Final Scientific Report

"Theoretical Description of the Fission Process"
NNSA/SSAA Grant DE-FG03-03NA00083
Principal Investigator: Witold Nazarewicz (University of Tennessee)
7/1/2006-6/30/2009

1. Executive summary

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. In this work, we studied the phenomenon of spontaneous fission using the symmetry-unrestricted nuclear density functional theory (DFT). 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 estimated spontaneous fission half-lives, and good agreement with experimental data was found. We also predicted a new phenomenon of trimodal spontaneous fission for some transfermium isotopes. Our calculations demonstrate that fission barriers of excited superheavy nuclei vary rapidly with particle number, pointing to the importance of shell effects even at large excitation energies. The results are consistent with recent experiments where superheavy elements were created by bombarding an actinide target with 48-calcium; yet even at high excitation energies, sizable fission barriers remained. 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

2. Brief summary of the goals and accomplishments of the project

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 will use recently developed Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) codes.

ii. Systematic self-consistent calculations of binding energies and fission barriers of actinide and trans-actinide nuclei using modern density functionals. This will be followed by calculations of spontaneous fission lifetimes and mass and charge divisions using dynamic adiabatic approaches based on the WKB approximation.

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.

We are pleased to report substantial progress in the all areas of the program. One measure of this progress is publications and invited material. Our research resulted in 18 refereed publications, including one Phys. Rev. Letters, and one Phys. Rev. C rapid communication. We presented our research in 37 invited and contributed talks at international meetings, colloquia, and seminars. The main accomplishments are listed below in Sec. 5.A. More specifically, in the area (i), the main accomplishments are Refs. 4, 5, 9, 10, 13, and 18; in the area (ii), the main accomplishments are Refs. 14, 15, 16, and 19; in the area (iiii), the main accomplishments are Refs. 6 and 7. 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.

3. List of project participants

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

- A. Baran (UT/University of Lublin)
- D. J. Dean (ORNL/UT)
- J. Dobaczewski (UT/University of Warsaw)
- J. McDonnell (UT)
- W. Nazarewicz (UT/ORNL, Principal Investigator)
- N. Nikolov (UT, graduate student; since January 2005)
- J. Pei (UT)
- N. Schunck (UT)
- J. Sheikh (UT)
- J. Skalski (Soltan Institute for Nuclear Studies, Warsaw)
- A. Staszczak (UT/University of Lublin)
- M. Warda (University of Lublin)

Two graduate students were involved in our fission research. Mr. Nikolov was fully supported by the grant. His main task, and also a principal part of his Ph.D. thesis, is to investigate the role of the surface-symmetry energy on fission properties of neutron-rich nuclei. Jordan McDonnell is a U.S. Department of Energy/NNSA Stewardship Science Graduate Fellow; his support comes from the Krell Institute. His main project is to describe fission pathways in highly excited nuclei. The grant fully supported one postdoc, Dr. Sheik, who was involved in a number of projects, including studies of fission barriers in superheavy nuclei and fission dynamics. Dr. Baran and Dr. Staszczak are senior researchers from Lublin/Poland who visited Tennessee for longer periods under this grant. Dr. Staszczak has been responsible for the fission barrier calculations; Dr. Baran carries out dynamic calculations of fission lifetimes. Dr. Dobaczewski, Dr. Schunck and Dr. Stoitsov are responsible for development of the HFB solver and improvements to the energy density functional. They were supported by the UNEDF SciDAC-2 project. Dr. Pei, another postdoc, was leading the temperature-dependent fission barrier calculations; his primarily support came from the Joint Institute for Heavy Ion Research. Dr. Skalski and Dr. Warda were visiting us under this grant.

