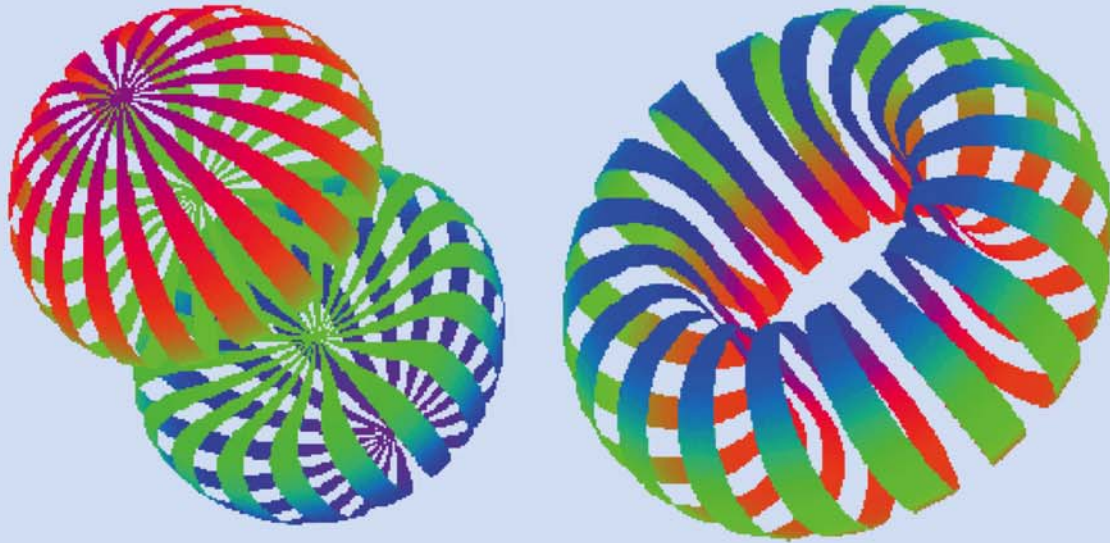# Report of the
Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop

Bethesda, Maryland

Co-sponsored by

Offce of Nuclear Physics
Office of Advanced Scientific Computing Research
U.S. Department of Energy Office of Science

Co-chairs

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Ewing Lusk

August 10-12, 2006

Office of Science
U.S. Department of Energy

Office of Nuclear Physics
Exploring Nuclear Matter - Quarks to Stars

ASCR

The colorful figures on the front cover represent two different shapes of the deuteron—the simplest nucleus containing a proton and a neutron—at a specific density. The left side shows the polarization state ±1, the right side state 0. These representations, resulting from modern nuclear theory, are a reminder that nuclear theory calculations, enabled by modern computing platforms, will be essential tools in any program related to advanced fuel cycles and nuclear power generation.

Contents

Executive Summary

The *Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop* was held in Bethesda, Maryland, on August 10–12, 2006, bringing together over 130 participants from universities, national laboratories, the private sector, and U.S. government agencies to explore basic research opportunities in nuclear physics and advanced computational science R&D as applied to the Department of Energy's activities in advanced fuel cycles. The workshop was sponsored by the Offices of Nuclear Physics and Advanced Scientific Computing Research, of the Department of Energy (DOE), Office of Science. The President's FY 2007 Budget Request identified programs within the Office of Science that are poised to participate in basic research activities that couple to applied programs with broad national interest, such as nuclear energy. A principal aim of this workshop was to bring together the applied and basic research communities with nuclear expertise to identify research opportunities that would be beneficial to DOE's Nuclear Energy program on advanced fuel cycles (AFCs). The primary objectives for the workshop were the following.

- Determine nuclear physics R&D needs of the AFC
- Determine how these needs can be met by existing programs
- Determine what facilities are appropriate for this research
- Identify computing resource needs for modeling and simulation

In order to accomplish these objectives, four working groups were established.

- Group A—Nuclear Data Needs in Support of AFC R&D
- Group B—Nuclear Measurements
- Group C—Nuclear Data
- Group D—Nuclear Theory and Computations

The reports of the four working groups, including identified research opportunities, are in the main body of this report. In addition, all presentations given at the workshop, both in plenary sessions and in parallel meetings of the four working groups, can be found on the workshop website, http://www-fp.mcs.anl.gov/nprcsafc/, along with early documents posted on the website to introduce workshop participants to ongoing activities in the AFC program.

Highlights of the Workshop

This was the first joint meeting between basic and applied researchers to discuss the AFC and possible contributions by the basic nuclear science community, as well as to explore potential contributions in the area of high-performance computing. This meeting was a necessary and important step in building a community of applied and basic researchers focused on important national issues related to the AFC, while providing new opportunities for basic nuclear physics research. Highlights from the four working groups are presented below.

Group A (Nuclear Data Needs): Advanced sensitivity analyses have helped to identify nuclear data needs due to both the characteristics of AFC reactors (high transuranic content and high fissile-to-fertile ratio in the cores) and the requirement to consider the reactor as well as the complete fuel cycle. A number of opportunities for basic nuclear physics R&D important to the AFC were identified, including the following:

- Cross-section covariance data (the highest priority)
- Cross-section evaluations
- Cross-section and covariance-processing tools
- Actinide nuclear data (major and minor)
- Structural material data (inelastic cross sections for standard reactor materials, for example, Fe, Na, Pb, and Si)
- Material detection and assay (R&D related to mockup of separation processes and determine data needs)
- Sensitivity analysis tools
- Criticality safety (sensitivity analysis to establish need for benchmark or cross-section measurements)

The nuclear physics R&D needs for the AFC defined by Group A provided the basis for the other working groups to identify appropriate research activities in their areas of expertise. Highlights from these groups follow.

Group B (Nuclear Measurements): Several experimental and theoretical opportunities (e.g., improved understanding of the complete fission process, level densities, radiative strength functions) were identified that will enable challenging and exciting basic research as well as meeting the needs of the AFC program. High-quality measurements, with both neutron and charged particle beams, will be driven by the new, stringent AFC data requirements. The following are examples of direct neutron measurements:

- Total cross sections (over full neutron energy range, meV's$\rightarrow$MeV's) to support detailed cross-section evaluations and improve the accuracy of such evaluations. Data are needed for a wide range of stable and radioactive nuclides.

- Elastic and inelastic cross sections for a range of intermediate mass nuclides. While some measurements exist, they are 30–40 years old and need to be updated with improved accuracy for the evaluated data files.

- Accurate fission cross-section measurements, particularly in the so-called resonance region for uranium and heavier actinides. Measurements down to 4–5%, and for some nuclides 1–2%, will be needed, calling for new and challenging experimental techniques.

- Capture cross-section measurements, particularly in the resonance region, at accuracies of 3–5%, and perhaps lower for some nuclides. These data are needed to study level densities and radiative strength functions in order to improve reaction models (with applications to both basic and applied nuclear physics).

Many reactions of importance to both basic nuclear physics and the AFC are not amenable to direct experimental measurement. The surrogate technique, developed as a way of determining cross sections of compound nuclear reactions, has the potential of being an important tool for tackling the problem of extracting experimentally inaccessible neutron-induced compound reactions of interest to the AFC, as well as addressing important questions in low-energy reaction and nuclear astrophysics.

The United States currently has a diverse and complementary collection of aging accelerator facilities, techniques, and associated personnel to address AFC issues. However, there exists a strategic need for investment in facilities, experimental equipment, and workforce. Otherwise, the basic scientific infrastructure will not be available to meet potential long-term AFC goals. These

issues, crossing governmental agencies and traditional research communities, should be the subjects of a future in-depth study or workshop to provide a comprehensive plan and set of tools for the AFC.

Group C (Nuclear Data): As stated above, there exists a high-priority need to produce nuclear data with covariances, in order to support reactor and fuel cycle design and to identify priorities for cross-section measurements and improved modeling of nuclear reactions. The following steps are called for:

- An aggressive program to provide covariance data for all evaluated nuclear data files (ENDF). At present, only 10–15 percent of the files have covariance data. Several-year efforts are envisioned.

- Further precision neutron cross-sections (fission, capture, and scattering). Precision data and their evaluation, for both major and minor actinides, are important for precise simulations of nuclear criticality, transmutation rates, and radiation damage and heating—all vital for the AFC.

- Consolidation of data for decay data, delayed neutrons, fission yields, and photon production.

- Extensive international collaborations for covariance work—particularly with Europe and Japan. A Global Nuclear Data Initiative is being considered that will couple modeling tools, codes, input libraries, and databases to an integrated system for evaluated data.

- Processing covariance data so they can be used by application codes for reactor design and development.

The close coupling of nuclear data measurements and evaluated nuclear data with covariances is essential for the future success of the AFC program.

Group D (Nuclear Theory and Computations): A more fundamental and accurate description of nuclear reactions would be beneficial to several DOE missions, including: basic nuclear physics in the Office of Science, the AFC in Nuclear Energy, and Science-based Stockpile Stewardship in the National Nuclear Security Administration. For the AFC program, a wall-to-wall simulation of the reactor core, with potential impact on safety and economy, will require advanced nuclear theory calculations of relevant cross sections where experimental evaluated data do not exist. While some tools exist, these cross-section calculations will require the development of both theoretical and computational methods to approach the required AFC accuracy. In turn, cross sections feed into the data evaluations that are input to the simulations of reactor cores. Currently, no single institution in the United States or elsewhere has either the expertise or the personnel to address the theoretical needs of such a nuclear reactions effort, requiring the coordination of nuclear physics and computational sciences. The following are required for development of the next generation of reaction theory needed for the AFC:

- Development of a new generation of theoretical tools and several new computational codes for modern computational platforms.

- Establishment of graduate and postdoctoral fellowships to train the next generation of computational nuclear scientists.

- Enhanced support in the nuclear theory base for nuclear structure and reaction theory development.

- Coordinated effort or framework approach to bring together all reaction-code components under one computational umbrella—providing a strategy for common input/output data files, common language interfaces, and common algorithms.

The material in the workshop report encompasses a large body of scientific opportunities in nuclear physics and related computational activity with application to DOE's advanced fuel cycle efforts. Hence, it can be used as a resource by the appropriate offices of DOE and the research community as they map out future research in this area. This workshop was, however, only a start in bringing the basic and applied nuclear science communities together to address a common problem. Further workshops and perhaps even topical meetings will be needed to help chart the way forward as this cross-cutting program develops.

Introduction

Nuclear energy has been a key component of the mix of electrical power generation in the United States for over fifty years. Future energy needs project an increasing role for nuclear power well into this century. A basic understanding of nuclear physics was, and continues to be, essential for the development of this energy source. The connections between basic and applied research, focused on nuclear power generation, was the theme of the *Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop,* the report of which is presented in this document.

In 2005 the Department of Energy (DOE) Office of Science undertook a study of how its basic research activities could benefit the applied programs in DOE's Office of Nuclear Energy (NE). In September 2005, this culminated in a workshop entitled *The Path to Sustainable Nuclear Energy, Basic and Applied Research Opportunities for Advanced Fuel Cycles*, with participation from university, national laboratory, and industrial researchers, as well as the DOE [1]. One of the goals of the workshop was to "identify new basic science that will be the foundation for advances in nuclear fuel-cycles technology in the near term (i.e., the next 20 years). Scientific areas within the Office of Science that were found to affect advanced fuel cycles (AFCs) included materials, separations, modeling and simulation, and proliferation resistance of the overall nuclear cycle [1]. Within these four principal areas, modeling and simulation was found to provide scientific opportunities in two areas for nuclear physics and its computational connections— *nuclear data* and *multiscale modeling with uncertainties*. These became the focus of the present workshop.

An important event in the evolution of the present workshop process was the submission of the President's FY 2007 Budget Request in February 2006. In that document, the following statement can be found regarding DOE's Nuclear Physics program: "Funding is provided within the Low Energy subprogram to support research efforts that are also relevant to the design of next generation nuclear reactors. This research can help to provide the nuclear data and knowledge required for advanced nuclear fuel cycles. Additional funding is provided for this effort in the Theory subprogram for Nuclear Data activities."

As a follow-up to the workshop of September 2005, and with the stimulus provided by the President's FY 2007 Budget Request, three workshops were convened to explore the connections between basic and applied research related to nuclear energy. The first, sponsored by DOE's Office of Basic Energy Sciences, was held July 30–August 2, 2006, and was titled Workshop on Basic Research Needs for Advanced Nuclear Energy Systems. The second workshop, sponsored by the Offices of Nuclear Physics and Advanced Scientific Computing Research, was held August 10–11, 2006, and was titled Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop. The third workshop, sponsored by the Offices of Nuclear Energy and Advanced Scientific Computing Research, was held on August 15–17, 2006, and was titled Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems. Separate reports have been written for each of the workshops.

The report presented here summarizes the discussions of the second workshop. The principal goals of this workshop were fourfold.

- Determine nuclear physics R&D needs of the AFC
- Determine how these needs can be met by existing programs
- Determine what facilities are appropriate for this research
- Identify computing resource needs for modeling and simulation

In order to meet these goals, four working groups were established:

- Group A—Nuclear Data Needs in Support of AFC R&D
- Group B—Nuclear Measurements
- Group C—Nuclear Data
- Group D—Nuclear Theory and Computations.

