1. Cover Page

Final Scientific Technical Report

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2. Accomplishments

a. The main goals of the project

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 based on the WKB approximation.

iii. Develop the description of spontaneous and compound-nucleus fission within the nuclear DFT framework combined with stochastic approach based on Langevin dynamics.

iv. Develop codes and technology that can be freely used by NNSA researchers and, generally, by the low-energy nuclear physics community.

v. Educate junior scientists and students in nuclear many-body techniques to describe low-energy nuclear phenomena in specific areas of research relevant to stockpile stewardship.

b. Accomplishments

1. In J. Phys. G 42, 077001 (2015), we suggested 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 this guide as a living document, which will need to be updated as more useful information becomes available, and as fidelity of fission theory improves.

2. 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. In Phys. Rev. C 91, 044323 (2015), 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. 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. In Phys. Rev. C 92, 045806 (2015), 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. Reflecting the breadth of research opportunities in the field of superheavy element research, the special issue Nucl. Phys. A 944, 1-690 (2015) 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. In 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. A recent high-resolution α, X-ray, and γ-ray coincidence-spectroscopy experiment at GSI offered the first glimpse of excitation schemes of isotopes along α-decay chains of Z=115. To understand these observations and to make predictions about shell structure of superheavy nuclei below ^{288}115, in Nucl. Phys. A 953, 117 (2016) we employed nuclear DFT. We found that the presence and nature of low-energy E1 transitions in well-deformed nuclei around Z=110, N=168 strongly depends on the strength of the spin-orbit coupling; hence, it provides an excellent constraint on theoretical models of superheavy nuclei.

7. In Phys. Rev. C 93, 011304(R) (2016), 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.

8. Nuclear masses play a fundamental role in understanding how the heaviest elements in the Universe are created in the r process. In Phys. Rev. Lett. 116, 121101 (2016), 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.

9. 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 in Phys. Rev. C 93, 054304 (2016) 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.

10. In nuclear astrophysics, the quantum simulation of large inhomogenous dense systems as present in the crusts of neutron stars presents big challenges. The feasible number of particles in a simulation box with periodic boundary conditions is strongly limited due to the immense computational cost of the quantum methods. In Comput. Phys. Comm. 223, 34 (2018), we described the techniques used to parallelize Sky3D, a nuclear density functional theory code that operates on an equidistant grid, and optimize its performance on distributed memory architectures. We also describe cache blocking techniques to accelerate the compute-intensive matrix calculation part in Sky3D. Presented techniques allow Sky3D to achieve good scaling and high performance on a large number of cores, as demonstrated through detailed performance analysis on Edison, a Cray XC30 supercomputer.

11. Electron localization measure was originally introduced to characterize chemical bond structures in molecules. In Phys. Rev. C 94, 064323 (2016), we introduced a nucleon localization based on Hartree-

Fock densities introduced to investigate α-cluster structures in light nuclei. Compared to the local nucleonic densities, the nucleon localization function has been shown to be an excellent indicator of shell effects and cluster correlations. In particular, we investigated the emergence of fragments in fissioning heavy nuclei using the self-consistent energy density functional method with a quantified energy density functional optimized for fission studies. We studied the particle densities and spatial nucleon localization distributions along the fission pathways of ^{264}Fm, ^{232}Th, and ^{240}Pu. We demonstrated that the fission fragments were formed fairly early in the evolution, well before scission. To illustrate the usefulness of the localization measure, we showed how the hyperdeformed state of ^{232}Th could be understood in terms of a quasimolecular state made of ^{132}Sn and ^{100}Zr fragments. Compared to nucleonic distributions, the nucleon localization function more effectively quantifies nucleonic clustering: its characteristic oscillating pattern, traced back to shell effects, is a clear fingerprint of cluster/fragment configurations. This is of particular interest for studies of fragment formation and fragment identification in fissioning nuclei.