4. Outreach

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 DNP/APS meetings, Advanced Fuel Cycles Workshop, NNSA Annual Workshop, NNSA/ASCR workshop on *Scientific Grand Challenges in National Security: the Role of Computing at the Extreme Scale*, and other meetings (see below).
- A research topic related to the theory of fission has been listed on the website of the UTK Physics Department: http://www.phys.utk.edu/graduateprogram_research_projects.html.
- We developed a set of graduate-level lectures on modern nuclear science, including topics covered by this grant, see http://www.phys.utk.edu/witek/NP621/NuclPhys621-2008.html.
- We organized the annual fission workshop at the Joint Institute for Heavy Ion Research.
- We established a fission project website, http://www.phys.utk.edu/witek/fission/fission.html, that popularizes our research.
- We contributed to outreach activities at HRIBF, see http://www.phy.ornl.gov/hribf/science/abc/. In particular, we prepared a popular flyer on bimodal fission: http://www.phy.ornl.gov/hribf/science/abc/2007/bimodalfission.pdf.
- Dean and Nazarewicz, together with Bertsch, wrote a popular article on high-performance computing in nuclear structure that also features our fission research. The article appeared in SciDAC Review, Issue 6, 42, 2007. Another SciDAC Review article, on fission research, is in preparation.
- Our work on fission barriers in compound superheavy nuclei was featured in *Defense Science Quarterly*, Summer 2009, p. 6.
- We prepared a high-lever brochure for DOE Office of Science on Nuclear Physics Highlights, which also highlight nuclear fission theory, see http://www.phys.utk.edu/witek/Brochure/NPH_basic version.pdf

5. Deliverables

We made progress in the area of the nuclear energy density functional; we performed systematic studies of particle-number fluctuations and developed the particle-number-projected (before variation) Skyrme-HFB formalism; we established and implemented a method to calculate the zero-point energy correction and inertia tensor; and we produced several self-consistent HFB mass tables involving particle number projection. We began systematic barrier computations for the heavy and superheavy elements. In particular, we succeeded in calculating three-dimensional self-consistent potential energy surfaces (in the space of elongation, mass asymmetry, and necking). We produced the first microscopic estimates of spontaneous fission lifetimes based on the adiabatic collective action. Finally, we studied fission barriers in compound nuclei.

We are pleased to report substantial progress in all areas of the program. One measure of this progress is publications and invited material. Our research resulted in 18 refereed publications, including one Phys. Rev. Letters, and one Phys. Rev. C rapid communication. They are listed in Sec. 4.A. We presented our research in 37 invited and contributed talks at international meetings, colloquia, and seminars., see Sec. 4.C. Section 4.D talks about code development work and Sec. 4.E describes the workshop supported by this project.