The central theme of the workshop was associated with DOE's program in advanced fuel cycles. Figure 1 provides an overview [2] of the elements of the fuel cycle: mining of fissile material→enrichment and fabrication of reactor fuel→burning of the fuel in a reactor (e.g., today's fleet of light water reactors)→separation of the spent nuclear fuel (SNF)→storage of waste in appropriate repositories. Once fuel is burned, intermediate processes are envisioned that can greatly reduce high-level radioactive waste, thereby lowering the levels of radiotoxicity and associated heat loads for a geological repository and possibly eliminating the need for additional repositories.
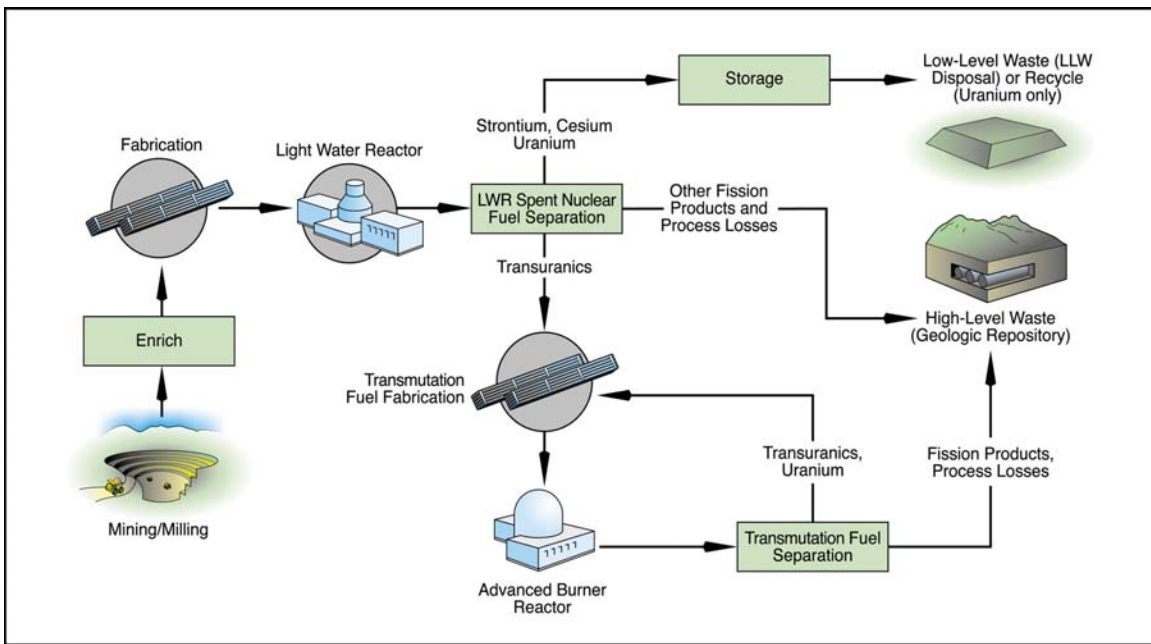
Fig.1. Overview of possible nuclear fuel cycle [2]

With transmutation the used fuel reaches the toxicity level of the natural fuel within a few centuries. Figure 2 shows such an example [3].
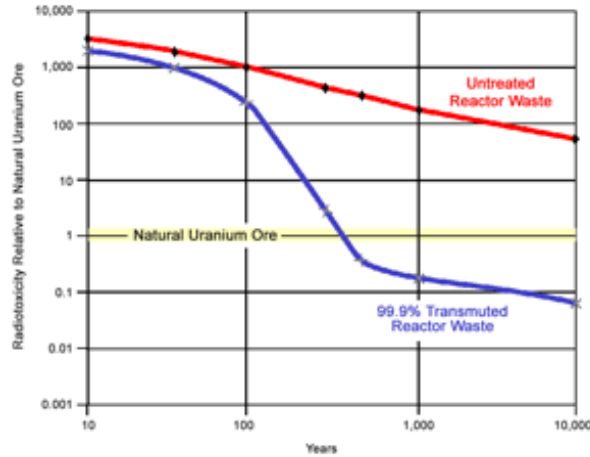
Fig. 2. Untreated vs transmuted nuclear waste

Clearly, knowledge of the basic underlying nuclear physics processes will be important for effective utilization of nuclear power and reduction of its waste. In addition, it is expected that advanced computational tools can be used to improve our understanding of the many physical processes encountered in the fuel cycle—further helping to reduce the time and costs in this program.

Attending the meeting were 133 participants from U.S. universities, national laboratories, and the private sector, DOE and other federal agencies, and foreign countries. Representation from these groups was as shown in Figure 3.
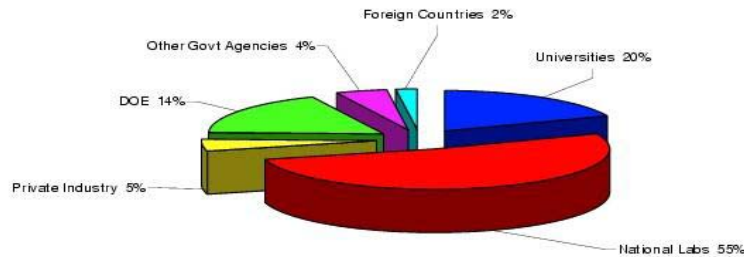
Data collected from 133 participants

Fig. 3. Representation of participants at workshop

The first day of the workshop, August 10, 2006, was spent in plenary session. The presentations were tailored to provide participants with updated information on the AFC program, identify the needs for and status of nuclear data, and indicate possible advanced scientific tools—experimental, theoretical, and computational—that could be brought to bear on nuclear fuel cycle problems. Ample time was allowed for discussions after each talk. The second day of the workshop, August 11, 2006, was devoted to parallel meetings of the four working groups. Each group was charged with developing a set of scientific opportunities that could form the basis for

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basic R&D activities related to the fuel cycle. A majority of the time was spent hearing presentations specific to each group's topical area, followed by development of the scientific opportunities. At the end of that afternoon the working groups presented their results in a plenary session. This completed the formal workshop.

On August 12, 2006, the organizers met in the morning with the leaders of the four working groups to discuss the workshop results and establish a time line for each group to write its contribution to the overall report. In addition, time was spent with representatives of DOE discussing the highlights of the meeting. The expectation is that this report will form the basis of a resource document that both DOE and the research community can use to map out R&D efforts between basic and applied research in the area of nuclear fuel cycles.

R&D Highlights from the Workshop

Before presenting the individual write-ups of each working group, a synopsis of the R&D highlights from these reports is appropriate. These findings, related to future basic nuclear physics R&D for the AFC, flow from the presentations and discussions in the plenary and parallel sessions, particularly those related to the 'needs of the AFC identified by Group A.

Group A (Nuclear Data Needs in Support of AFC R&D): Advanced sensitivity analysis, performed for reactor systems (including fast spectrum reactors of interest to the GNEP) over a wide range of integral parameters, shows that the impact of assumed uncertainties in nuclear cross-section data is, in some cases, significant. This clearly identifies nuclear data, both measured and evaluated, as a high-priority activity for the AFC. Specific scientific opportunities for basic nuclear physics R&D, important to the AFC, were identified, along with appropriate timelines. These opportunities include the following:

- Cross-section covariance data (identified as the highest priority). Over the near term (2007–2012), full covariance data should be implemented for a broad range of nuclides within ENDF/B-VII. New covariance data should be completed over thermal, resonance, and high neutron energy ranges for ^{253}U, ^{238}U, and ^{239}Pu. Over the longer term (2012–2020) covariance files should be updated and expanded as new data and models become available. A potential need for supercomputing exists for some of these activities.

- Cross-section evaluations for actinide fission and capture, prompt neutrons per fission, delayed neutrons, and photon production as new data become available over the near term (2007–2012).

- Various measurements over the near term (2007–2012) spanning fission, capture, delayed neutron fractions, and other decay data for both major and minor actinides at accuracies of 2–4%. Over the longer term (2012–2020), minor actinide data should be improved as determined from sensitivity analyses. Isotopically pure targets may be needed to achieve required data accuracy.

- Inelastic cross-section data for structural and coolant materials. The main data needs are for Fe, Na, Pb, and Si cross sections.

- Development of sensitivity analysis tools, for both Monte Carlo and deterministic methods. A group of experts, over the near term, should be established with the goal of providing a consistent method of analysis and validation of nuclear data. Over the longer

term, the potential of relating reactor physics experiments to nuclear model parameters should be explored. This effort will require collaborations between the basic nuclear physics, computational science, and reactor engineering communities.

- Various data for material detection and assay (accountability issues) and criticality safety. Data needs will be determined as processes or appropriate benchmarks are established (both activities span the near and long term).

Higher-precision data and associated techniques can be expected to provide new opportunities for basic research with a strong coupling to computational science. For example, the new requirement that the complete fuel cycle be taken into account for uncertainty assessment requires the propagation of uncertainties throughout complex systems (e.g., reactors, temporary storage, and repository). Early studies point to formidable computing challenges, requiring the development of appropriate sensitivity and uncertainty propagation techniques. These in turn, point to major opportunities for development of novel high-performance computational techniques. The requirements brought on by the need of very high accuracy for data, as well as new ways of handling the production of such nuclear data, suggest an approach using high-accuracy integral experiments that utilize nuclear model parameters, rather than matrices of nuclear cross sections. Such an approach presents both a scientific and a computational challenge to basic science and high-performance computing.

The nuclear physics R&D needs for the AFC, provided by Group A, were used by the other working groups to identify appropriate basic science R&D activities within their area of expertise. The highlights from these groups are presented below.

Group B (Nuclear Measurements): This working group concentrated on identifying basic research opportunities related to measurements, facilities, and associated instrumentation needed to provide the nuclear data needs of the AFC. The group identified experimental and theoretical opportunities that would form the basis for challenging and exciting basic research activities, while meeting the needs of the AFC program. High-quality measurements, with both neutron and charged particle beams, will be needed to meet the new, stringent AFC data requirements. The following represent examples of measurements requiring direct neutron beams:

- Total cross-section measurements, over the full neutron energy range (meV's→MeV's), to support detailed cross-section evaluations and improve their accuracy (e.g., reliable neutron widths are needed for calculating important experimental effects such as self-shielding and multiple scattering). Data are needed for a range of stable and radioactive nuclides. On the theoretical side total cross sections are important for understanding the nuclear optical model, which is needed for better evaluated data. In order to meet AFC data needs, some cross sections need to be known to a 1% absolute accuracy. Currently, four U.S. facilities (ORELA, LANSCE, Kentucky, and Rensselaer) have the capability of making such measurements, but investments will be needed to provide this capability over the full neutron energy range.

- Elastic and inelastic neutron cross-section measurements are needed for a range of intermediate mass nuclides, particularly for AFC processing operations. While some data exist, they are 30–40 years old and must be updated with improved accuracy for the evaluated data files. The ability to make doubly differential elastic scattering measurements in the United States is currently limited (ORELA, Rensselaer, and Ohio University), and investment in facility infrastructure would be required to extend elastic scattering measurements over the full neutron energy range.

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- Accurate fission cross section measurements, particularly in the resonance region for uranium and heavier actinides, will be needed for AFC development. Measurements down to 4–5%, and for some nuclides 1–2%, will be needed, thus calling for new and challenging experimental techniques. At present, no single experiment or facility can cover the full energy range, with the required resolution, for the fission process. New techniques must be developed to reduce fission cross section measurement uncertainties. The three major sources of error are particle ID, target thickness, and the use of ^{235}U as a reference point. Early studies suggest that a gas-filled time projection chamber could reduce these sources of error. Developing such a detector, with application to AFC problems, would constitute a strong instrumentation challenge, with potentially high scientific returns.

- Measurement of neutron capture cross-sections is important, particularly in the resonance region, at accuracies of 3–5%, and perhaps lower for some nuclides. These data are needed to study level densities and strength functions, in order to improve reaction models, with applications to both basic (nuclear astrophysics) and applied (AFC) nuclear physics. At present, the 4π BaF$_2$ detector (DANCE) at LANSCE is deployed for such measurements. An equivalent portable 4π array would further extend the capability of such measurements, particularly for the resonance region.

Many reactions, important to basic nuclear physics and the AFC, cannot be directly measured. The surrogate technique, developed to determine cross sections of compound nuclear reactions, may be useful for extracting experimentally inaccessible neutron-induced compounds of interest to the AFC, while addressing scientific questions associated with low-energy reaction and nuclear astrophysics. A recent variation, the surrogate ratio technique, has been applied to (n, fission) reactions on actinide nuclei and yields cross sections with uncertainties of at 5% over the energy interval 7–25 MeV.

Group C (Nuclear Data): As stated in Group A's list of needs, there exists a high-priority need to produce nuclear data with covariances. Such data is needed to support reactor and fuel cycle design, identify priorities for cross section measurements for the AFC program, improve modeling of nuclear reactions, and support criticality and national security applications. In the area of nuclear data the following steps are called for:

- An aggressive program to provide covariance data for all evaluated nuclear data files (ENDF). At present, only 10–15% of the files have covariance data. A several-year effort is envisioned to accomplish this task. Three key steps are seen for this program: adopt a flexible approach, establish a strong dialog with users, and produce usable results in each phase.

- Further precision neutron cross-sections (fission, capture, and scattering). Precision data and their evaluation, for both major and minor actinides, are needed for high-accuracy simulations of nuclear criticality, transmutation rates, and radiation damage and heating—all vital for the AFC.

- Consolidation of data for nuclear decay, delayed neutrons, fission yields, and photon production.

- Extensive international collaborations on covariance work—particularly with Europe and Japan. A Global Nuclear Data Initiative (GNDI) is being considered that will couple modeling tools, codes, input libraries, and databases to an integrated system for evaluated data.

- Processing convariance data so they can be used by application codes for reactor design and development.

The close coupling of nuclear data measurements and evaluated nuclear data with covariances is seen as being essential for the future success of the AFC program.

Group D (Nuclear Theory and Computations): Neutron-nucleus cross sections, particularly for the heavy transuranics, rare actinides, and certain light elements, play an important role in determining reactor design and safety parameters. Indeed, a more fundamental and accurate description of nuclear reactions would be beneficial to several DOE missions, including: basic nuclear physics in the Office of Science, the AFC program in Nuclear Energy, and Science-based Stockpile Stewardship in NNSA. For basic nuclear physics a deeper and more reliable description of nuclear reactions can provide a powerful tool for understanding the processes that power stars. For the AFC program, a wall-to-wall simulation of the reactor core, with potential impact on safety and economy, will require advanced nuclear theory calculations of relevant cross sections where experimental evaluated data are nonexistent. While some tools exist, these cross-section calculations will require the development of theoretical and computational methods to approach the accuracy required for the AFC. These cross sections, which feed into data evaluations, are themselves input to the simulations of reactor cores. Currently, no single institution in the United States or elsewhere has the expertise or personnel to adequately address the theoretical needs of such a nuclear reactions modeling effort, requiring the coordination of nuclear physicists and computational scientists. The development of the next generation of reaction theory needed for the AFC requires the following actions:

- Development of a new generation of theoretical tools and new computational codes for modern computational platforms. In particular, for the neutron-induced reactions of interest to the AFC, improved theoretical descriptions are needed for the nuclear optical potential, statistical decay of the compound nuclear systems, pre-equilibrium reactions, fission, and direct nonstatistical reactions.

- Establishment of graduate and postdoctoral fellowships to train the next generation of computational nuclear scientists.

- Enhanced support of nuclear theory base for nuclear structure and reaction theory.

- Coordinated effort or framework approach to bring together all reaction-code components under a single computational umbrella—providing a strategy for common input/output data files, common language interfaces, and algorithms.

Facilities, Instrumentation, and the Research Community

In order to carry out a program of measurements for the AFC, neutron and charged particle facilities, as well as appropriate nuclear instrumentation and computing resources, will be required in the coming years. In addition, a knowledgeable and trained research community must be available to perform the complex measurements that will be needed for this effort.