12. Nuclear density functional theory (DFT) is the tool of choice in describing properties of complex nuclei and intricate phases of bulk nucleonic matter. It is a microscopic approach based on an energy density functional representing the nuclear interaction. An attractive feature of nuclear DFT is that it can be applied to both finite nuclei and pasta phases appearing in the inner crust of neutron stars. While nuclear pasta clusters in a neutron star can be easily characterized through their density distributions, the level of clustering of nucleons in a nucleus can often be difficult to assess. To this end, we use the concept of nucleon localization. In Chapter 5 of *Nuclear Particle Correlations and Cluster Physics*, we demonstrated that the localization measure provides us with fingerprints of clusters in light and heavy nuclei, including fissioning systems. Furthermore, we investigated the rod-like pasta phase using twist-averaged boundary conditions, which enable calculations in finite volumes accessible by state of the art DFT solvers.

13. To interpret charge radii in ^{52,53}Fe measured with bunched-beam collinear laser spectroscopy, in Phys. Rev. Lett. 117, 252501 (2016), we employed nuclear density functional theory with Fayans and Skyrme energy density functionals. We demonstrated that the trend of charge radii along the Fe isotopic chain results from an interplay between single-particle shell structure, pairing, and polarization effects. This work employed results of our systematic DFT calculations stored in the massexplorer database.

14. In Phys. Rev. C 96, 024306 (2017), we revealed mechanisms behind the formation of central depression in nucleonic densities in light and heavy nuclei. To this end, we introduced several measures of the internal nucleonic density. Through the statistical analysis, we studied the information content of these measures with respect to nuclear matter properties. We demonstrated that the central depression in medium-mass nuclei is very sensitive to shell effects, whereas for superheavy systems it is firmly driven by the electrostatic repulsion. An appreciable semibubble structure in proton density is predicted for 294Og, which is currently the heaviest nucleus known experimentally.

15. In Phys. Rev. C 96, 061301(R) (2017), we used the stochastic Langevin framework to simulate the nuclear evolution after the system tunnels through the multidimensional potential barrier. For a representative sample of different initial configurations along the outer turning-point line, we defined effective fission paths by computing a large number of Langevin trajectories. We extracted the relative contribution of each such path to the fragment distribution. We then used nucleon localization functions along effective fission pathways to analyze the characteristics of prefragments at prescission configurations. We found that non-Newtonian Langevin trajectories, strongly impacted by the random force, produce the tails of the fission fragment distribution of ^{240}Pu. The prefragments deduced from

nucleon localizations are formed early and change little as the nucleus evolves towards scission. On the other hand, the system contains many nucleons that are not localized in the prefragments even near the scission point. Such nucleons are distributed rapidly at scission to form the final fragments. Fission prefragments extracted from direct integration of the density and from the localization functions typically differ by more than 30 nucleons even near scission.

16. In Phys. Rev. Lett. 120, 053001 (2018), fermion localization functions were used to discuss electronic and nucleonic shell structure effects in the superheavy element oganesson, the heaviest element discovered to date. Spin-orbit splitting in the 7p that Og is expected to show uniform-gas-like behavior in the valence region with a rather large dipole polarizability compared to the lighter rare gas elements. The nucleon localization in Og is also predicted to undergo a transition to the Thomas-Fermi gas behavior in the valence region. This effect, particularly strong for neutrons, is due to the high density of single-particle orbitals.

17. Until recently, ground-state nuclear moments of the heaviest nuclei could only be inferred from nuclear spectroscopy, where model assumptions are required. Laser spectroscopy in combination with modern atomic structure calculations is now able to probe these moments directly, in a comprehensive and nuclear- model-independent way. In Phys. Rev. Lett. 120, 232503 (2018) we reported on unique access to the differential mean-square charge radii of $^{252;253;254}$No, and therefore to changes in nuclear size and shape. State-of-the-art nuclear density functional calculations describe well the changes in nuclear charge radii in the region of the heavy actinides, indicating an appreciable central depression in the deformed proton density distribution in $^{252;254}$No isotopes. Opportunities for training and professional development provided by the project.

18. Four new elements with atomic numbers Z = 113, 115, 117 and 118 have recently been added to the periodic table. The questions pertaining to these superheavy systems are at the forefront of research in nuclear and atomic physics, and chemistry. The Perspective published in Nature Phys. 14, 537 (2018) offers a high-level view of the field and outlines future challenges.