A. Completed projects - Publications

1. *"Pairing Properties of Superheavy Nuclei"*, A. Staszczak, J. Dobaczewski, and W. Nazarewicz, **Int. J. Mod. Phys. E 16, 310 (2007)**. In this work, we investigated whether pairing properties of even-even superheavy N=184 isotones are studied within the Skyrme-Hartree-Fock+BCS approach. In the particle-hole channel we took the Skyrme energy density functional SLy4, while in the particle-particle channel we employed the seniority pairing force and zero-range delta-interactions with different forms of density dependence. We concluded that the calculated static fission trajectories weakly depend on the specific form of the delta-pairing interaction. We also investigated the impact of triaxiality on the inner fission barrier and found a rather strong atomic number dependence of the effect.
2. *"Bimodal Fission in the Skyrme-Hartree-Fock Approach*", A. Staszczak, J. Dobaczewski, and W. Nazarewicz, **Acta. Phys. Pol. B, 38, 1589 (2007)**. Spontaneous-fission properties of ^{256}Fm, ^{258}Fm, and ^{260}Fm isotopes were studied within the Skyrme-Hartree-Fock+BCS framework. In the particle-hole channel we took the Skyrme SkM* effective force, while in the particle-particle channel we employ the seniority pairing interaction. Three static fission paths for all investigated heavy fermium isotopes were found. The analysis of these fission modes allows us to explain the observed asymmetric fission of ^{256}Fm, as well as bimodal fission of ^{258}Fm and symmetric fission in ^{260}Fm.
3. *"Collective Inertia and Fission Barriers Within the Skyrme-Hartree-Fock Theory"*, A. Baran, A. Staszczak, J. Dobaczewski, and W. Nazarewicz, **Int. J. Mod. Phys. E16, 443 (2007)**. In this work, spontaneous fission barriers, quadrupole inertia, and zero-point quadrupole-energy corrections were calculated for ^{252,256,258}Fm in the framework of the self-consistent Skyrme-Hartree-Fock+BCS theory. Two ways of computing dynamical inertia were employed: the Gaussian Overlap Approximation to the Generator Coordinate Method and cranking ansatz. The Skyrme results were compared with those of the Gogny-Hartree-Fock-Bogoliubov model.
4. *"Particle-Number Projection and the Density Functional Theory*", J. Dobaczewski, M. V. Stoitsov, W. Nazarewicz, and P. -G. Reinhard, **Phys. Rev. C 76, 054315 (2007)**. In the framework of the Density Functional Theory for superconductors, we studied the restoration of the particle number symmetry by means of the projection technique. Conceptual problems were outlined and numerical difficulties discussed. Both are related to the fact that neither the many-body Hamiltonian nor the wave function of the system appear explicitly in the Density Functional Theory. Similar obstacles are encountered in self-consistent theories utilizing density-dependent effective interactions.
5. *"Variation After Particle-Number Projection for the Hartree-Fock-Bogoliubov Method with the Skyrme Energy Density Functional"*, M. V. Stoitsov, J. Dobaczewski, R. Kirchner, W. Nazarewicz, and J. Terasaki, **Phys. Rev. C 76, 014308 (2007).** Variation after particle-number restoration was incorporated for the first time into the Hartree-Fock-Bogoliubov framework employing the Skyrme energy density functional with zero-range pairing. The resulting projected HFB equations can be expressed in terms of the local gauge-angle-dependent densities. Results of projected calculations are compared with those obtained within the Lipkin-Nogami method in the standard version and with the Lipkin-Nogami method followed by exact particle-number projection.
6. *"Adiabatic Fusion Barriers from Self-Consistent Calculations"*, J. Skalski, **Phys. Rev. C 76, 044603 (2007)**. We studied adiabatic fusion barriers within the static Hartree-Fock method with the effective Skyrme interactions SkM* and SLy6. We discussed the problem of kinetic energy of the relative motion becoming spurious for separate fragments, relevant for fusion and fission barriers. We also discussed specific assumptions necessary to compensate for the non-uniqueness of the static method. Barriers obtained with two forces agree to within 2 MeV and seem nearly decoupled from errors in binding energies specific to each force. For a number of reactions, comparisons are made with experimental estimates of barriers and barriers calculated with the frozen densities. The adiabatic barriers are generally lower than the experimental estimates. The offset amounts to less than 3 MeV in lighter systems and varies between zero and ~10 MeV in heavy ones. We also

calculated HF energy surfaces for three heavy systems looking for a relation between the adiabatic potential and the fusion hindrance at large $Z_T Z_P$. One can see a link between quasi-fission and the force opposing fusion, acting inside the Coulomb barrier. One surface illustrates the identity of the adiabatic fusion barrier with the fission saddle of a compound nucleus.