A number of U.S. university and national laboratory accelerator facilities, represented at this workshop, can be expected to participate in an AFC-related program. They are the following:

- Argonne National Laboratory (ATLAS and IPNS)
- Lawrence Berkeley National Laboratory (88-Inch cyclotron)
- Los Alamos National Laboratory (LANSCE)
- Oak Ridge National Laboratory (HRIBF, ORELA, SNS)
- Ohio University (Edwards Accelerator Laboratory)
- Rensselaer Polytechnic Institute (Gaerttner Linear Accelerator Laboratory)
- Triangle Universities Nuclear Laboratory (TUNL)
- University of Kentucky.

Other accelerator facilities in the United States may also be potential participants. Principal support for these facilities comes from various offices of DOE's Office of Science, Office of Nuclear Energy, and NNSA, as well as other, non-DOE institutions. Many of these facilities support basic and applied programs and deliver beams to a wide variety of users. In addition, several are run as national user facilities and have substantial advanced nuclear instrumentation that could be brought to bear on issues related to the AFC. Presentations at the workshop stressed, however, that several of the accelerator facilities needed further investment, in their accelerator complex and advanced nuclear instrumentation, to enable them to meet the demands of a full-scale, creditable AFC measurement program. At the same time, there can be no research effort without an adequate research community. Time and again at the meeting concern was raised regarding a "lost generation of nuclear researchers." Some way must be found to attract students back to the nuclear physics programs at our universities and national laboratories. One key to this situation is a future with a job. The expected demand for nuclear expertise, in a 21st century hungry for additional energy resources, can be filled only by a cadre educated and trained at our national laboratories and universities.

In summary, the United States currently has a diverse and complementary set of aging accelerator facilities, techniques and associated personnel to start to address AFC issues. However, there exists a strategic need for investment in facilities, experimental equipment, and workforce. Otherwise, the basic scientific infrastructure will not be available to meet potential long-term AFC goals. These issues, crossing government agencies and traditional research communities, should be subjects of a future in-depth study or workshop to provide a comprehensive plan and future set of tools for the AFC.

Plan of This Document

The remainder of this document is devoted to the reports of each of the working groups and represents the discussions and conclusions that resulted from their working sessions on the second day of the workshop. The writeups provide background information specific to the working group and a vision of basic research R&D activities focused on the nuclear fuel cycle. Seven appendixes are attached to this report:

- Acronym List
- Appendix 1—charge to the workshop
- Appendix 2—agenda for the plenary sessions of the workshop
- Appendix 3—agendas of the parallel working groups
- Appendix 4—list of workshop cochairs and working group leaders
- Appendix 5—participant list
- Appendix 6—cross-cutting educational proposal

The workshop website http://www-fp.mcs.anl.gov/nprcsafc/ contains all plenary and parallel (working group) presentations. The website also includes informational documents related to nuclear data and the AFC, which were posted there before the meeting.

We emphasize that this workshop was the initial step in bringing the basic and applied research communities together around the central theme of advanced nuclear fuel cycles. By necessity this workshop was restricted in time and with a large phase space of material to cover. As already noted, further workshops and even topical meetings will need to be held as this program develops and helps contribute to a brighter future for the nation's energy supply.

1. Group A: Nuclear Data Needs in Support of Advanced Fuel Cycle Research and Development

Working Group A focused on nuclear data needs in support of the DOE Advanced Nuclear Fuel Cycle. This information was developed primarily from initial sensitivity analyses performed as part of the Advanced Nuclear Fuel Cycle Initiative (AFCI) in collaboration with the Organisation for Economic Co-operation and Development-Nuclear Energy Agency (OECD-NEA). These analyses have been performed for reactor systems including fast spectrum systems of interest to the Global Nuclear Energy Partnership (GNEP) [4, 5]. The results obtained on a wide range of integral parameters show that the impact of assumed cross-section data uncertainties is, in some cases, significant. Parameters included in the analysis were K_{eff}, Doppler reactivity, coolant void reactivity, burnup, transmutation rate, peak power, spent fuel decay heat, radiation source level, and radiotoxicity. In addition, the data needs for criticality safety and material accounting (safeguards) were discussed during the course of the workshop. A summary list of the nuclear data needs, in order of priority, is given in Table 1. This list, divided into near term and long term, should be revisited and updated on an annual basis.

Table 1. Summary of Nuclear Data Needs

Activity	Near Term (2007–2012)	Long Term (2012–2020)	Comments
Cross-Section Covariance Data	• Implement full covariance data file for a broad set of isotopes within ENDF/B-VII. Need an early first (rough) set of data that is generated with a consistent systematic approach. • Complete new covariance data over thermal, resonance, and high neutron energy ranges for ^{235}U, ^{238}U, ^{239}Pu. • Complete covariance for all isotopes of high-priority isotopes as established in the ad hoc OECD-NEA working group.	• Complete, update. and improve covariance files as new data and models become available.	• Need to increase the number of experts qualified to perform this activity. • Potential need for supercomputing. • The availability of covariance data can be used both for design optimization and for validation experiment planning. • Need to re-evaluate need for better ^{235}U resonance data with ENDF/B-VII (JAEA).
Cross-Section Evaluations	As new data become available, perform evaluations of actinide fission and capture, prompt neutrons per fission, delayed neutrons, and photon production data.	• Further needs as outcome of system design development.	• Interface between core and reflector in fast reactor is sensitive to the photon transport. • Supercomputer time may be needed to evaluate resonance data.

Cross-Section and Covariance Processing Tools	• Test and validate the methodology. Extend if necessary.	• Update as needed.	
Actinide Nuclear Data	• Fission of ^{239}Pu at 2% accuracy or better • ^{240}Pu capture at the first resonance • Fission of ^{241}Pu at 4% accuracy or better • Fission of ^{241}Am at 4% accuracy or better • Fission of ^{242m}Am at 4% accuracy (below 1 MeV), 10% accuracy (above 1 MeV) • ^{243}Am capture in the "fast" and "thermal" range • ^{238}U capture between 2 and 200 keV and between 10 eV and 400 eV • ^{238}U inelastic • Delayed neutron fractions, decay constants and spectra • Decay data and fission yields for (minor) actinides improvements	• Provide improvements in minor actinide data as determined from sensitivity analyses. • Inelastic scattering in structural materials and higher actinides.	• Isotopically pure targets may be needed to achieve required data accuracy (i.e., ^{240}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{237}Np).
Structural Material data	As for structural/coolant materials, the most significant data needs are • Fe inelastic • Na elastic • Pb inelastic • Si inelastic cross sections.	• Potential further needs as outcome of system design development.	

Material Detection and Assay	• Perform research using mockups of separation processes. Investigate photon, neutron, and passive interrogations techniques. • Establish feasibility. • Determine data needs after processes have been established. • Improved delayed neutron and delayed neutron spectra may be needed.	• Provide data needs as determined by the design and feasibility studies.	• Gamma fission, fast neutron fission, detection of prompt neutrons, delayed neutrons, photons, gamma-gamma prime, nuclear resonance fluorescence, and so on are all being considered for material assay and detection measurements.
Sensitivity Analysis Tools Development	• Establish working group of experts to collaborate on the development of sensitivity analysis tools, both Monte Carlo and deterministic methods [6-9]. Goal is to establish consistent method of analysis and validation.	• Explore potential of relating reactor physics experiments to nuclear model parameters.	
Criticality Safety	• Perform sensitivity analysis to establish need for benchmark and/or cross-section measurements.	• Perform experiments to meet data needs as determined from sensitivity analyses.	• Critical safe configurations are needed for separations and fuel fabrication processes. Data relevant to transuranic solutions and fuels may be needed to reduce uncertainties.

1.1 Data Uncertainties

To date, sensitivity and uncertainty analyses have been performed with relatively sparse or ad hoc covariance information. Thus, as shown in Table 1, a top priority in the near term is to provide a consistent set of covariance data for a broad set of isotopes and to standardize tools used for analyses and data evaluation. The covariance data should be reliable, complete, and consistent (see Figure 4). We stress that better uncertainty data will play an essential role both in assessing needs for new data with reduced uncertainties and in making design-oriented statistical data adjustments.

With respect to nuclear data, sensitivity analyses performed to date (albeit with the ad hoc covariance) have shown that the uncertainties in the data are significant for a few parameters related to both fast and thermal spectrum reactors. These are as follows:

- K_{eff} for all systems (in the case of thermal systems, at the end of the irradiation cycle as a result of high burnup)
- Burnup reactivity swing and related isotope density variations during core depletion

- Void coefficient on reactivity in fast systems
- Neutron source for thermal systems at fuel unloading (to a lesser extent,)

In order to reduce uncertainties to acceptable levels, the analysis shows that new data are needed for a few minor and major actinides. These are shown in Table 1 with required accuracies.
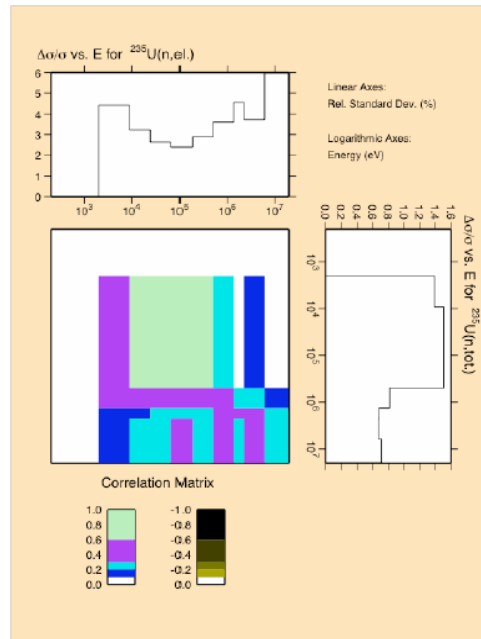
Fig. 4. Cross correlation between uncertainties in the elastic and total cross sections of 235U (P.Talou,T.Kawano, and P.G.Young)

1.2 Data Needs and the Relation to Basic Science

In order to meet the data needs for advanced fuel cycles, several challenges must be addressed by advances in basic science.

- **Covariance data:** There exists a significant challenge to (a) provide, together with sensitivity analysis, a tool to identify uncertainties that can have an immediate impact at the level of a preconceptual system design and a later impact on design (reactor and fuel cycle) optimization and margin reduction; and (b) identify and quantify data improvements (by isotope, type of reaction, range of energy) and their respective priorities in order to meet design target accuracies. Developments in basic science will help improve the theoretical base, which currently relies on the methods of producing covariance data.

- **Differential cross sections:** Very high accuracy plutonium fission and capture cross-section improvements are needed in the range 5–0.5 keV. The required accuracy presents a serious problem for most current experimental techniques. Hence, a basic science challenge is to develop innovative techniques (e.g., new detectors) that will allow a breakthrough in this field.

- **Minor actinide data improvements:** Some specific needs have already been pointed out, for example, for ^{241}Am and ^{242m}Am, and additional needs for higher mass actinides (Cm and beyond) are expected because of the characteristics of advanced fuel cycles, which in some cases have not yet been fully defined. The field of higher mass actinide nuclear interaction cross-sections is one where little is known, both for theoretical and experimental reasons. It is certainly a relevant scientific challenge to explore this field, and it is a challenge for basic science to develop new experiments and techniques. An example is exploration of the use of accelerator mass spectroscopy to get information on the capture cross-sections of minor actinides up to ^{252}Cf.

- Inelastic cross sections: For some intermediate mass nuclei (e.g., ^{23}Na or ^{56}Fe) inelastic scattering cross-section accuracies of the order of 10% are needed. Moreover, there exists a general need to improve the knowledge of inelastic scattering for actinides. Relevant experiments have proven particularly difficult. It would be worthwhile for the basic science community to investigate whether current challenges could be met with new and innovative measurement techniques.

- Other nuclear data: Basic science R&D can contribute to data improvement in other areas including decay and delayed neutron data, fission product yields, and neutron-induced photon production data, which will be useful for both reactor and material accounting needs. For example, in the field of beta decay data, some progress has been made by exploiting fundamental physics developments; this work needs to be continued and expanded.

- Computing: The expression of data improvements and related techniques opens two new and very challenging fields where basic science can provide added value.

  o The new requirement to take into account the complete fuel cycle for uncertainty assessment requires the propagation of uncertainties (e.g., nuclear data) throughout complex systems that include reactors, fuel fabrication and reprocessing facilities, temporary storages, and repository. Preliminary investigations have pointed to formidable computing challenges in order to develop appropriate sensitivity and uncertainty propagation methods. As an example, the Bayesian approach currently in use for the detection of sparse patterns could be extended to the detection of the effective patterns of sensitivity matrices. In this field, there are significant opportunities for the development of novel high-performance computation techniques.

  o The requirements for very high accuracy and the vision of a new paradigm to handle the production of nuclear data suggest a new approach that can use specific, high-accuracy integral experiments in order to provide information, not at the level of multigroup cross sections (statistical multigroup data adjustments), but at the level of nuclear model parameters. In this case, scientific and computational challenges represent an original opportunity for both basic science and high-performance computation.

- **Simulation:** Related to the interplay of nuclear data uncertainty reduction and transport method improvement, any design target accuracy includes both the uncertainties coming from nuclear data and the approximations in the simulation. In order to translate most of the requirements on the nuclear data uncertainty reduction, the simulation-induced uncertainties must be minimized. Achieving this objective implies significant parallel efforts in the high-fidelity simulation field where basic science plays a significant role.

2. Group B: Nuclear Measurements

Working Group B focused on measurements, facilities, and instrumentation to enhance the scientific basis and provide nuclear data needed to support the advanced fuel cycle. This working group brought together over 40 researchers from national laboratories and universities in the fields of nuclear science and nuclear engineering. Many researchers from the basic science community said they were eager to participate in such research; their first question was "How can we help?" The basic science community is poised to inject improved understanding of nuclear processes (in terms of models for reactions, structure and decay), new detector concepts, and specialized facilities, which will be essential for making the significant advances in nuclear data needed for reactor development. These researchers also expressed their interest in helping develop a vision for the longer-term future of nuclear energy in this country. Their talents and capabilities, coupled with those at large national laboratory facilities, offer the potential for significant advances and for a re-establishment of U.S. leadership in developing nuclear power. At the same time, the reactor applications community will orient all researchers to the requirements of improved materials properties and data precision that will provide the basis for a successful enhanced utilization of nuclear energy in the United States.

2.1 Background and Nuclear Data Needs

Within the Advanced Fuel Cycle Initiative in DOE/NE, now encompassed by the Global Nuclear Energy Partnership, nuclear data needs are established and ranked by the Physics Working Group under the direction of the National Technical Director for Transmutation Engineering. This working group normally meets twice a year and updates its priority list based on any changes in program direction, new results from nuclear data sensitivity analyses, and so forth. Sensitivity analyses apply a generalized perturbation theory to assess the sensitivity of quantities of interest (e.g., criticality, reactivity coefficients, reactivity loss with burnup) to uncertainties in nuclear data. When combined with estimates of the cost of measuring a particular cross section to within a target accuracy and an estimate of the best achievable accuracy for specific cross sections, this procedure produces a quantifiable ranked list of needed cross-section measurements, with target accuracies, within specific neutron energy bands.