19. The non-perturbative method to compute Adiabatic Time Dependent Hartree Fock Bogoliubov (ATDHFB) collective inertias is extended to the Generator Coordinate Method (GCM) including the case of density dependent forces. In Phys. Lett. B 787, 134 (2018), the two inertias schemes are computed along the fission path of the 234U and compared with the perturbative results. We find that the non-perturbative schemes predict very similar collective inertias with a much richer structure than the one predicted by perturbative calculations. Moreover, the non-perturbative inertias show an extraordinary similitude with the exact GCM inertias computed numerically from the energy overlap. These results indicate that the non-perturbative inertias provide the right structure as a function of the collective variable and only a phenomenological factor is required to mock up the exact GCM inertia, bringing new soundness to the microscopic description of fission.

20. In Phys. Rev. C 98, 034318 (2018), we considered 10 global models based on nuclear density functional theory with realistic energy density functionals as well as two more phenomenological mass models. The emulators of two-neutron separation energy residuals and Bayesian confidence intervals defining theoretical error bars were constructed using Bayesian Gaussian processes and Bayesian neural networks. By establishing statistical methodology and parameters, we carried out extrapolations toward the two-neutron dripline. While both Gaussian processes (GP) and Bayesian neural networks reduce the root-mean-square (rms) deviation from experiment significantly, GP offers a better and much more stable performance. The increase in the predictive power of microscopic models aided by the statistical treatment is quite astonishing: The resulting rms deviations from experiment on the

testing dataset are similar to those of more phenomenological models. We found that Bayesian neural networks results are prone to instabilities caused by the large number of parameters in this method. Moreover, since the classical sigmoid activation function used in this approach has linear tails that do not vanish, it is poorly suited for a bounded extrapolation. The empirical coverage probability curves we obtain match very well the reference values, in a slightly conservative way in most cases, which is highly desirable to ensure honesty of uncertainty quantification. The estimated credibility intervals on predictions make it possible to evaluate predictive power of individual models and also make quantified predictions using groups of models. The proposed robust statistical approach to extrapolation of nuclear model results can be useful for assessing the impact of current and future experiments in the context of model developments. The new Bayesian capability to evaluate residuals is also expected to impact research in the domains where experiments are currently impossible, for instance, in simulations of the astrophysical r process.

c. Dissemination of results

The results of our work were published in peer-reviewed scientific journals .We reported the status of microscopic fission theory at several meetings, including SSAA Annual Workshop and several conferences in the U.S., Europe, Asia, and Australia (see below). Other notable outcomes include:

- 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 ou postdoc 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.
- Chunli Zhang received Sherwood K Haynes Award from Physics Department, MSU, for her Ph.D. work
- Nazarewicz served as a co-lead of a section on Nuclear Structure and Reactions of *Nuclear Physics, DOE Exascale Requirements Review report*. June 15-17, 2016.

- Our SSAA project has been highlighted in NSCL's GreenSheet.
- Nazarewicz has been awarded the G.N. Flerov Prize from the Joint Institute for Nuclear Research for outstanding research in nuclear physics. He was cited for his *theoretical studies of the atomic and nuclear properties of the heaviest elements*.
- Our publication on electron and nucleon localization functions of oganesson was highlighted as Editors' suggestion. It was featured in Physics (phys.aps.org) as Viewpoint: Heaviest Element Has Unusual Shell Structure; featured on the cover of Phys. Rev. Lett. 120(5) issue, and featured by MSUToday, Physics Today, Nature, Physics World, Science News, Gizmodo, Phys.org, Chemistry World, and many international news outlets.
- Our publication on cluster formation in pre-compound nuclei in the time-dependent framework was highlighted as Editors' suggestion. It was featured in Physics (phys.aps.org) as Physics Focus: Video-Nuclear Fusion in Hi-Def, and also highlighted by GSI.
- Our paper on sizes and shapes of nobelium isotopes was highlighted as Editors' suggestion. It was featured in Physics (phys.aps.org) as Physics Focus and by Science News.
- Our Perspective in Nature Physics on the limits of nuclear mass and charge was featured by MSUToday, ScienceAlert, Phys.org, and many international news outlets.
- Our publication on Bayesian approach to model-based extrapolation of nuclear observables was highlighted as Editors' suggestion.