7. *"Nuclear fission with mean-field instantons",* J. Skalski, **Phys. Rev. C 77, 064610 (2008).** We presented a description of nuclear spontaneous fission, and generally of quantum tunneling, in terms of instantons - periodic imaginary-time solutions to time-dependent mean-field equations - that allows for a comparison with more familiar and used generator coordinate (GCM) and adiabatic time-dependent Hartree-Fock (ATDHF) methods. It is shown that the action functional whose value for the instanton is the quasiclassical estimate of the decay exponent fulfils the minimum principle when additional constraints are imposed on trial fission paths. In analogy with mechanics, these are conditions of energy conservation and the velocity-momentum relations. In the adiabatic limit the instanton method reduces to the time-odd ATDHF equation, with collective mass including the time-odd Thouless-Valatin term, while the GCM mass completely ignores velocity-momentum relations. This implies that GCM inertia generally overestimates instanton-related decay rate. The very existence of the minimum principle offers a hope for a variational search for instantons, and sharply contrasts with absence of a suitable functional for real-time mean-field dynamics. After the inclusion of pairing, the instanton equations and the variational principle can be expressed in terms of the imaginary-time-dependent Hartree-Fock- Bogolyubov (TDHFB) theory. The adiabatic limit of this theory reproduces ATDHFB inertia.
8. *"Relative Motion Correction to Fission Barriers",* J. Skalski**, Int. J. Mod. Phys. E 17, 151 (2008).** We discuss the effect of kinetic energy of the relative motion becoming spurious for separate fragments on the selfconsistent mean-field fission barriers. The treatment of the relative motion in the cluster model is contrasted with the necessity of a simpler and approximate approach in the mean-field theory. A scheme of the energy correction to the Hartree-Fock is proposed. The results obtained with the effective Skyrme interaction SLy6 show that the correction, previously estimated as ~8 MeV in A=70-100 nuclei, amounts to 4 MeV in the medium heavy nucleus ^{198}Hg and to null in ^{238}U. However, the corrected barrier implies a shorter fission half-life of the latter nucleus. The same effect is expected to lower barriers for multipartition (i.e. ternary fission, etc) and make hyperdeformed minima less stable.
9. "Broyden's method in nuclear structure *calculations*", A. Baran, A. Bulgac, M. McNeil Forbes, G. Hagen, W. Nazarewicz, N. Schunck, and M.V. Stoitsov, **Phys. Rev. C 78, 014318 (2008).** In a collaborative effort of several groups, Broyden's method, widely used in quantum chemistry for the numerical solution of nonlinear equations in many variables, was applied in the context of the nuclear many-body problem. Much faster convergence has been achieved in comparison with the linear-mixing procedure, which is often used in such types of calculations.
10. *"Deformed Coordinate-Space Hartree-Fock-Bogoliubov Approach to Weakly Bound Nuclei and Large Deformations,"* J. C. Pei, M. V. Stoitsov, G. I. Fann, W. Nazarewicz, N. Schunck, and F. R. Xu, **Phys. Rev. C 78, 064306 (2008).** The coordinate space formulation of the HFB method enables self-consistent treatment of mean-field and pairing in well deformed systems whose properties are affected by the particle continuum space. To describe such systems theoretically, we developed an accurate 2D lattice Skyrme-HFB solver HFBAX based on B-splines. Compared to previous implementations, we made a number of improvements aimed at boosting the solver's performance. These include: explicit imposition of axiality and space inversion, use of the modified Broyden's method to solve self-consistent equations, and a partial parallelization of the code. HFBAX has been benchmarked against other HFB solvers, both spherical and deformed, and the accuracy of the B-spline expansion was tested by employing the multiresolution wavelet method. Illustrative calculations are carried out for stable and weakly bound nuclei at spherical and very deformed shapes, including constrained fission pathways.
11. *"Adiabatic Mass Parameters for Spontaneous Fission",* A. Baran, J.A. Sheikh, and W. Nazarewicz,

Int. J. Mod. Phys. E 18, 1054 (2009). The collective mass tensor derived from the adiabatic time-dependent Hartree-Fock-Bogoliubov theory, perturbative cranking approximation, and the Gaussian overlap approximation to the generator coordinate method is discussed. Illustrative calculations are carried out for ^{252}Fm using the nuclear density functional theory with Skyrme interaction SkM* and seniority pairing.