The following materials have been identified as needing improved cross-section data with corresponding uncertainty (i.e., covariance) information.

^{232}Th, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242}mAm, ^{243}Am, ^{242}Cm, ^{243}Cm, ^{244}Cm, ^{245}Cm, Pb, Bi, ^{56}Fe, ^{57}Fe , ^{58}Ni, ^{52}Cr, Zr, Mo, ^{15}N, Si, C, O, Na, ^{10}B ^{1}H , Ti (5 isotopes), ^{85}Rb, ^{87}Rb

The data needs for these materials span the complete energy range, and cross-section measurements are needed in the resonance region and at high energies above the resonance range.

Recently, the DOE/NE Advanced Fuel Cycle Initiative and Generation-IV (GEN-IV) reactor program initiated efforts to improve cross-section data to support the transmutation of spent nuclear fuel (SNF) and reactor core analysis, respectively. Currently the priority list defines cross section measurements for ^{242}Pu, ^{240}Pu, and ^{241}Pu fission, ^{240}Pu and ^{241}Pu capture, Mo(n,xα), inelastic scattering for ^{56}Fe and ^{23}Na, and ^{239}Pu(n,2n). In the past year or so it has become evident that safeguards and materials accountability of spent fuel reprocessing and transmutation fuel fabrication facilities may require higher-fidelity nuclear data of the fission process. In particular, in order to achieve the stringent goals for materials accountability, new sensitivity analyses may be needed to determine neutron multiplicity distributions, the energy distributions of emitted

neutrons as a function of multiplicity, photo-fission cross sections, delayed neutron fractions, and the energy distributions of delayed neutrons.

In addition to these data needs, the AFCI/GEN-IV Physics Working Group determined that there exists a need for better characterization of the minor actinide fission process. In particular, new measurements are needed to determine fission product yields, prompt energy release, and decay heat associated with the minor actinide fission process.

Following the President's State of the Union address in January 2006, the United States initiated an effort to develop an advanced nuclear fuel cycle that will present nuclear data challenges in addition to the established nuclear data needs identified within the AFCI and GEN-IV programs. Moreover, basic science R&D will be needed to support closing the fuel cycle (e.g., SNF reprocessing, transportation, and handling). Establishing the safety basis for licensing applications for AFC operations will require the verification and validation of radiation transport modeling software (e.g., MCNP at Los Alamos, SCALE at Oak Ridge) and associated nuclear data with benchmark-critical or subcritical experiments. Because the AFC will involve novel fissile material processes, there will be integral data needs (e.g., benchmark critical or subcritical experiments and reactivity worth experiments) and differential data needs (i.e., cross-section measurements) for supporting AFC applications. The integral data needs are vital to AFC research and development; however, these needs are more applied in nature and hence do not fall within traditional DOE Office of Science research activities. Therefore, the measurement panel focused attention on the differential nuclear data needs that mainly involve basic science.

Although significant research has been performed by DOE/NE to identify reactor nuclear data needs, the nuclear data needs (i.e., including accuracy requirements) for the rest of the fuel cycle have not yet been clearly defined. Nevertheless, scientific opportunities for basic R&D can be identified based on existing measurement capabilities and the current state of nuclear data in the evaluated databases.

The AFC data needs span energies from thermal to high energies. As part of the AFC plan, the fuel cycle will be closed thereby requiring that SNF be reprocessed to produce new fuel for nuclear reactors. During reprocessing, two situations develop.

- Isotopes of plutonium, americium, and curium with higher mass numbers build up.

- The transition from fluid to solid form in the fuel reprocessing involves systems that establish intermediate- and thermal-energy neutron spectra.

The nuclear data for many of the actinides anticipated in the fuel reprocessing streams are not well known at intermediate energies that encompass the resonance region. Moreover, the safety basis for efficiently sized equipment, in terms of inventory and throughput, will require the demonstration of acceptable margins of subcriticality.

The novel process streams in SNF processing facilities and fuel fabrication plants may challenge the accuracy limits of existing detection techniques needed to monitor the proliferant material. As previously noted, the safeguards and material accountability applications may drive the need for better nuclear data:

- (γ, f) and (γ, n)
- Neutron multiplicity and associated energy distributions
- Delayed neutron fraction and associated energy distributions.

In addition to the reprocessing component of the advanced fuel cycle, operations will involve material handling and SNF transportation in approved shipping casks. The following are possible issues that should be investigated to assess differential data needs for advanced fuel cycle applications:

- Improved fuel exposure prediction of spent fuel isotopics (actinides and fission products)

- Improved prediction of spent fuel reactivity worth for criticality safety burnup credit (BUC) that is needed for transportation in addition to efficient sizing of reprocessing equipment

- Improved prediction of neutron radiation source terms, required neutron shielding and subsequent neutron reflection in criticality evaluations

- Improved cross-section data for isotopes acting as chemical reagents (important for neutron moderation and absorption).

BUC, in particular, will be a significant issue for the transportation and handling of SNF. BUC consists of taking credit for the reactivity decrease associated with the presence of fission products in the SNF. For current licensing applications, the SNF must be modeled as fresh fuel, an approach that is very conservative and limiting in terms of material throughput in transportation and handling operations. If BUC can be implemented in the licensing process, the cost savings for shipping the current U.S. inventory of SNF could be several hundred million dollars. The fission products that are the major contributors for BUC are ^{103}Rh, ^{133}Cs, ^{143}Nd, ^{149}Sm, ^{151}Sm, and ^{155}Gd. Unfortunately, the quality of fission product cross-section data for these major contributors is very poor. In addition, better capture cross-section data for ^{153}Eu and ^{155}Eu is required for improved isotopic prediction for ^{155}Gd, which is an important fission product for BUC. Clearly, nuclear data measurement in the resonance region will be needed to support advanced fuel cylce R&D.

Studies indicate that full-range nuclear data measurements (from the low eV region to the MeV region) are needed in order to address current AFC data needs. As new AFC studies are performed, one can expect additional data needs to be identified. The basic science community must be ready to respond to these emerging needs in a timely manner. In addition, the basic science data community must stay engaged with the applied AFC community to assess and quantify data needs and to establish priorities for research and development. To this end, the working group felt strongly that follow-on workshops need to be held at least annually.

2.2 Direct Neutron Measurements—Techniques and Instrumentation

The United States has a diverse portfolio of neutron and γ−ray measurement capabilities located at national laboratories and universities. As a result, DOE and the associated research community are poised to make significant advances in experimental areas relevant to the AFC. We note that all operating monoenergetic neutron source capabilities in the United States are located at universities (Ohio State University, the University of Kentucky, and Triangle Universities Nuclear Laboratory). Thus, university facilities will also be needed to advance the basic neutron science frontier.

Table 2 lists general neutron science measurement areas needed to support the AFC. In the past several years most R&D has focused on measurements of neutron capture and fission cross-sections (see Figure 5).

Table 2: AFC nuclear data measurement capability needs. Status column: A: established capability that is part of current DOE/NE AFC research efforts; B: partially studied under other R&D programs, but additional work may be needed to support AFC research; C: area where very little or no R&D is in progress. In most cases, the capability cannot be addressed without additional investment.

| **Needed Measurements for Neutron Data**	**Status**		
	A	B	C
Total cross sections		X	
Elastic scattering angle distributions			X
Inelastic scattering and distributions of emitted neutron energies		X	
Fission			
• Cross-section measurements	X		
• Gamma and neutron output (nu-bar, P(nu); energy distributions)		X	
• Fragment yields and kinetic energies			X
Capture			
• Cross-section measurements	X		
• Gamma-ray energy distributions		X	
• Capture-to-fission ratios		X	
(n,z) hydrogen and helium gas production	X		
(n, xn) for transmutation [e.g., Am(n,2n)]		X	
Data for safeguards and material accountability			
• Delayed neutron spectra		X	
• Gamma-ray induced reactions			X
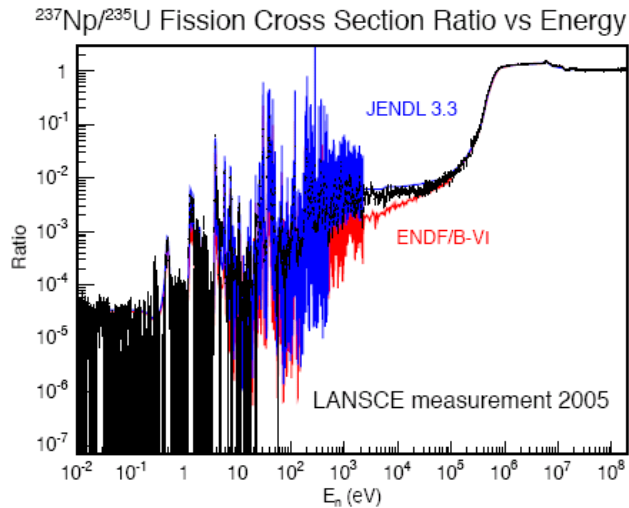
Fig. 5. Ratio of the fission cross section of ^{237}Np relative to the standard ^{235}U over 10 orders of magnitude in incident neutron energy. Data obtained in the DOE/NE AFCI program at LANSCE.

In addition, a dedicated effort has focused on hydrogen and helium gas production measurements from (n,z) reactions. Therefore, the neutron science community can make immediate contributions to address the AFC data needs for capture, fission, and gas production. Continuing R&D efforts will be needed in these areas to ensure that the United States does not lose the capability to perform capture, fission, and gas production measurements. Significant opportunities exist for additional researchers to participate in these measurements and to develop advanced detectors to improve the science output of this program.

Active measurement capabilities also are partially supported by other research programs. Although this research does not specifically address AFC objectives and needs (e.g., accuracy requirements), it could be refocused with existing personnel and capabilities. Some key measurements, however, are not being addressed at present. Additional R&D effort will be needed (e.g., total cross section measurements) that will require additional investment at one or more existing facilities.

In the following subsections, the measurement needs identified in Table 2 are discussed in more detail, with emphasis on capabilities and suggestions for research and development.

2.2.1 Total Cross Sections

Scientific Challenges

Total cross-section measurements are vital for supporting detailed cross-section evaluation efforts, and total cross-section data will be needed to improve the accuracy of neutron evaluations. For example, reliable neutron widths are important for calculating experimental effects such as self-shielding and multiple scattering in the sample under investigation. In addition, when capture measurements are too difficult to measure, total cross-section measurements will be critical for developing a cross-section evaluation. Total cross-section data are also essential for improved understanding of the nuclear optical model, which in turn is used to provide better evaluated data. The capability for performing these measurements in the United States is limited to a few facilities:

- LINAC lab at Rensselaer Polytechnic Institute (RPI) can perform transmission or total cross-section measurements from thermal energies up to ~1 keV (e.g., see Fig. 6).

- ORELA at Oak Ridge National Laboratory can perform transmission measurements from thermal up to several MeV, with demonstrated ability to measure total cross-sections to the sub-percent level for certain isotopes.

- ANSC at Los Alamos National Laboratory has measured total cross-sections, but that capability would need to be re-established to provide total cross-sections from 0.1 to 20 Mev.

- The Van De Graaff accelerator at the University of Kentucky has measured total cross-sections 0.25 to 20 MeV, and is most suited to common structural targets (e.g., Fe, Cr) as opposed to actinide targets (at 5–15% accuracy).
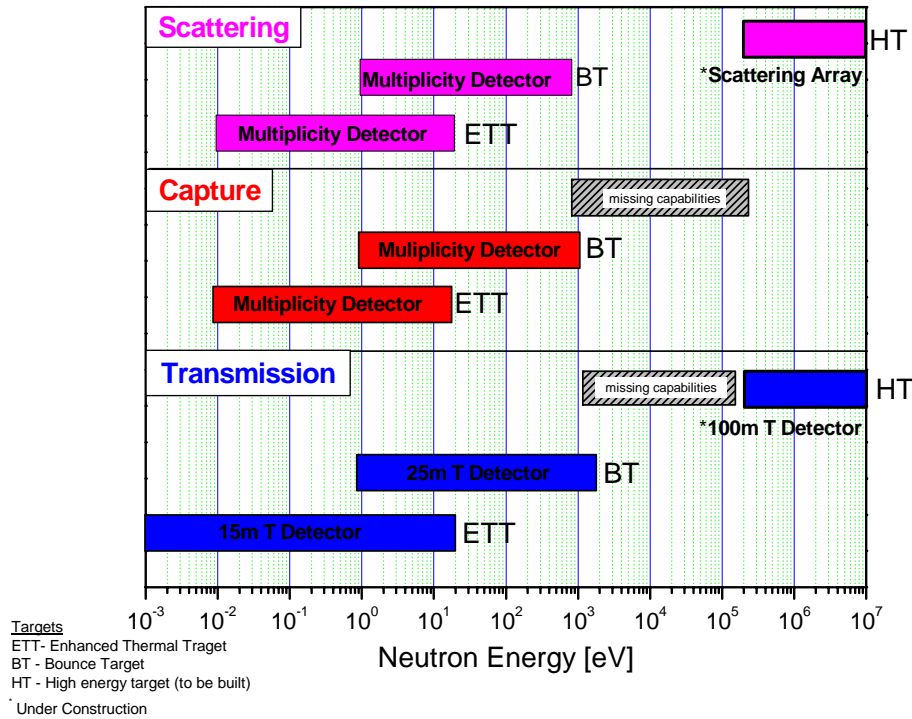
Fig. 6. Example of nuclear measurement capabilities (RPI)

Scientific Opportunities

Two issues associated with total cross-section measurements must be addressed. First, additional R&D will be needed to reconstitute a comprehensive transmission capability over the entire neutron energy range for a wide variety of nuclides. Second, in many cases, for AFC data needs and for improving the nuclear optical model, total cross-section accuracies need to be improved down to 1% absolute accuracy. Many factors contribute to cross-section measurement uncertainty. In most cases, a study to understand, measure, and correct background data is needed in conjunction with a study of the systematic effects on the measurements. Such R&D studies could involve collaborations between national laboratory and university facilities or groups, effectively using the expertise and infrastructure that resides in each to help move this AFC effort forward.