3. Products

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 20 publications (Section 3.A). We presented our research in 38 invited and contributed talks at international meetings, colloquia, and seminars (Section 3.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.

A. Completed projects - Publications

1. *Benchmarking Nuclear Fission Theory*, J. Phys. G 42, 077001 (2015), G.F. Bertsch, W. Loveland, W. Nazarewicz, and P. Talou.
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).
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].
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).
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).
6. *Recoil-alpha-fission and recoil-alpha-alpha-fission events observed in the reaction ^{48}Ca + ^{243}Am*, U. Forsberg, D. Rudolph, L.-L. Andersson, A. Di Nitto, Ch.E. Dullmann, J.M. Gates, P. Golubev, K.E. Gregorich, C.J. Gross, R.-D. Herzberg, F.P. Hessberger, J. Khuyagbaatar, J.V. Kratz, K.

Rykaczewski, L.G. Sarmiento, M. Schadel, A. Yakushev, S. Aberg, D. Ackermann, M. Block, H. Brand, B.G. Carlsson, D. Cox, X. Derkx, J. Dobaczewski, K. Eberhardt, J. Even, C. Fahlander, J. Gerl, E. Jager, B. Kindler, J. Krier, I. Kojouharov, N. Kurz, B. Lommel, A. Mistry, C. Mokry, W. Nazarewicz, H. Nitsche, J.P. Omtvedt, P. Papadakis, I. Ragnarsson, J. Runke, H. Schaffner, B. Schausten, Y. Shi, P. Thorle-Pospiech, T. Torres, T. Traut, N. Trautmann, A. Turler, A. Ward, D.E. Ward, and N. Wiehl, Nucl. Phys. A 953, 117 (2016).

7. *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).
8. *Impact of Nuclear Mass Uncertainties on the r Process,*D. Martin, A. Arcones, W. Nazarewicz, and E. Olsen, Phys. Rev. Lett. 116, 121101 (2016).
9. *Time-dependent density functional theory with twist-averaged boundary conditions*, B. Schuetrumpf, W. Nazarewicz, and P.-G. Reinhard, Phys. Rev. C. 93, 054304 (2016).
10. *Nucleon localization in light and heavy nuclei*, C. Zhang, B. Schuetrumpf, and W. Nazarewicz, Phys. Rev. C 94, 064323 (2016).
11. *Charge Radii of Neutron-Deffcient* ^{52,53}*Fe Produced by Projectile Fragmentation*, K. Minamisono, D. M. Rossi, R. Beerwerth, S. Fritzsche, D. Garand, A. Klose, Y. Liu, B. Maass, P. F. Mantica, A. J. Miller, P. Muller, W. Nazarewicz, W. Nortershauser, E. Olsen, M. R. Pearson, P.-G. Reinhard, E. E. Saperstein, C. Sumithrarachchi, and S. V. Tolokonnikov, Phys. Rev. Lett. 117, 252501 (2016).
12. *Formation and distribution of fragments in the spontaneous fission of* ^{240}*Pu*, J. Sadhukhan, C.L. Zhang, W. Nazarewicz, and N. Schunck, Phys. Rev. C 96, 061301(R) (2017).
13. *Central depression in nucleonic densities: Trend analysis in the nuclear density functional theory approach*, B. Schuetrumpf, W. Nazarewicz, and P.-G. Reinhard, Phys. Rev. C 96, 024306 (2017).
14. *Clustering and pasta phases in nuclear density functional theory*, B. Schuetrumpf, C. Zhang, and W. Nazarewicz, in: Nuclear Particle Correlations and Cluster Physics, Chapter 5, p. 135 (2017).
15. *Electron and nucleon localization functions of oganesson: Approaching the Thomas-Fermi limit*, P. Jerabek, B. Schuetrumpf, P. Schwerdtfeger, and W. Nazarewicz, Phys. Rev. Lett. 120, 053001 (2018). [Editors' Suggestion, Featured in Physics].
16. *Scalable Nuclear Density Functional Theory with Sky3D*, M. Afibuzzaman, B. Schuetrumpf, and H.M. Aktulga, Comput. Phys. Comm. 223, 34 (2018).
17. *The limits of nuclear mass and charge*, W. Nazarewicz, Nature Phys. 14, 537 (2018).
18. *Probing sizes and shapes of nobelium isotopes by laser spectroscopy*, S. Raeder, D. Ackermann, H. Backe, R. Beerwerth, J. C. Berengut, M. Block, A. Borschevsky, B. Cheal, P. Chhetri, Ch.E. Dullmann, V.A. Dzuba, E. Eliav, J. Even, R. Ferrer, V.V. Flambaum, S. Fritzsche, F. Giacoppo, S. Gotz, F.P. Hessberger, M. Huyse, U. Kaldor, O. Kaleja, J. Khuyagbaatar, P. Kunz, M. Laatiaoui, F. Lautenschlager, W. Lauth, A.K. Mistry, E. Minaya Ramirez, W. Nazarewicz, S.G. Porsev, M.S. Safronova, U.I. Safronova, B. Schuetrumpf, P. Van Duppen, T. Walther, C. Wraith, and A. Yakushev, Phys. Rev. Lett. 120, 232503 (2018). [Editors' Suggestion. Featured in Physics].
19. *Non-perturbative collective inertias for fission: a comparative study*, S. A. Giuliani, L. M. Robledo, Phys. Lett. B 787, 134 (2018).
20. *Bayesian approach to model-based extrapolation of nuclear observables*, L. Neufcourt, Y. Cao, W. Nazarewicz, and F. Viens, Phys. Rev. C 98, 034318 (2018). [Editors' Suggestion].

