopic Description of Fission Process,” W. Nazarewicz, Stewardship Science Academic Programs (SSAP) Symposium, Bethesda, Maryland, Feb. 17, 2016.
5. “Theory of nuclear ground state properties,” W. Nazarewicz, X International Workshop on Application of Lasers and Storage Devices in Atomic Nuclei Research,” Poznań, Poland, May 16-19, 2016.
6. “Superheavy Element Research: Future Aspects,” W. Nazarewicz, Nobel Symposium NS160: Chemistry and Physics of Heavy and Superheavy Elements, Bäckaskog Castle, Sweden, May 29 - June 3, 2016.
7. “Massexplorer: A Website for Theoretical Nuclear Physics Calculations,” E. Olsen, 2016 NUCLEI Annual Meeting, Argonne National Laboratory, June 6-9, 2016.
8. “TDHF with Twist-Averaged Boundary Conditions,” B. Schuetrumpf, 2016 NUCLEI Annual Meeting, Argonne National Laboratory, June 6-9, 2016.
9. “Nuclear structure and fission for r process,” Witold Nazarewicz, ICNT program, The r-process: connecting FRIB with the cosmos, MSU, June 13, 2016.

3. Participants

Research was carried out by the principal investigator, two research professors, two postdocs, two graduate students, and a number of collaborators. A list of personnel involved in the research covered by this grant includes:

- J. Dobaczewski (University of Warsaw/ University of Jyväskylä)
- Z. Matheson (MSU, graduate student)
- W. Nazarewicz (MSU, Principal Investigator)
- E. Olsen (MSU, postdoc; graduated in 2014)
- J. Sadhukhan (Kolkata; visiting Research Professor)
- B. Schuetrumpf (MSU, Postdoc)
- J. Sheikh (Srinagar; visiting Research Professor)

Training of next-generation nuclear theorists is an important part of our undertaking. Two graduate students were involved in our fission research. **Erik Olsen** was involved in developing software for our DFT and QRPA work. He was responsible for benchmarking energy density functionals in the context of fission, proton emission, and beta decay. He also contributed to various software developments. He completed his Ph.D. in 2014, and is currently working on DFT developments at MSU as a postdoc. **Zach Matheson** is a new graduate student at MSU. His fist project is the analysis of fission yields around ^{180}Hg, in collaboration with experimental groups from ISOLDE and JAEA. We are currently working on recruiting the second graduate student to join our fission project.

Dr. Bastian Schuetrumpf joined our group in 2015. He is currently working on incorporating twisted angle boundary conditions into our DFT codes used for fission, including the fast-Fourier transform code. Dr. Jhilam Sadhukhan was working with us as a postdoc and, recently, as research professor; he came from Variable Energy Cyclotron Centre, Kolkata, India. Dr. Dobaczewski is the head of nuclear theory group at the University of York, UK, and University of Jyväskylä, Finland; Dr. Sheikh is a Dean of the Faculty at the University of Kashmir, Srinagar, India and expert in nuclear self-consistent calculations. We collaborate with Dr. Nicolas Schunck (LLNL) and Dr. Patrick Talou (LANL) on microscopic theory of fission.

4. Impact

Advanced theoretical methods and high-performance computers may finally unlock the secrets of nuclear fission, a fundamental nuclear decay that is of great relevance to society. Under this project, we study the phenomenon of spontaneous fission using the symmetry-unrestricted nuclear density functional theory. Our results show that many observed properties of fissioning nuclei can be explained in terms of pathways in multidimensional collective space corresponding to different geometries of fission products. From the calculated collective potential and collective mass, we estimate spontaneous fission half-lives by minimizing the collective action integral. Our calculations demonstrate that fission barriers of excited nuclei vary rapidly with particle number, pointing to the importance of shell effects even at large excitation energies. Not only does this reveal clues about the conditions for creating new elements, it also provides a wider context for understanding other types of fission.

Understanding of the fission process is crucial for many areas of science and technology. Fission governs existence of many transuranium elements, including the predicted long-lived superheavy species. In nuclear astrophysics, fission influences the formation of heavy elements on the final stages of the r-process in a very high neutron density environment. Fission applications are numerous. Improved understanding of the fission process will enable scientists to enhance the safety and reliability of the nation's nuclear stockpile and nuclear reactors. The deployment of a fleet of safe and efficient advanced reactors, which will also minimize radiotoxic waste and be proliferation-resistant, is a goal for the advanced nuclear fuel cycles program. While in the past the design, construction, and operation of reactors were supported through empirical trials, this new phase in nuclear energy production is expected to heavily rely on advanced modeling and simulation capabilities.

Much of the research carried out under this grant has applications that can impact NNSA programs in stockpile stewardship and non-proliferation. Specifically, the research described in this proposal supports the research goals of the SSAA Program in Topic Research Area Low-Energy Nuclear Science, sub-area Physics of the fission process, including division of mass and charge as a function of excitation, production of energy, and the reaction properties of prompt fission products..

The principal impact is in the delivery of fission models capable of providing nuclear data not only of a higher quality, but also with quantified uncertainties. For many NNSA applications, the required data on fission cross sections or fission products cannot be obtained via experiment, because very neutron-rich nuclei with short half-lives are required. Understanding fission and in particular properties of fission fragments is essential to successfully analyzing fission yields under a variety of conditions.

5. Changes/Problems

There are no changes from the DOE approved application.

6. Special reporting requirements

N/A

7. Budgetary Information

We estimate around $30K of unobligated balances remaining at the end of the budget period.