2.2.2 Elastic Scattering and Distributions of Neutron Energies

Scientific Challenges

Elastic scattering measurements may be very important for providing improved scattering data for AFC or GEN-IV moderating materials. As an example, efforts are under way to investigate graphite for advanced reactor designs. Unfortunately, the scattering data for graphite in the evaluated nuclear data files are based on measurements performed more than 40 years ago. Moreover, the material composition of graphite can vary substantially, thereby impacting the scattering distributions. The scattering distributions for many nuclides in the intermediate range may be important for advanced fuel cycle processing operations. As previously noted for total

cross-section measurements, the capability to directly measure doubly differential elastic scattering cross-section data is limited to a few select facilities (primarily Oak Ridge, RPI, and Ohio University).

Scientific Opportunities

Currently, the United State does not have a full energy-range measurement capability to measure exit angle distributions from elastic scattering. Moreover, elastic scattering measurements cannot be performed from the eV range to ~0.2 MeV. Re-establishment of this capability will require investment in existing facility infrastructure. Improved electronics and instrumentation (with increased acceptance) would need to be part of such a package. Further study may be needed to realize this potential for application to the basic science AFC effort.

2.2.3 Fission

Scientific Challenges

Accurate fission cross-section data will be important for AFC development. Recently, fission measurements in direct support of DOE/NE R&D efforts have been conducted at LANSCE (see Figure 5). Although LANSCE can measure the full-range fission cross-section with very high accuracy, the energy resolution in the resonance region is insufficient to support a resonance evaluation for the fission cross section. RPI has the capability to measure fission from 0.01 eV to 1 keV, but this energy range will not cover the entire resonance region. ORELA has conducted high-resolution fission cross-section measurements from the eV region to several hundred keV using long flight paths. At present, however, no single experiment or facility can cover the full energy range, with the required resolution, for the fission process.

In an alternative approach, Idaho National Laboratory (INL) researchers have been investigating the measurement of fission parameters at the Intense Pulsed Neutron Source using neutron-induced reactions with a multiparameter coincidence system of several detector types. In order to determine cross-section data, the INL method uses correlated data for neutron-induced reactions on nuclide targets. Recently, they have performed measurements of discrete gamma rays from fission and capture (see Section 2.2.4) on ^{239}Pu. This method could be used to determine branching ratios as well as neutron multiplicity and fission yields. The method is, however, a nontraditional approach for measuring cross-sections, and additional work will be needed to determine whether the measurements can be used to produce evaluated cross-section data files.

Information beyond fission cross-section data and correlated coincidence data will be needed to gain a better understanding of the complex fission process especially for minor actinides. Some non-AFC research has been devoted to measuring gamma and neutron production from fission. However, the research does not address AFC accuracy requirements. Likewise, little or no research is being performed to determine fission fragment yields and associated kinematics data, which is needed for a better understanding of fission processes.

Scientific Opportunities

Based on projected AFC data needs, fission cross-section data may need to be measured to less than 5% accuracy and to within 1–2% accuracy for some nuclides. Therefore, additional R&D will be needed to improve cross-section measurement accuracies to support AFC work. The following opportunities exist:

- Currently, LANSCE has the capability to perform fission cross-section measurements over the full range of interest to the AFC. Additional R&D focused on instrumentation, such as novel fission chambers (e.g., time-projection chambers or dual-arm spectrometers), will be needed to achieve the projected AFC target accuracies. A complete covariance matrix is being developed for these measurements and will provide new insights into the uncertainties of these precise data.

- Existing lead slowing-down spectrometers at RPI and LANSCE can be used to measure fission cross-sections on very small samples of actinides. This capability, together with innovative detectors, could be used also to study other aspects of the fission process.

- New techniques can be developed to reduce fission cross-section measurement uncertainties. Three of the major contributors to fission cross-section measurement uncertainty are particle identification, target thickness, and the use of ^{235}U as a normalizing reference. Collectively, these three sources of error are the limiting factors that currently prohibit fission measurements to better than 1% accuracy. Preliminary studies indicate that the development and use of a time projection chamber (TPC) could reduce the error associated with these sources—with the potential to reduce fission cross-section measurements to the sub-1% level. In addition, the TPC has the potential (often in conjunction with other detectors) to measure other properties of the fission process (e.g., fission fragments, photons from fission, emitted neutron spectra, and the number of neutrons per fission). Currently, a TPC has not been developed for use at any of the traditional cross-section measurement facilities. One possible research opportunity involves a multilaboratory and university collaboration to develop a TPC measurement capability and demonstrate fission cross-section measurements to within 1% uncertainty. In order to demonstrate improved fission cross-section measurements over the entire energy range, a TPC measurement capability would need to be demonstrated at continuous-in-energy and monoenergetic neutron facilities. If successful, the TPC would advance the current fission measurement capability beyond the traditional fission chamber approach.

- INL researchers have measured discrete gamma rays from fission and capture to study neutron-induced reactions with a multiparameter coincidence system of several detector types. Before this methodology is accepted for cross-section measurements to produce evaluated nuclear data files, work is needed to demonstrate the development of a cross-section evaluation from the INL measurements. For example, a significant challenge exists in the resonance region where detailed energy resolution is required for evaluators to extract resonance parameters. Additional measurements on other isotopes would be needed, and these measured results must be validated against cross-section measurements from other neutron science facilities.

Additional opportunities for fission measurements using surrogate techniques are identified in Section 2.3.

2.2.4 Capture

Scientific Challenges

As with fission, active R&D is devoted to performing capture cross-section measurements at various neutron facilities. Although preliminary AFC reactor studies indicate that uncertainties in the 10% range may be acceptable for some nuclides, ^{241}Am capture measurements will be needed to within 5% uncertainty, and higher-precision measurements for some nuclides may be needed

for other parts of the AFC. Therefore, the challenge will be to perform capture cross-section measurements to less than 5% uncertainty. The DANCE detector at LANSCE is relatively new (~3–5 years old), and future R&D will be performed to develop a covariance matrix for capture that will provide additional insights into the uncertainties of these precise capture measurements. ORELA has demonstrated capture cross-section measurements to ~3% accuracy. We note that 3–5% accuracy is believed to be the highest accuracy attainable with current measurement techniques in the resonance region.

Scientific Opportunities

- LANSCE has demonstrated the capability of measuring capture cross sections and fission-to-capture ratios on very small actinide samples. The present DANCE program includes a detailed R&D study to understand, measure, and make corrections for the background data to extend experiments to the 100 keV region. Substantial opportunities exist in the present DANCE detector for studies of level densities and radiative strength functions to improve reaction model physics—an ideal area for university-laboratory cooperation.

- ORELA can be used to obtain reliable average resonance parameters such as level densities, neutron strength functions, and average widths, which are the input parameters for nuclear model calculations. This area is ideal for university-laboratory cooperation.

- Developing a new state-of-the-art 4π BaF$_2$ detector ball could complement the DANCE detector at the Lujan Center. With the appropriate detailed energy resolution throughout the resonance region coupled with low backgrounds and well-shielded flight paths, a BaF$_2$ detector ball would advance the present state of the art for resonance region capture measurements. Such a large-scale undertaking could arise from a collaborative effort between the national laboratory and university communities. It would serve as a training ground for next-generation researchers, as well as providing a first-class instrument for both basic and applied science. Portability of such a device, to take advantage of existing neutron source capabilities, would be a key issue.

- In addition to capture cross-section measurements, some non-AFC related research has been devoted to measuring gamma energy distributions resulting from capture as well as capture-to-fission ratios (e.g., DANCE). Other neutron science facilities also could be used to make such measurements but by less comprehensive methods. Gamma production data will be relevant for power distribution assessments at reactor interfaces (e.g., reactor core/reflector boundary). Before a new AFC experimental program is initiated for these measurements, interactions between the basic science community and the AFC R&D community will be needed to quantify these data needs and target accuracies.

Additional opportunities for capture measurements using surrogate techniques are identified in Section 2.3.

2.2.5 (n, z) Hydrogen and Helium Gas Production

Scientific Challenges

Detailed modeling of radiation damage in structural materials and in cladding includes atomic displacement and nuclear transmutation, the latter changing the elemental composition of the material. One class of transmutation reactions is those that produce the light elements, hydrogen and helium, both of which have been identified as potentially significant contributors to changes in materials properties. Credible values for these production cross sections are therefore essential

as the source term in modeling radiation damage. These cross sections are often small fractions of the total reaction cross-section, and nuclear reaction model codes have had great difficulty in predicting them even to within a factor of two because of uncertainties in the nuclear level densities, in the optical model, and in the ratio of pre-equilibrium-to-equilibrium reaction mechanisms. Experimental measurements with new, multidetector arrays allowing one to identify final states via event-by-event measurements of neutrons and charged particles, in coincidence with γ-rays, would be valuable in calibrating the reaction and decay codes.

Scientific Opportunities

- Hydrogen and helium production cross-sections are being measured over a wide range of structural materials at LANSCE. The energy and angular distributions are integrated to obtain values for the production of these gases. The data have sufficient statistics for the production cross sections but are marginal for testing nuclear reaction models. With a more efficient (larger solid angle) set of detectors, the experimental data would serve as benchmarks for statistical and pre-equilibrium models. Furthermore, measurements with improved physics content should be done where possible with isotopically enriched samples.

- Reactions that produce these charged-particles should be compared with (n,n') and other reactions to identify the reaction mechanisms and to understand partial and total nuclear level densities.

2.2.6 (n, xn) for Transmutation

Scientific Challenges

The (n,2n), (n,3n), and other reactions transmute nuclei into other isotopes, which usually have different neutronic and nuclear decay properties. In most medium-weight nuclei, the cross sections can be calculated with some degree of certainty except near thresholds. For actinides and some other nuclides where these reactions compete with fission, the calculations are very uncertain. Measurements are required to reduce these uncertainties. Two approaches are activation and measurement of gamma- and x-rays in the residual nuclides. The latter data give the production cross-sections of these radiations, and the (n,xn) cross section is deduced from those data using a nuclear reaction model that incorporates the available nuclear structure and decay information.

Scientific Opportunities

- (n,2n), (n,3n) and other reactions can in many cases be studied by activation. Monoenergetic neutron sources are required for this work. At the workshop, researchers from Ohio University, the University of Kentucky, and Triangle Universities Nuclear Laboratory presented talks highlighting their respective measurement capabilities. Each of the university laboratories is poised to make R&D contributions in this area.

- The measurement of prompt gamma rays from de-excitation of excited states in the residual nuclei is used to deduce these (n,xn) cross sections. Both continuous-in-energy and monoenergetic sources are required for these studies; and, in both cases, high-resolution gamma- and x-ray detectors are essential. Detector system upgrades would increase the quantity and quality of the data, for example, in the detection of coincident gamma rays to identify the reaction more cleanly (such as (n,2n) in competition with fission).

2.2.7 Data for Safeguards and Material Accountability

Scientific Challenges

Process streams in the fuel cycle, both front and back end, have large quantities of actinides that are potential proliferant materials. The challenge is to measure the input and output of these isotopes and to ensure that none are diverted. The measurement in this approach needs to be extremely accurate at each end, probably better than 0.1%.

Scientific Opportunities

New ideas are needed on how to measure the important actinides to an accuracy of 0.1%. This is probably the subject of a new metrology rather than an improvement in our understanding of nuclear physics.

2.3 Surrogate and Other Charged Particle Reaction Measurements—Techniques and Instrumentation

The surrogate technique is an indirect method for determining cross sections of compound-nuclear reactions that are difficult or impossible to measure directly. Many scientific questions relevant to basic nuclear reaction physics, to nuclear astrophysics, and to the AFC are associated with compound-nuclear reactions. For many of these reactions a direct measurement of the cross section is impractical or impossible. In these cases the surrogate technique offers an alternative approach.

The surrogate technique was pioneered in the 1970s as a method to extract cross sections for neutron-induced cross sections on unstable nuclei. Over the past several years, there has been a resurgence of theoretical and experimental activity at several national laboratories and with their numerous university collaborators. This technique has been applied in a variety of forefront scientific areas, including the use of inverse kinematics reactions with rare isotope beams, with some considerable success.

One new approach has been the recent development of the surrogate ratio technique, which eliminates many of the systematic uncertainties in the original method. Figure 7 illustrates the current accuracy achievable by the surrogate ratio method for fission studies. Plotted is the experimentally measured ratio of the cross sections $^{234}U(\alpha,\alpha'f)/^{236}U(\alpha,\alpha'f)$, surrogate for $^{233}U(n,f)/^{235}U(n,f)$ (blue points) compared to the ratio of the accepted values from ENDF-B7 (red points). Except for the lowest energies, the agreement is excellent, typically within 5%, over an excitation energy range from 7 to 25 MeV. Recently the validity of the surrogate ratio approach has been theoretically studied for (n,f) reactions on actinide nuclei.

The surrogate technique can be employed to determine indirectly the cross section for a two-step reaction that proceeds through an equilibrated (compound) nuclear state. The direct, desired, reaction is $a + A \rightarrow B^* \rightarrow c + C$, where the target nucleus A is unstable. The surrogate reaction produces the same compound system B^* but via a different reaction involving a stable beam target combination, $d + D \rightarrow B^* + b$, and the subsequent decay $B^* \rightarrow c + C$ is observed in coincidence with the outgoing particle b When the target nucleus A is unstable or in an excited short-lived state, direct measurements of the reaction $a + A \rightarrow B^* \rightarrow c + C$ are extremely difficult or impossible. In addition, calculations of the cross section are too difficult or too inaccurate when several possible decay channels must be considered. Fission, which obviously plays an important role in the actinide region, in particular introduces large theoretical uncertainties.
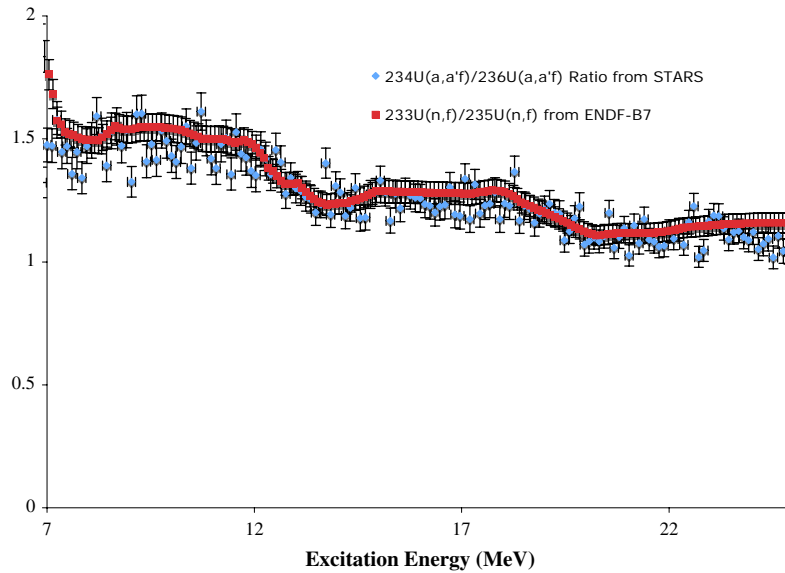
Fig. 7. Experimental ratio of $^{234}U(\alpha,\alpha'f)/^{236}U(\alpha,\alpha'f)$ measured using the STARS detector array compared to the ratio of accepted $^{233}U(n,f)/^{235}U(n,f)$ values from ENDF-B7.
(S.R. Lesher et al., to be published)

Scientific Challenges

Although the basic idea is simple, significant challenges exist. In particular, three key theoretical challenges must be addressed in order to provide a reliable framework for planning and analyzing surrogate experiments. Clearly these theoretical developments need to go hand in hand with additional experimental information.