12. *"Fission Quadrupole Mass Parameters in HF+BCS and HFB Methods",* A. Baran, J.A. Sheikh, A. Staszczak, and W. Nazarewicz, **Int. J. Mod. Phys. E 18, 1049 (2009).** The self-consistent Hartree-Fock+BCS and Hartree-Fock-Bogoliubov methods are compared at large nuclear deformations. The calculations are carried out for the fission pathway and quadrupole mass parameter of ^{252}Fm.
13. *"Solution of the Skyrme-Hartree-Fock-Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis. (VI) HFODD (v2.38j): a new version of the program",* J. Dobaczewski, W. Satuła, B.G. Carlsson, J. Engel, P. Olbratowski, P. Powalowski, M. Sadziak, J. Sarich, N. Schunck, A. Staszczak, M. Stoitsov, M. Zalewski, and H. Zduńczuk, **Comput. Phys. Commun. 180, 2361 (2009)**. This paper describes the new version (v2.38j) of the code HFODD, which solves the nuclear Skyrme-Hartree-Fock or Skyrme-Hartree-Fock-Bogolyubov problem by using the Cartesian deformed harmonic-oscillator basis. In the new version, we have implemented: (i) projection on good angular momentum (for the Hartree-Fock states), (ii) calculation of the GCM kernels, (iii) calculation of matrix elements of the Yukawa interaction, (iv) the BCS solutions for state-dependent pairing gaps, (v) the HFB solutions for broken simplex symmetry, (vi) calculation of Bohr deformation parameters, (vii) constraints on the Schiff moments and scalar multipole moments, (viii) the D2h transformations and rotations of wave functions, (ix) quasiparticle blocking for the HFB solutions in odd and odd-odd nuclei, (x) the Broyden method to accelerate the convergence, (xi) the Lipkin-Nogami method to treat pairing correlations, (xii) the exact Coulomb exchange term, (xiii) several utility options, and we have corrected two insignificant errors.
14. *"Fission barriers of compound superheavy nuclei",* J.C. Pei, W. Nazarewicz, J.A. Sheikh, and A.K. Kerman, **Phys. Rev. Lett. 102, 192501 (2009).** The dependence of fission barriers on the excitation energy of the compound nucleus impacts the survival probability of superheavy nuclei synthesized in heavy-ion fusion reactions. In this work, we investigated the isentropic fission barriers with nuclear DFT. For nuclei around ^{278}112 produced in "cold fusion" reactions, we predicted a more rapid decrease of fission barriers with excitation energy as compared to the nuclei around ^{292}114 synthesized in "hot fusion". The relationship between isothermal and isentropic descriptions has been demonstrated. The effect of the particle gas is found to be negligible in the range of temperatures studied.'
15. *"Systematic study of fission barriers of excited superheavy nuclei",* J.A. Sheikh, W. Nazarewicz, and J.C. Pei, **Phys. Rev. C 80, 011302(R) (2009).** In this paper, we performed systematic study of fission-barrier dependence on excitation energy using the self-consistent finite-temperature Hartree-Fock+BCS (FT-HF+BCS) formalism. The calculations have been carried out for even-even superheavy nuclei with Z ranging between 110 and 124. For an accurate description of fission pathways, the effects of triaxial and reflection-asymmetric degrees of freedom have been fully incorporated. Our survey demonstrates that the dependence of isentropic fission barriers on excitation energy changes rapidly with particle number, pointing to the importance of shell effects even at large excitation energies characteristic of compound nuclei. The fastest decrease of fission barriers with excitation energy is predicted for deformed nuclei around N=164 and spherical nuclei around N=184 that are strongly stabilized by ground-state shell effects. For nuclei ^{240}Pu and ^{256}Fm, which exhibit asymmetric spontaneous fission, our calculations predict a transition to symmetric fission at high excitation energies due to the thermal quenching of static reflection asymmetric deformations.
16. *"Microscopic description of complex nuclear decay: Multimodal fission",* A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz, **Phys. Rev. C 80, 014309 (2009).** In this paper, we described a study of spontaneous fission using the symmetry-unrestricted nuclear density functional theory. Our

results show that the observed bimodal fission can be explained in terms of pathways in multidimensional collective space corresponding to different geometries of fission products. We also predict a new phenomenon of trimodal spontaneous fission for some rutherfordium, seaborgium, and hassium isotopes.