B. Presentations

1. “Nuclear Structure Theory: today and tomorrow,” W. Nazarewicz, ISOLDE Workshop and Users Meeting 2014, CERN, Geneva, Switzerland, Dec. 15, 2014
2. “Microscopic Description of Fission Process,” W. Nazarewicz, JINA, MSU, Jan. 26, 2015.
3. “Microscopic Description of Fission Process,” W. Nazarewicz, 2015 Stewardship Science Academic Programs Symposium, Santa Fe, NM, March 12, 2015.
4. “Superheavy Nuclei: Theoretical Challenges,” W. Nazarewicz, Super Heavy Nuclei Symposium, Texas A&M University, College Station, TX, March 31, 2015.
5. “Study of nuclear fission with DFT,” J. Sadhukhan, 2015 NUCLEI Collaboration Meeting, NSU, June 10-13, 2015.
6. “Nuclear Pasta with twisted average Boundary Conditions,” B. Schuetrumpf, 2015 NUCLEI Collaboration Meeting, NSU, June 10-13, 2015.
7. “Information content of a nuclear observable and uncertainty quantification of nuclear models,” W. Nazarewicz, Nuclear Structure and Dynamics III, Portoroz, Slovenia, June 14-19, 2015.
8. “Nuclear Structure Theory: today and tomorrow,” W. Nazarewicz, Reflections on the Atomic Nucleus, Liverpool, UK, July 28-30, 2015.
9. “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
10. “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.
11. “Concluding Remarks,” W. Nazarewicz, Information and statistics in nuclear experiment and theory ISNET-3, ECT*, Trento, Italy, Nov. 16-20, 2015.
12. “Microscopic Description of Fission Process,” W. Nazarewicz, Stewardship Science Academic Programs (SSAP) Symposium, Bethesda, Maryland, Feb. 17, 2016.
13. “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.
14. “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.
15. “Massexplorer: A Website for Theoretical Nuclear Physics Calculations,” E. Olsen, 2016 NUCLEI Annual Meeting, Argonne National Laboratory, June 6-9, 2016.
16. “TDHF with Twist-Averaged Boundary Conditions,” B. Schuetrumpf, 2016 NUCLEI Annual Meeting, Argonne National Laboratory, June 6-9, 2016.
17. “Nuclear structure and fission for r-process,” Witold Nazarewicz, ICNT program, The r-process: connecting FRIB with the cosmos, MSU, June 13, 2016.
18. “Massexplorer: A Website for Theoretical Nuclear Physics Calculations,” E. Olsen, Nuclear Data Workshop, U. Notre Dame, Aug. 10, 2016.
19. “Nuclear Structure & Reactions: Breakout Report,” W.Nazarewicz, Exascale Requirements Review for Nuclear Physics, Gaithersburg, MD, June 15-17, 2016.
20. “Prospects for breakthroughs in understanding nuclei”, W. Nazarewicz, 26th International Nuclear Physics Conference, Adelaide, Australia (plenary talk), Sep. 11-16, 2016
21. “Microscopic Description of the Fission Process,” W. Nazarewicz, HIAS 2016, ANU, Canberra, Australia, Sep. 18-20, 2016.
22. “Nucleon localization within nuclear density functional theory,” C. Zhang, 2016 Fall Meeting of the APS Division of Nuclear Physics, Vancouver, BC, Canada, Oct. 14, 2016.
23. “Survey of Reflection-Asymmetric Nuclear Deformations,” E. Olsen, 2016 Fall Meeting of the APS Division of Nuclear Physics, Vancouver, BC, Canada, Oct. 14, 2016.