- **Accounting for the J^π population mismatch.** In most cases the surrogate reaction will populate states in the compound nucleus differently than the direct reaction. In particular, the angular-momentum and parity (J^π) populations will be mismatched. Since the J^π population influences the decay probabilities of the compound nucleus, models have to be developed that account for the differences between the reactions. This is a nontrivial theoretical task because a proper treatment of direct reactions leading to highly excited states in the intermediate nucleus requires a description of particle transfers and inelastic scattering to unbound states.

- **Role of pre-equilibrium reactions (Is the intermediate nucleus truly in a compound state?)** Central to the surrogate method is the assumption that the formation and decay of the intermediate nuclear state—in both the direct and the surrogate reaction—are independent of each other. This assumption is valid only if the intermediate nucleus equilibrates before it decays into the final reaction products. Rapid (pre-equilibrium) decay of the intermediate configuration before a compound nucleus can be formed could invalidate the surrogate analysis (but perhaps not the surrogate ratio method). Theoretical estimates of the probability that a compound nucleus is actually formed in a particular reaction, together with the effects of pre-equilibrium decays on J^π populations, can be used to guide experiments to test these estimates.

- **Choice of the reaction.** In many cases, several possible surrogate reactions can produce the relevant compound nucleus. Improved theoretical inputs are required to assess the suitability of the different options and to determine the optimal conditions for carrying out surrogate-reaction experiments.

Physics Objectives Addressed by the Technique

The surrogate technique addresses several fundamental nuclear physics objectives, is of relevance to nuclear astrophysics, and can enable several important measurements relevant to the AFC program. The surrogate technique and particularly the surrogate ratio technique may be most useful in the energy range of $E_{neutron}$ greater than several hundred keV, with some hope of extending to lower energies, for heavy nuclei (A > 100), and for cases where the half life of the direct target nucleus is less than ~100,000 years. Many reactions relevant to the AFCI program require light-ion stable beams (e.g., d, ^{3}He, α) and associated facilities.

The surrogate approach, and the surrogate ratio technique in particular, offer a unique opportunity to combine a proven approach toward measuring (n,f) cross sections in a fast reactor neutron spectrum with a basic science program that can answer critical questions in low-energy reaction and nuclear astrophysics. The surrogate ratio technique has been shown to be valid for obtaining (n,f) cross sections and may hold special promise in obtaining (n,γ) cross sections at high energies (E>100 keV).

The nuclear data needs for the AFCI are similar to the needs of a program measuring s-process branch point cross sections for developing stellar nucleosynthesis models. In both cases the (n,γ) cross-sections on radioactive nuclei of importance are adjacent to more long-lived stable nuclei and require data in energy regions considerably above "normal" reactor energies (30 keV < kT < 6 MeV).

A well-designed program of benchmarking the surrogate technique by comparison to known (n,γ) cross sections would open a new highly versatile tool for addressing nuclear data needs for both Generation IV reactor design and stellar nucleosynthesis. In addition, this program would address several important nuclear physics questions:

- How can one quantitatively describe the equilibration process of the intermediate nucleus following the direct reaction?
- What are the spin-parity (J^{π}) distributions of highly excited (continuum) nuclear states following a direct reaction?
- How were the elements from iron to uranium made?
- What role does convective flow play in stellar nucleosynthesis models?
- What are the benchmark experiments that test the theoretical predictions?

Scientific Opportunities

- Theory
  - Improve and extend current reaction theories.
  - Develop models to predict the population of unbound states in direct (transfer and inelastic scattering) reactions.
  - Develop theoretical descriptions of the equilibration of a highly excited nucleus
  - Improve the input (optical model, level densities, etc.) for Hauser-Feshbach calculation.

- Experiment
  - Develop a program of experiments to benchmark the technique for (n,f) (n,nγ) and (n,xnγ) reactions on a broad range of targets broad range of target nuclei.
  - Extend these measurements into new energy regions.
  - Look at different reaction mechanisms, including inverse kinematics with rare isotope beams.
  - Develop experiments that explicitly test theoretical predictions of, for example, spin-parity distributions, or level densities.

2.4 Nuclear Reaction Models

A brief review of the current status of nuclear models pointed to future needs for the AFC program and for continued progress in the basic science. Additional discussions on nuclear modeling calculations were addressed in the parallel Nuclear Data Panel Session and Nuclear Theory and Computations—Nuclear Reactions Panel Session and can be found in Sections 3 and 4 of this report.

The following needs were identified by the measurements working group (B):

- Improved modeling of fission and all aspects of the fission process.

- Improved understanding of neutron capture, including radiative strength functions, the optical model, and competing channels where open, such as inelastic scattering. In order to support capture modeling, a key issue will be the ability to perform measurements to obtain better level density data and radiative strength functions.

- Extension of reaction models for neutrons interacting with nuclides off the valley of stability, focusing in particular on fission-product nuclides.

- Neutron capture and (n,2n) reactions, especially in the actinide region for transmutation needs. Understanding how (n,2n) cross sections rise from threshold (where the (n,2n) reaction overlaps the tail of the fission neutron energy distribution) may be important. Current models have limited predictive capability in this case; predictions depend on the details of nuclear structure and level densities near threshold. The experimental facilities and apparatus to perform direct measurements by directly counting the two neutrons in the exit channel no longer exist in this country. [241]Am was identified as having particular relevance to the AFC program.

- Surrogate reactions, and the surrogate ratio technique in particular, for neutron energies > a few hundred keV. The surrogate ratio technique had been shown to be valid for obtaining (n,f) cross sections and may hold special promise in obtaining (n,γ) cross sections at energies above a few hundred keV. The technique has yet to be proved for (n,2n) reactions. Comparisons of theoretical calculations and extensive experimental benchmarking are required. It is particularly interesting to test the theory for capture reactions for energies above ~200 keV.

- A comprehensive description of the fission process including scission and postfission observables.

- Improved shell model Monte Carlo techniques.

2.5 Structure and Decay Properties

The databases on nuclear structure and decay data refer to a complexity of nuclear-level schemes and tables of numerical values that quantify fundamental properties of atomic nuclei, such as level energies, quantum numbers and state lifetimes, as well as various decay modes and associated radiations. These data are the core result of basic nuclear structure research; they are the best evaluated summary of many experimental observations. The information plays a seminal role in many applied R&D technologies for the AFC including nuclear energy production, reactor design and safety, material accountability and safeguards, and material analysis. The nuclear structure and decay data are frequently used as standards in cross-section measurements, and their interpretation, where the activations and neutron induced prompt gamma-ray (n,xnγ) techniques are utilized. These data also provide important input to various nuclear reaction calculations, including information on nuclear level densities, γ-ray radiation strength functions, deformation parameters, and angular momentum distributions and populations.

Decay data of fission products (FP) and transactinide (TA) nuclides are at the core of decay heat evaluations in AFC of both thermal and fast reactors. Accurate calculation of the decay heat is needed for predicting the residual power in these reactors in case of shutdown and for designing heat-removal systems during the handling and interim storage of spent fuel and during fuel transport. Although extensive measurement efforts have been developed over the past 50 years in response to the increasing need of the nuclear technology community for accurate data, differences exist between the decay heat standards and experiments, depending on the irradiation and cooling times, and the fissile actinides considered. The experimental data are particularly scarce for short cooling times (less than 3000 s) where the decay of neutron-rich FP dominates owing to the large β-decay Q values (~4–10 MeV) and the fact that β-decay feeding intensities into the high-energy region of the daughter nuclei are frequently missing ("pandemonium effect"). This is the case for almost half of all known FP involved in the fission process (~1200 nuclides). Attempts made in past to resolve data deficiencies using high-resolution γ-ray spectroscopy techniques were partly successful, due to the low efficiency and sensitivity of the detector systems used in these measurements and the lack of pure, and intense sources. The Total Absorption Gamma-ray Spectrometry (TAGS) method, which is in principle free from the "pandemonium" problem, has been applied in the past for 50 cases, albeit this technique is compromised when isomers are present or β-decay delayed neutrons are emitted. For cooling times longer than 3000 s the contributions from TA decays dominate. The ongoing IAEA Coordinated Research Project on "Updated Decay Data Library for Actinides" outlined specific needs for future measurements (mostly dealing with half-lives, branching ratios and emission probabilities) of selected TA nuclides that need to be performed.

Scientific Opportunities

- A significant advancement of our understanding of nuclear decay of nuclei far off stability could result by combining high-resolution discrete γ-ray spectroscopy with the high-efficiency event-by-event measurement of neutrons and charged particles identifying the decay channel. A high-efficiency, 4π detector for neutrons and charged particles is needed that can be used with a set of discrete high-resolution γ-ray detectors.

- Complementary information may be obtained by using high-resolution γ-ray spectroscopy with state-of-the art multi-detector systems, currently operating at DOE's accelerator facilities, along with total absorption γ-ray spectrometry. This goal can be accomplished at radioactive beam facilities, such as CARIBU at Argonne and HRBIF at Oak Ridge, where high-intensity and pure beams of neutron-rich fission fragments can be

produced and delivered to dedicated β-decay counting stations. Technically, this is the essential tool to significantly improve and resolve deficiencies in the fission product decay data that are needed for decay heat evaluation in reactor applications. With a modest upgrade, the world's most powerful γ-ray spectrometer for nuclear structure research, GAMMASPHERE, can be used as a powerful spectrometer for β-decay studies of neutron-rich fission products. The development and operation at these facilities of a dedicated total absorption gamma-ray spectrometer, in conjunction with neutron detection system for β-decay delayed neutrons, would be a substantial asset for both basic and applied science.

- Dedicated measurements of decay properties of selected transactinide nuclei using pure, mass-separated sources and state-of-the art detector equipment need to be encouraged and supported.

2.6 Facilities

The DOE and other federal agencies, as well as several universities in the United States, support and operate facilities that are essential to the basic and applied neutron science programs associated with the AFC. For an expanding AFC capability, these facilities will be even more important. The present workshop—with its emphasis on the identification of scientific potential in the AFC for nuclear physics and its associated computational aspects—was not asked to critique the status of these facilities. Such a critique should be the focus of a future workshop. Nevertheless, detailed descriptions with links to individual facilities can be found on the Background Documents link on the workshop website at http://www.mcs.anl.gov/nprcsafc/. See also the presentation by Paul Koehler (ORNL) in the plenary session.

2.7 Cross-Cutting Nuclear Chemistry and Target Sample Preparation

In addition to the measurement facility and manpower issues is the concern over target sample availability for experiments. Nuclear materials science is also rapidly disappearing from the United States, and only a handful of experienced personnel remain available to prepare target samples for measurements. Further, the number of facilities available to produce actinide and other radioactive target samples is very limited. Under the AFCI/GEN-IV program, Idaho National Laboratory has been preparing target samples for cross-section measurements. Moreover, a portion of the material for target preparation has been supplied by Oak Ridge National Laboratory. As an example of the decline in target material capabilities, we note that much of the actinide and radioactive target sample preparation capability has been discontinued at Oak Ridge in recent years. One factor was the increasing regulatory rigor and costs, concurrent with a decrease in funding with the discontinuation of the nuclear weapons testing program, which had provided some baseline support for facilities and capabilities. Another factor was the elimination of basic science R&D support to isotope-related activities when the Isotope Program and the Revolving Fund concept was adopted in FY90, centralizing isotope activities as a NE program.

The situation with stable isotope target samples is better because the capabilities to perform chemical and materials processing has been maintained, however, there is no new production of enriched stable isotopes. All current material is being drawn from the existing inventory of stable isotopes that had previously been enriched on the Oak Ridge calutrons, which last operated in 1998. Although the nuclear chemistry/materials science issue falls outside the scope of the measurement panel workshop, the lack of target samples may prove to be a key limiting factor in future measurements.

2.8 Cross-Cutting Educational Opportunities

As critical as facilities and advanced instrumentation are to present and future AFC efforts, none of these can occur without a dedicated and well-educated cadre of nuclear science and engineering researchers. While not directly a charge of this workshop, the topic was much discussed in plenary and parallel sessions. An initial proposal addressing the subject was developed in the meeting of the measurements group and brought forward by Professor Jolie Cizewski of Rutgers University. This proposal is presented in Appendix 7 of this document.

2.9 Summary of R&D Opportunities

The following summarizes the scientific opportunities identified by the measurements working group for AFC nuclear data measurement R&D.

Short Term (1–3 years)

- In order to facilitate identification of basic science R&D needs of the AFC program, dialog must continue between the basic science and applied communities, and a priority ranking should be established for measurements with accuracy requirements. Additionally, follow-on workshops should be conducted, possibly on an annual basis, to clarify the data needs and measurement requirements.

- The need for radiochemical facilities for isotopic enrichment and sample development and fabrication is an issue that cuts across all proposed measurements. This issue needs more study.

- A comprehensive total or transmission measurement capability is needed for the entire energy range and a wide range of nuclides (i.e., including highly radioactive samples).

- In many cases, for AFC data needs and for the nuclear optical model, total cross-section accuracies need to be improved toward 1% absolute accuracy. Many factors contribute to cross-section measurement uncertainty. In most cases, a study to understand, measure, and correct for background data is needed in conjunction with a study of the systematic effects on the measurements. Specific details for R&D opportunities are noted in Section 2.2.

- A doubly differential elastic- and inelastic-scattering measurement capability is needed for the entire energy range.

- Additional R&D is needed to improve fission cross-section measurement accuracy to within 1%. Multilaboratory and university R&D with novel fission chambers (such as time-projection chambers or dual-arm spectrometers) will be needed to achieve projected AFC target accuracies.

- Systematic errors associated with traditional (n,f) measurements need to evaluated and understood in order to undertake (n,f) measurements with the required accuracy. Preparation and handling of radioactive samples also play a large role, as do safety concerns.

- A more efficient (larger solid angle) set of detectors is needed at LANSCE to support detailed energy and angular distribution measurements for hydrogen and helium gas production measurements. The resulting experimental data would serve as benchmarks

for statistical and pre-equilibrium models. Furthermore, measurements with improved physics content should be done where possible with isotopically enriched samples.