17. "Toroidal super-heavy nuclei in Skyrme-Hartree-Fock approach", A. Staszczak and C. Y. Wong, **Acta Phys. Polonica B 40, 753 (2009).** Within the self-consistent constraint Skyrme–Hartree–Fock+BCS model, we found equilibrium toroidal nuclear density distributions in the region of superheavy elements. For nuclei with a sufficient oblate deformation, it becomes energetically favourable to change the genus of nuclear surface from 0 to 1, i.e., to switch the shape from a biconcave disc to a torus. The energy of the toroidal (genus = 1) SHF+BCS solution relative to the compact (genus = 0) ground state energy is strongly dependent both on the atomic number Z and the mass num- ber A. We discuss the region of Z and A where the toroidal SHF+BCS total energy begins to be a global minimum.
18. "Towards the universal nuclear energy density functional", M. Stoitsov, J. Moré, W. Nazarewicz, J. C. Pei, J. Sarich, N. Schunck, A. Staszczak, and S. Wild, SciDAC 2009, **J. Phys. Conf. Series 180, 012082 (2009)**. The UNEDF SciDAC project to develop and optimize the energy density functional for atomic nuclei using state-of-the art computational infrastructure is briefly described. The ultimate goal is to replace current phenomenological models of the nucleus with a well-founded microscopic theory with minimal uncertainties, capable of describing nuclear data and extrapolating to unknown regions
19. *"Thermal Fission Pathways in ^{232}Th*", J.D. McDonnell, W. Nazarewicz, J.A. Sheikh, Proc. 4th International Workshop on Fission and Fission Product Spectroscopy, **AIP Conference Proceedings 1175, 371, (2009).** Two-dimensional thermal potential energy surfaces have been investigated for ^{232}Th using the finite temperature HF+BCS approach with Skyrme energy density functional SkM*. At low excitation energy, the calculated static fission path goes through families of triaxial and reflection-asymmetric shapes. With increasing excitation energy, the shallow third minimum associated with a nonzero octupole moment becomes washed out, and the static fission valley moves towards the axial and reflection-symmetric limit.

B. Talks/Posters

1. "Theoretical Description of the Fission Process," W. Nazarewicz, 2006 Division of Nuclear Physics Annual Meeting, October 25-28, 2006; Nashville, Tennessee, BAPS **51**, 93 (2006).
2. "Theoretical Challenges in the Physics of Nuclei," W. Nazarewicz, invited talk at DNP Town Meeting on Nuclear Astrophysics/Study of Nuclei, Chicago, IL, January 19-21, 2007.
3. "Modern Approaches to Fission," W. Nazarewicz, invited talk at Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop, Bethesda, Maryland, August 10-12, 2006.
4. "Theoretical Description of the Fission Process," W. Nazarewicz, 2007 Stewardship Science Academic Alliance Symposium, Washington, DC, Feb. 6, 2007.
5. "Nuclear Structure '07: Exciting, Broad, Relevant," W. Nazarewicz, Fourth International Conference on Fission and Properties of Neutron-Rich Nuclei, Sanibel Island, Florida, Nov 11-17, 2007.
6. "LACM-NNSA Program," W. Nazarewicz, First International JUSTIPEN-LACM Meeting, Oak Ridge, Tennessee, March 5-8, 2007.
7. "Computing Atomic Nuclei", W. Nazarewicz, IOP Annual Nuclear Physics Group Conference, Liverpool, UK, April 1, 2008.
8. "Science of rare isotopes: connecting nuclei with the universe", W. Nazarewicz, plenary talk,