24. “Prospects for Breakthroughs in (Low-Energy) Nuclear Theory,” W. Nazarewicz, Sixth International Conference on Fission and Properties of Neutron-Rich Nuclei, Sanibel Island, Florida, November 6-12, 2016.
25. “Prospects for Breakthroughs in Low-Energy Nuclear Theory,” W. Nazarewicz, First Tsukuba-CCS-RIKEN joint workshop on microscopic theories of nuclear structure and dynamics, RIKEN Nishina Center, Japan, Dec. 12, 2016
26. “Large scale static and time-dependent Hartree-Fock calculations with twist-averaged boundary conditions,” B. Schutrumpf, First Tsukuba-CCS-RIKEN joint workshop on microscopic theories of nuclear structure and dynamics, Tsukuba, Japan, Dec. 14, 2016
27. “The nucleon localization function in (time-dependent) DFT,” B. Schutrumpf, FUSION17, Hobart, Tasmania, Australia, Feb. 23, 2017
28. “At the End of the Nuclear Chart,” W. Nazarewicz, International Festive Colloquium Dedicated to the naming of the New Elements with Atomic Numbers 115, 117 and 118, RAS, Moscow, Russia, March 2, 2017
29. “Superheavy Element Research: Perspectives,” W. Nazarewicz, JINR, FLNR, Dubna, Russia, March 3, 2017
30. “Microscopic Description of Fission Process,” W. Nazarewicz, Stewardship Science Academic Programs (SSAP) Symposium, Naperville, IL, April 12-13, 2017
31. “Time-dependent description nuclear collisions and infinite nucleonic systems,” B. Schutrumpf, ARIS 2017, Keystone, CO, USA, May 31, 2017.
32. “Scalable nuclear density functional theory based on the code Sky3D,” B. Schutrumpf, NUCLEI Meeting, Santa Fe, NM, USA, June 7, 2017.
33. “Superheavy Element Research: Perspectives (Theory, a 10 km view)”, W. Nazarewicz, SHE2017, Kazimierz Dolny, Poland, Sep. 10-14, 2017.
34. “Fermion localizations in nuclear DFT and TDDFT”, W. Nazarewicz, FiDiPro Winter Symposium on Nuclear Structure Physics, University of Jyvaskyla, Finland, Dec. 11-15, 2017.
35. “Microscopic Description of the Fission Process,” W. Nazarewicz, Stewardship Science Academic Programs (SSAP) Symposium, Bethesda, MD, February 21-22, 2018.
36. “(i) Fermion localization in nuclear DFT and TDDFT; (ii) and Bayesian approach to model-based extrapolations”, W. Nazarewicz, Nuclear Structure and Reactions for the 2020s, GANIL, Caen, France, July 2-6, 2018.
37. “Bayesian approach to model-based extrapolation of nuclear observables”, FRIB-TA Workshop `FRIB and the GW170817 kilonova', MSU, July 16-27, 2018.
38. “Applications of Nuclear Density Functional Theory”, W. Nazarewicz, International School of Nuclear Physics, 40th Course, The Strong Interaction: From Quarks and Gluons to Nuclei and Stars, Erice, Italy: September 16-24, 2018.