- Reactions that produce charged-particles (i.e., gas production reactions) need to be compared with (n,n') and other reactions to pin down the reaction mechanisms and to understand partial and total nuclear level densities.

Intermediate Term (1–5 years)

- Direct (n,f) measurements.

- Surrogate and charge particle techniques. These are of value when direct measurements are difficult or impossible to carry out. They are important for theory—current reaction theories need to be improved and extended. They are also important for experiment, including: benchmark experiments for surrogate reactions and other charged particle techniques for (n,f), (n,γ) and (n,xnγ) reactions on a broad range of nuclei.

- Multilaboratory and university collaboration to establish a 4π BaF_2 detector array for detailed energy resolution cross-section measurements in the resonance region to complement the existing DANCE detector.

- Measurement of gamma energy distributions resulting from capture as well as capture-to-fission ratios.

- R&D for (n,xn) for transmutation. In many cases, (n,2n), (n,3n), and other reactions can be studied by activation. Monoenergetic neutron sources, currently located at universities, are required for this work.

- R&D for (n,xn) for transmutation. Measurement of prompt gamma rays from de-excitation of excited states in the residual nuclei is used to deduce these (n,xn) cross sections. Both continuous-in-energy and monoenergetic sources are required for these studies, and in both cases high-resolution gamma- and x-ray detectors are essential. Upgrades of existing detector systems would increase the quantity and quality of the data, for example, in the detection of coincident gamma rays to identify the reaction more cleanly, such as (n,2n), in competition with fission.

- Data for safeguards and material accountability. Process streams in the fuel cycle, both front and back end, have large quantities of actinides that are potential proliferant materials. The challenge is to measure the input and output of these isotopes and to ensure that none are diverted. The measurement accuracy in this approach needs to be extremely accurate at each end (i.e., possibly better than 0.1%). This challenge is an opportunity for new approaches on how to measure the important actinides to such high accuracy.

- Measurements to support nuclear reaction modeling, which will improve the understanding of fission processes, neutron capture and (n,2n) reactions, surrogate reactions and the surrogate ratio technique, and use of shell model Monte Carlo techniques. Further investments will be required to carry out some of these activities for the AFC; for example, no facilities or experimental equipment currently exists for directly measuring the two neutrons in (n,2n) reaction studies.

- Measurements to support nuclear structure and decay R&D, including highly excited nuclear systems. Development of high efficiency 4π neutron and charged particle detectors, in conjunction with discrete high-resolution γ-detectors will be of considerable effectiveness for such a program. Upgrades for existing detector systems for such measurements should be explored. Dedicated measurements of decay properties of selected transactinide nuclei using pure, mass-separated sources along with state-of-the-art detector systems should be considered.

3. Group C: Nuclear Data

Nuclear data represents a bridge between basic nuclear sciences and advanced fuel cycle as well as Global Nuclear Energy Partnership applications. The U.S. nuclear data community's Cross Section Evaluation Working Group is currently completing development of a next-generation evaluated nuclear data library for nuclear science and technology, ENDF/B-VII. Nuclear data integrate a number of activities, including measurement of microscopic cross sections, nuclear reaction theory, statistical analysis, radiation transport physics, computer code and database development, processing of nuclear data, and fundamental and integral validation against experiments that include criticality and neutron transmission (shielding) measurements.

The new ENDF/B-VII library, to be released in December 2006, represents a major improvement over the ENDF/B-VI library released in 1990. An extensive paper on ENDF/B-VII that is under preparation [10] concludes that despite numerous improvements in the library, considerable challenges remain, of which probably the most important is to produce high-quality covariance data for neutron-induced reactions. This conclusion is well in line with the findings of the present workshop.

The working group established nuclear data priorities for AFC and GNEP applications considering two factors.

- AFC user requirements as formulated by M. Salvatores in his workshop plenary talk and as reiterated in the report of Group A

- Nuclear physics and nuclear data research topics that are in line with the mission of the DOE Office of Science

Covariance data were identified as the first priority. Other data needs are discussed in approximate order of decreasing priority. The underlying issues represent considerable opportunities and challenges to be addressed by nuclear physics research and nuclear data communities.

3.1 Covariance Data

A covariance matrix specifies uncertainties and correlations for a collection of physical quantities such as cross sections and average number of neutrons released per fission. The importance of covariances is twofold. First, they are required for design and operational optimization of AFC systems by correct assessment of uncertainties of integral quantities. Second, they are required for identification of data needs for these systems and subsequent planning of experiments as well as evaluation work. The error estimation of calculated quantities relies on the uncertainty information obtained from the analysis of experimental data and is stored as variance and covariance data in the basic nuclear data libraries such as ENDF/B-VII.

General properties of covariance matrices and early procedures for generating nuclear data covariances were widely discussed in the 1970s and 1980s. Accordingly, many of the existing covariance data were developed about 30 years ago for the ENDF/B-V library. This earlier activity languished during the 1990s because of the limited interest of the users and the constrained resources available to nuclear data evaluators. More recently, intensive interest in the design of a new generation of nuclear power reactors, as well as in criticality safety and national security applications, has stimulated a revival in the demand for covariances.

Table 3 shows the considerable lack of the covariance data in evaluated data libraries. Evaluation methodology must be developed and validated and covariance data produced for a large set of isotopes. To this end, nuclear cross-section evaluated data files need to be generated that incorporate uncertainties and correlations, for the actinides and other isotopes of interest. Such covariance data files need to be generated by using available experiments and nuclear theory modeling information, and methods need to be improved within radiation transport codes to utilize these data.

Table 3. Neutron cross-section covariance files in the ENDF/B-VI and ENDF/B-VII libraries.
Only quality data were migrated (13 files), and 13 new files were produced.

	ENDF/B-VI	**ENDF/B-VII**	**Comment**
Total number of files	328	393	
Files with covariances	48	26	13 new files in VII.0

The U.S. nuclear data community has started developing such capabilities, but currently these capabilities are still in their infancy. Much attention needs to be devoted to this area to bring this capability to fruition within ~2 years, to benefit reactor design work. Methods needed include Bayesian analysis approaches that can combine uncertainty information available from both small-scale fundamental experiment and theory, with integral constraints from integral experiments. This work can build on capabilities developed at the NNSA labs that have been important for the methodology known as quantification of margins and uncertainties.

Covariance data files need to be created for all isotopes, and they should be added into the ENDF/B-VII library. Major and minor actinides are the highest priority, but an initial coarse-grained approach should be used to obtain covariances for all isotopes (with an aggressive goal to produce the initial complete database within about one year—by the end of 2007). This goal could be achieved by building on the recently developed BNL-LANL covariance methodology for the entire neutron energy range, summarized in Fig. 8. At low energies this method uses uncertainties of the thermal values and resonance parameters from the recent *Atlas of Neutron Resonances* [11]; at higher energies the code EMPIRE [12] is used to produce sensitivity matrices. In the entire energy region the code KALMAN [13] is used to propagate uncertainties and generate correlations.
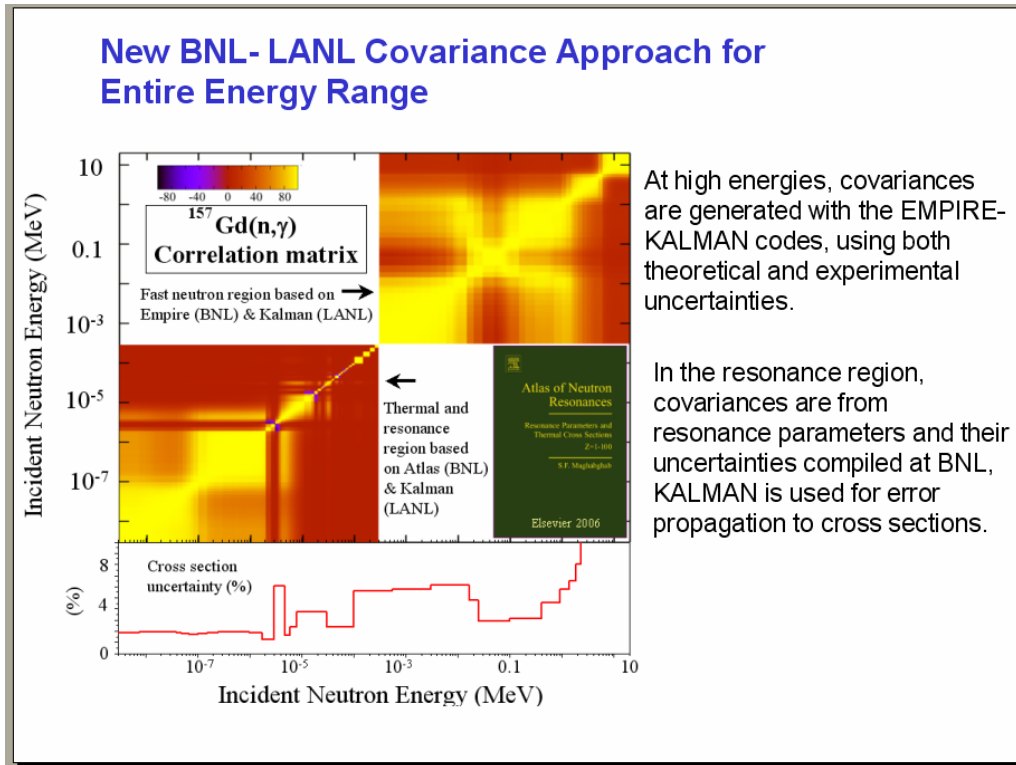
Fig.8. Summary of the recently developed BNL-LANL covariance methodology for the entire neutron energy range illustrated on the $^{157}Gd(n,\gamma)$ reaction.

Once crude covariances have been completed, they should be improved, until high-quality covariance data for ENDF/B-VII are produced, as shown in Fig. 9, which summarizes the recently prepared Covariance Vision of the U.S. Nuclear Data Program [14]. For major actinides, we should build on recent progress at LANL and ORNL. Of interest is also the Monte Carlo approach in the fast neutron region, proposed by Argonne and being pursued in Europe by Koning, as well as the ORNL retroactive method in the resonance region. For a simple estimate one could use the ORNL method based on integral data in the thermal and resonance region, although this is already superseded by a more complex BNL-LANL approach described above.

An important ingredient of the covariance work is processing of these data so that they can be used by application codes. To this end, the NJOY data processing code [15] needs to be extended to process covariances, including utilization of the ERRORJ module [16] to handle the resonance region. An alternative approach would represent the resonance processing code PUFF by ORNL [17].

Any future work on covariances will also build on extensive international collaboration. In particular, one was completed in 2005, and three international working groups on covariances are ongoing under the NEA Working Party on Evaluation Cooperation (WPEC).

- SG20, covariance methodology in the resonance region, chair T. Kawano, Los Alamos
- SG24, covariance methodology in the fast neutron region, chair M. Herman, Brookhaven
- SG26, nuclear data needs for Gen-IV reactors, chair M. Salvatores, Argonne
- SG27, processing of covariances in the resonance region, chair M. Dunn, Oak Ridge

Although in each of these groups the United States is playing a leadership role, Europe and Japan are making important contributions.

Covariance Vision

Proceed in 3 steps, adopt flexible approach, establish strong dialog with users, produce usable results in each step.

1. **1st year:** Produce crude, yet reasonable covariances for all nuclei in ENDF/B-VII.0 (Chadwick's idea, LANL), make results available via ENDF/A library, establish dialog with users, release in 2007.

2. **Next 2-3 years:** Improve all covariances so that they are of solid quality to justify their inclusion into ENDF/B-VII.1, release in ~2010.

3. **Next 4-5 years:** Produce quality results, include into ENDF/B-VII.2, release ~2015.

Manpower and cost
- 2-4 FTE scientists, 1-2 post-docs
- cost initially ~$0.9 mil, increasing to ~$1.8 mil in last years

Leverage
- Leverage from CSEWG and international effort (NEA Paris, IAEA Vienna)
- Expertise in databases and services, tailored to user needs

Fig. 9. Covariance Vision recently prepared by the U.S. Nuclear Data Program

3.2 Actinides

Accurate nuclear cross-sections are needed for precise simulations of nuclear criticality, transmutation rates, and radiation damage and heating. Some of the most important cross sections are still not known to the level of precision that are needed for AFC design, and the DOE Office of Science community has capabilities that can address this deficiency. The two main areas needed are major actinides and minor actinides.

3.2.1 Major Actinides

Improvement of Poor Thermal and Intermediate ^{239}Pu Criticality. Much of the ENDF/B-VII data testing points to weaknesses in ^{239}Pu data in the thermal (and possibly intermediate) region—K_{eff} are overpredicted significantly. Although very fast assemblies exist (e.g., Jezebel) that indicate our cross sections perform well in the high-energy region, there are very few lower-energy, more intermediate assemblies involving ^{239}Pu. Some assemblies in the ICSBEP benchmark book [18] in the intermediate region are also largely overpredicted. This situation suggests that for GNEP plans involving fast reactors with significant ^{239}Pu content, an improved ^{239}Pu evaluation is needed, possibly in the resolved and unresolved resonance regions.

^{239}Pu(n,γ) Reaction. ^{239}Pu(n,γ) is needed to less than 8% above about 1 keV. Our current covariance analysis provides covariance data indicating uncertainties of ~10–15% in this range, so more work is needed.