2008 APS April Meeting St. Louis, Missouri, April 12, 2008.

9. "Computing atomic nuclei", W. Nazarewicz, Zakopane Conference on Nuclear Physics, Zakopane, Poland, Sep. 1-4, 2008.
10. "Nuclear Structure in the Era of Terascale Computing", W. Nazarewicz, Colloquium, University of Jyväskylä, Jyväskylä, Finland, Oct. 2008
11. "Applications of the Density Functional", W. Nazarewicz, 5th ANL/MSU/JINA/INT FRIB Workshop on Bulk Nuclear Properties, MSU, East Lansing, USA, November 19-22, 2008.
12. "Fission Barriers of Compound Heavy Nuclei; Pairing Reentrance Phenomenon in Heated Rotating Nuclei", W. Nazarewicz, Nuclear Physics Seminar, GANIL, Caen, France, May 2009.
13. "Microscopic description of nuclear fission", W. Nazarewicz, The University of the West of Scotland, Paisley, UK, July 9, 2009.
14. "Nuclear Structure Theory 2009: Progress Report and Challenges", W. Nazarewicz, The Scottish Universities Physics Alliance Invited Lecture, Scotland (webinar), July 2009
15. "Nuclear Structure Theory", W. Nazarewicz, National Nuclear Physics Summer School, MSU, June 28-July 10, 2009.
16. "Frontiers of nuclear physics", keynote talk, W. Nazarewicz, The 10th International Conference on Nucleus-Nucleus collisions, Beijing, China, Aug. 16-21, 2009.
17. "Microscopic description of nuclear fission", W. Nazarewicz, Meeting on Scientific Grand Challenges in National Security: The Role of Computing at the Extreme Scale, Washington D.C., Oct. 6-8, 2009.
18. "Pairing Properties of Superheavy Nuclei," A. Staszczak, 13th Nuclear Physics Workshop, September 27th - October 1st, 2006, Kazimierz Dolny, Poland.
19. "Collective Inertia and Fission Barriers Within the Skyrme-Hartree-Fock Theory," A. Baran, 13th Nuclear Physics Workshop, September 27th - October 1st, 2006, Kazimierz Dolny, Poland
20. "Bimodal Fission in the Skyrme-Hartree-Fock Approach," A. Staszczak, Zakopane Conference on Nuclear Physics, September 4-10, 2006, Zakopane, Poland.
21. "Coordinate-Space HFB Calculations of Weakly Bound and Very Deformed Systems", J. Pei, 5-th ANL/MSU/JINA/INT FRIB Workshop on Bulk Nuclear Properties Michigan State University, November 19-22, 2008.
22. "Fission Barriers of Compound Superheavy Nuclei", J. Pei, 10th international conference on nucleus-nucleus collisions, Beijing, China, August, 17-21, 2009.
23. "Bimodal Fission in the Skyrme-Hartree-Fock Approach," A. Staszczak, First International JUSTIPEN-LACM Meeting, Oak Ridge, Tennessee, March 5-8, 2007.
24. "Toroidal SHE in Skyrme-Hartree-Fock approach", A. Staszczak, Zakopane Conference on Nuclear Physics, Zakopane, Poland, Sept. 1-7, 2008.
25. "Multimodal fission", A. Staszczak, 15th Nuclear Physics Workshop "*Marie & Pierre Curie*", Kazimierz Dolny, Poland, Sept. 24-28, 2008.
26. "Below-barrier paths: multi-modal fission and doughnut nuclei", A. Staszczak, FIDIPRO-UNEDF collaboration meeting on nuclear energy-density-functional methods, Jyväskylä, Finland, Oct. 9-11, 2008.
27. "Multi-modal fission of heavy and super-heavy nuclei", A. Staszczak, The 3rd LACM-EFES-JUSTIPEN Workshop, Oak Ridge, TN, Feb. 23-25, 2009.
28. "Spontaneous fission half-lives of fermium isotopes in the Skyrme-HFB theory", A. Staszczak, 16th Nuclear Physics Workshop "*Marie & Pierre Curie*", Kazimierz Dolny, Poland, Sept. 23-27, 2009.
29. "Collective Inertia and Fission Barriers Within the Skyrme-Hartree-Fock Theory," A. Baran, First International JUSTIPEN-LACM Meeting, Oak Ridge, Tennessee, March 5-8, 2007.
30. "Adiabatic mass parameters for spontaneus fission", A. Baran, 15th Nuclear Physics