C. Websites

We established a fission project website, https://people.nscl.msu.edu/~witek/fission/fission.html, that popularizes our research.

In an effort to share this data with other research groups, the website http://massexplorer.frib.msu.edu has been launched. Created by Dr. Erik Olsen and students, it contains mass table data obtained with several 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.

4. 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 York, Professor)
- S. Giuliani (MSU, Research Associate)
- Z. Matheson (MSU, graduate student)
- W. Nazarewicz (MSU, Principal Investigator)
- E. Olsen (MSU, Research Associate)
- J. Sadhukhan (Kolkata; visiting Research Professor)
- B. Schuetrumpf (MSU, Research Associate; currently GSI, Germany)
- C. Zhang (MSU, graduate student; Ph.D. November 2017; currently at Google)

Training of next-generation nuclear theorists is an important part of our undertaking. Two graduate students were involved in our fission research. **Zach Matheson** is a 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. Zach was selected to receive the DOE Office of Science Graduate Student Research (SCGSR) award. The enabled him to conduct a "program for spontaneous fission calculations using density functional theory" at Lawrence Livermore National Laboratory in a collaboration with Dr. Nicolas Schunck. The award covered Zach's stay at LLNL during the Spring Semester 2017. The award letter states: "Your selection is in recognition of your outstanding academic accomplishments and the merit of the research proposed in your SCGSR application, and reflects your potential to advance in your Ph.D. studies and make important contributions to the mission of the DOE Office of Science."

The second graduate student was **Chunli Zhang**. This grant provided partial support for her work on the fission fragment localization. This project constituted a part of her Ph.D. thesis, which was successfully defended in November 2017.

Three research associates were involved in our fission research. **Erik Olsen** has been responsible for developing software for our DFT and QRPA work and for benchmarking energy density functionals in the context of fission, proton emission, and beta decay. He also contributed to various software developments. He is responsible for maintaining website massexplorer.frib.msu.edu, which stores our DFT results. **Bastian Schuetrumpf** joined our group in 2015. He succeeded in incorporating twisted angle boundary conditions into our DFT codes used for fission, including the fast-Fourier transform code. He left us in 2017 to assume a postdoctoral position at GSI, Germany. His replacement is Dr. **Samuel Giuliani**, who joined us in the Fall of 2017. 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. We collaborate with Dr. Nicolas Schunck (LLNL) and Dr. Patrick Talou (LANL) on microscopic theory of fission.

We will continue to encourage MSU students to join our SSAA effort. In this context, we designed a undergraduate/graduate-level nuclear physics survey course at MSU (attended by 60-65 students annually) to expose students to nuclear physics challenges, including SSAA areas. It is crucial that there is a continuous influx of young, well-trained low-energy nuclear physicists entering the NNSA labs, and we will continue helping to maintain the pipeline of young scientific talent into fields of research relevant to Stockpile Stewardship.

We receive significant support from ASCR personnel collaborating with us on various collaborations, such as NUCLEI SciDAC-4 project. Locally at MSU, we collaborate with Metin Aktulga from Department of Computer Science and Engineering (on linear algebra and code scaling) and with Frederi Viens, Taps Maiti, and Leo Neufcourt and their group from the Department of Statistics and Probability (on uncertainty quantification and Bayesian inference).

5. 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.

6. Changes/Problems

There are no changes from the DOE approved application.

7. Special reporting requirements

N/A

8. Budgetary Information

We estimate no unobligated balances remaining at the end of the budget period.