Workshop “Marie & Pierre Curie”, Kazimierz Dolny, PL, Sep. 24-28, 2008.

31. “Dynamics of Spontaneous Fission”, J.A. Sheikh, 5th ANL/MSU/JINA/INT FRIB Workshop on Bulk Nuclear Properties, Michigan State University, November 19-22, 2008.
32. “Microscopic study of Collective Inertia and Fission Paths”, J.A. Sheikh, LANL-LLNL Fission Workshop, LANL, Feb. 3-4, 2009.
33. “Symmetry Projection in Density Functional Theory”, J.A. Sheikh, Workshop on Effective Field Theories and the Many-Body Problem at INT Seattle, June 2009.
34. “ATDHFB Collective Inertia and Fission Paths at Finite temperature”, J.A. Sheikh, the 3rd LACM-EFES-JUSTIPEN Workshop, Oak Ridge National Laboratory, February 23-25, 2009.
35. “Visualization and Analysis of Nuclear Quasi-Particle States”, poster, J.D. McDonnell, CNS-EFES08 Summer School, Tokyo, Japan, Aug. 28, 2008.
36. “Nuclear Fission at Finite Temperature”, poster, J.D. McDonnell, 4th International Conference on Fission and Fission Product Spectroscopy, Cadarache, France, May 13-16, 2009.
37. “Report on the 4th International Workshop on Nuclear Fission and Fission Product Spectroscopy”, J.D. McDonnell, Nuclear Physics Seminar, University of Tennessee, Knoxville, TN, Oct. 19, 2009.

C. Code developments

As stated in our original proposal, “*Developing codes and technology that can be freely used by NNSA is also one of our goals*.” We developed an accurate 2D lattice Skyrme-HFB solver HFBAX based on B-splines. We used this code to study fission barriers. In addition to providing new physics insights, HFBAX can serve as a useful tool to assess the reliability and applicability of coordinate-space and configuration-space HFB solvers, both existing and in development. Another code developed by our group is HFODD (v2.38j), which solves the Skyrme-Hartree-Fock-Bogoliubov equations in the Cartesian-deformed harmonic-oscillator basis. This code is currently used in all our advanced fission calculations that require breaking of most self-consistent symmetries. Based on HFODD, we developed codes to calculate collective inertia (tensor of mass parameters).

D. Annual workshop. As stated in our original proposal, “*We will hold workshops at the Joint Institute for Heavy Ion Research devoted to the fission problems that we will pursue under this proposal. We will solicit input from NNSA laboratory researchers on what is relevant to calculate*.” In 2007, 2008, and 2009, we held Joint JUSTIPEN-LACM Meetings at the Joint Institute for Heavy Ion Research in Oak Ridge. The meeting in 2007 was a merger of two workshops: (i) the US-Japan theory meeting under the auspices of the Japan-US Theory Institute for Physics with Exotic Nuclei (JUSTIPEN), and (ii) the annual NNSA-JIHIR meeting on the nuclear large-amplitude collective motion (LACM) with an emphasis on fission. The workshops were very well attended (60 participants in 2007, over 70 participants in 2008, and 90 participants in 2009) and involved participants from NNSA/DP Laboratories (LANL, LLNL, NNSA), as well as students and post-docs. The workshops were partly sponsored by this grant, and reference to NNSA support was displayed during the meeting. The program of the last workshop can be found at http://www.phy.ornl.gov/theory/papenbro/feb09.htm.