3.2.2 Minor Actinides

Theory Advances. Theory can be used to predict certain short-lived actinide fission and capture cross-sections. In particular, improved fission reaction model cross-section predictions are needed, to better determine cross sections where measurements are sparse and/or discrepant (e.g., [242m]Am). Advances in our understanding of the multidimensional fission potential (fission barrier), using macroscopic-microscopic and Hartree-Fock methods, will allow more accurate predictions for fission cross sections away from measured data (especially for minor actinides). Likewise, systematical trends of nuclear level densities both at equilibrium deformation, and at deformations typical of fissioning systems, will allow us to more accurately predict nuclear fission cross-sections off stability for chains of isotopes. This work builds on Office of Science nuclear data research where such models have been developed for nucleosynthesis models of r-process termination via fission. The nuclear reaction modeling codes within the DOE community will need to be extended to develop this improved predictive capability.
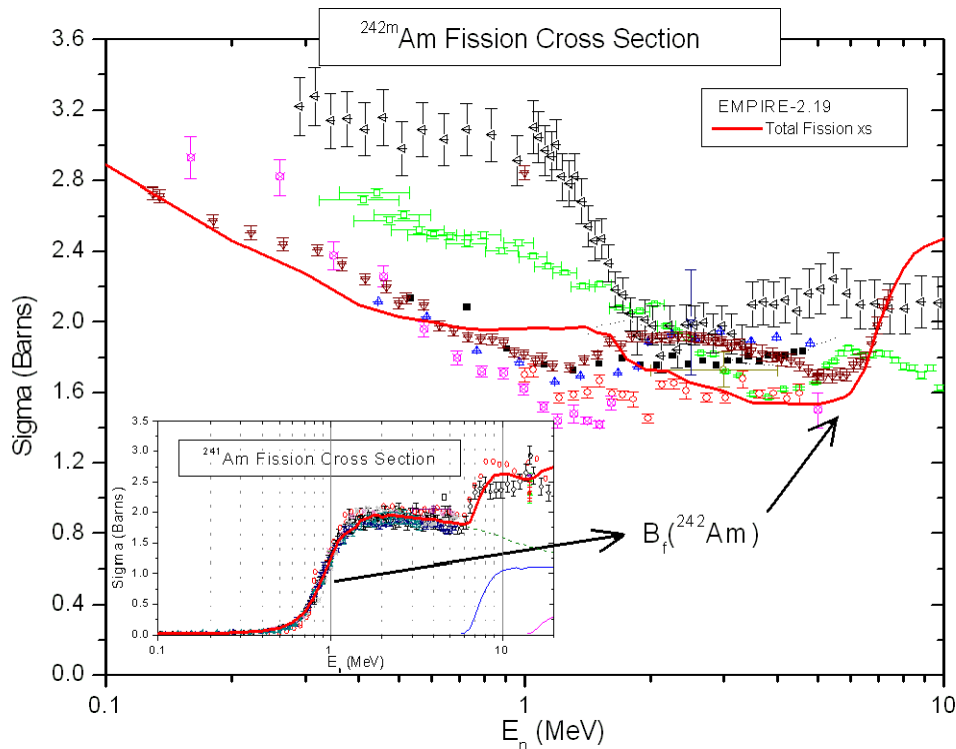
Fig.10. [242m]Am(n, fission) cross sections show considerable differences between experimental data and illustrate challenges faced by an evaluator to assess the best data.

Americium Data Improvements. [242m]Am fission and capture need improvements. Figure 10 illustrates challenges faced to produce recommended fission cross-sections on [242m] Am. The target uncertainties cited by Salvatores in the plenary session were significantly smaller than our current uncertainties, even with the recent evaluation work at Los Alamos for this isotope. Future work should build on the Los Alamos and Brookhaven reaction calculations and on planned measurements of capture and fission at the DANCE detector, using the target at Lawrence Livermore National Laboratory. The [241]Am capture reaction was also given high priority, and the target uncertainty Salvatores provided (~10%) requires additional modeling and experimental work.

Curium Data Improvements. ^{244,245}Cm data uncertainties appear to be important, but these isotopes have been ignored in the U.S. community in recent years. Future improved evaluations, especially of capture and fission and inelastic scattering, may be needed.

3.3 Computational Needs

The nuclear physics community has developed some sophisticated all-encompassing codes for predicting cross sections (EMPIRE, GNASH, etc.) that utilized input nuclear structure and reaction information (level densities, fission barriers, optical potentials, gamma-ray strength functions, etc.). The use of these codes often involves comparison with measured data, where available, in order to optimize the simulation predictions.

A Global Nuclear Data Initiative (GNDI) proposed by M. Herman (Brookhaven) would include a coupled set of codes (EMPIRE or GNASH, KALMAN, NJOY, MCNP, etc.) to allow global generation of nuclear data for all isotopes and all reactions, with optimization (global fitting) features that use fundamental measured data, as well as integral data (via MCNP simulations of integral experiments using the simulated cross-section data), to optimize the input model parameters used and thereby optimize the resulting evaluated database. The basic idea of GNDI, as illustrated in Fig. 11, is the following.

In the first loop, nuclear reaction modeling code such as EMPIRE is coupled to input parameter libraries and support databases such as the Reference Input Parameter Library (RIPL) [19], the Atlas of Neutron Resonances (Atlas) [11] and the EXFOR library of microscopic experimental cross sections [20]. This coupling allows one to obtain cross sections for the entire energy range of interest. Then, these cross sections are optimized by using the filtering code KALMAN. As the result, cross sections and their covariances are produced.

In the second loop, integral experiments are included. To this end, one has to employ a processing code such as NJOY, followed by simulation calculations with the code such as MCNP. Validation against integral experiments and optimization with the code KALMAN would allow the identification of deficiencies in microscopic data. This information would then be provided back to the first loop, input parameters would be adjusted and the procedure repeated.
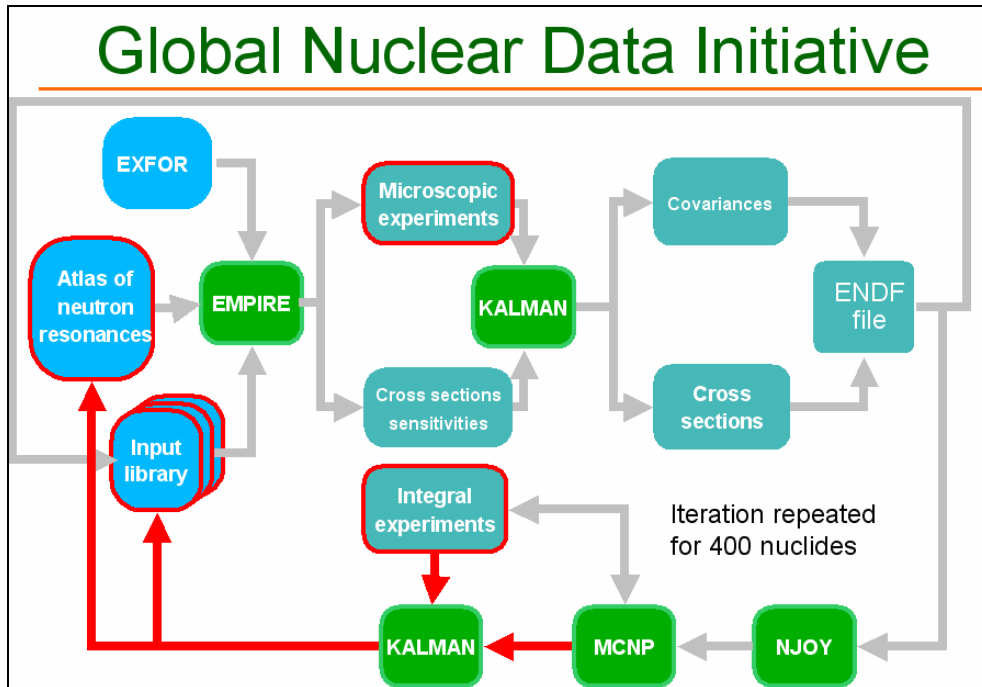
Fig.11. Global Nuclear Data Initiative couples available modeling tools, codes, input libraries, and databases to an integrated system for production of improved evaluated cross-sections.

Implementation of GNDI faces several challenges. Two involve the development of the two loops described above. A third challenge translates to the requirement that several support databases must be reviewed, improved, and maintained. On the top of this list is the library of experimental cross-sections, EXFOR. Here, the need for a thorough review, followed by removing of numerous deficiencies is the most pressing, and meeting this need will require an international effort. Also, the recently published *Atlas of Neutron Resonances* would benefit from an independent international review process. In addition, another important database, the Reference Input Parameter Library, for nuclear reaction model calculations will need continuing maintenance and inclusion of parameter uncertainties. A fourth challenge is the inclusion of high-precision measurements and related resonance parameter covariance analysis to produce refined covariances in the resonance region.

GNDI is an extremely exciting idea that potentially will bring huge benefits, but it will require high-end computation. An initial estimate is approximately 2,100 processors if one wants to make one iteration per week for a complete ENDF/B-VII library containing ~400 isotopes. Before the approach is usable in production mode, research is needed (and considerable CPU hours will be essential) to develop this capability.

3.4 Other Data and Activities

Integral Validation of Nuclear Data for AFC and GNEP. The new ENDF/B-VII library is performing extremely well in criticality benchmark applications. However, some deficiencies remain, mainly for Pu systems at intermediate and thermal energies. This situation is problematic for GNEP, which has a large Pu minor actinides fraction. New data testing is needed for GNEP for depletion inventories, reaction rates, and reactivity coefficients. A new publication of *Evaluated Reactor Physics Benchmark Experiments* [21] could be of help here.

Data Consolidation. There exists a need to put on a firmer basis several types of data of relevance to AFC, such as radioactive decay, delayed neutrons, fission yields and photon production. In particular, the following needs were identified.

- The new radioactive decay data library, recently produced for ENDF/B-VII by the NNDC, was used to calculate decay heat for ^{235}U and ^{239}Pu, indicating a deficit in gamma decay heat. Work on the library is needed to improve decay heat predictions as well as the decay of minor actinides of importance in AFC.

- Improvement in delayed neutrons is needed.

- Fission yields have not been improved in the ENDFB-VII library for more than 15 years, and an update would be desirable.

- Photon production has largely been neglected. Photons emitted in nuclear reactions are responsible for more than 10% of the heat released in power reactors. Current modeling techniques should be used to produce these data across the whole ENDF/B-VII library.

4. Group D: Nuclear Theory and Computations—Nuclear Reactions for the AFC Program

Neutron-nucleus cross sections, particularly in the heavy transuranics, rare actinides, and certain light elements, play an important role in determining reactor design and safety parameters. They are also inputs to reactor core design calculations. Neutron energies span orders of magnitude from the eV to the 20 MeV range, and therefore several reaction channels will be available for neutron-nucleus cross sections including resonant reactions, capture, (n,n′), (n,γ), (n,xn), and fission. While a number of these reactions can be studied experimentally, generally not all desired targets and energy ranges are assessable in the laboratory. Further, experiments tend to be labor intensive, time consuming, and expensive to perform. Thus, a more fundamental and accurate theoretical description of nuclear reactions would be beneficial to several DOE missions; in particular, the Advanced Fuel Cycle and Science-Based Stockpile Stewardship (SBSS) program and the basic science program supported by the Office of Nuclear Physics. Such an effort would remove the empiricism found in many reaction models and enable a predictive theory for calculating reaction cross sections. An enhanced theoretical effort will lead to accurate theoretical predictions (with their associated theoretical errors) that can provide a cost-effective basis for accurate reactor simulation and design that will also identify critical target nuclei that may require further investigation with experiment.

4.1 Scientific Challenges

Nuclear reactions play an important role in the science to be investigated in the physics of exotic nuclei, and in nuclear physics applications important to the SBSS and AFC programs. In the Nuclear Physics program of the Office of Science, current and future exotic beam facilities will study the properties of nuclei away from the valley of stability, with one goal to probe as close to the neutron drip line as possible. With such facilities, myriad new nuclear properties might be uncovered, such as disappearing shell closures. Furthermore, a future exotic beam facility will provide important data, such as masses and weak decay lifetimes, essential to understanding r-process nucleosynthesis, where neutron-capture on very exotic nuclei determines, in part, the elemental abundances. For AFC, certain key measurements or improvements in theory can significantly affect the reactor parameter uncertainties, which in turn will have major impact on cost of future reactors and their safety. For SBSS, an understanding of neutron-induced reactions is essential. For example, neutron-induced reactions on radio-chemical tracers in past underground tests provide important diagnostic information that can be used to calibrate modern simulation codes. In general, considerable overlap exists in the physics needs of laboratory nuclear physics, nuclear astrophysics, and the AFC and SBSS programs. In this regard, new theoretical developments utilizing leadership-class supercomputing coupled with a new generation of exotic beam facilities will provide a powerful new capability in the United States that will not only probe many unanswered questions about how nuclei are put together but will also provide new information important to astrophysics, AFC, and several NNSA supported programs.

The big picture for AFC and its relation to computing involves three key components. The first component involves theoretical calculations of cross sections. The second component is the feeding of nuclear theory to the nuclear data program. The third component addresses the application of Boltzmann transport, using the evaluated data, to model the core of a reactor. In this discussion, we focus on the cross section calculations.

Tying nuclear structure directly to nuclear reactions within a coherent framework applicable throughout the nuclear landscape is an important goal [22]. For light nuclei, ab initio methods hold the promise of direct calculation of low-energy scattering processes [23], including those important in nuclear astrophysics and tests of fundamental symmetries. In nuclear structure for heavier nuclei, the continuum shell model [24] and modern mean-field theories [25] allow for the consistent treatment of open channels, thus linking the description of bound and unbound nuclear states and direct reactions. On the reaction side, a better treatment of nuclear structure is equally crucial. The battleground in this task is the newly opening territory of weakly bound nuclei where the structure and reaction aspects are interwoven and the interpretation of future data will require advances in the understanding of reaction mechanisms.

At present, no single institution in the United States has either the expertise or the personnel to fully address the theoretical needs of a nuclear reactions program. There is a critical need to recreate a nuclear reactions capability within the United States, both at national laboratories and at the universities. The establishment of a national center combining the talents of several premier institutions is needed. The return from such an investment would be substantial, providing the United States with a renewed capability in nuclear structure and reactions that will provide several benefits:

- Solution to several outstanding and important problems in nuclear physics
- Foundation for establishing leadership in theoretical nuclear physics that will support future exotic beam facilities, NNSA programs, and AFC related efforts
- Enhancement of the AFC goals and mission
- Improvement of our understanding of the workings in the cosmos
- Infrastructure to train a new generation of scientists in a field important to the national interest

While practitioners in the nuclear physics and AFC communities might prefer verified experimental data, this situation is not always feasible. Complications arise from backgrounds due to the low event rates and screening due to atomic electrons. Similar to nucleosynthesis during the astrophysical s- and r-processes, radio-chemical diagnostics can trace a complex reaction network where capture (n,γ), inelastic scattering, fission, and nucleo-desynthesis $(n,2n)$ reactions can all occur on short-lived, exotic nuclei. Because of the short lifetimes for these target nuclei, many of these reactions are not amenable to direct measurement.

The present state of theory for the myriad relevant reactions is varied, but universally a comprehensive, picture based on the microscopic nature of nuclei is lacking. Present practice relies heavily on approximate theories that are empirically tuned to known data. Empirical tuning, while practical for nuclei where some information is available, diminishes the predictive power for these theories and introduces significant uncertainties into applications relevant for the exotic beam physics and the AFC programs. The primary reason for the present limited theoretical capability is that a proper treatment of the nuclear problem is complex and computationally daunting. Recent advances in computer technology, however, make it timely to take a fresh look at the theoretical program for low-energy nuclear structure and reactions. The complexity of the problem demands nothing less than a concerted effort to coordinate the research efforts between several subfields in nuclear physics and the computational sciences.

Applications of nuclear physics for AFC, and of overlapping interest for exotic beams, essentially fall into the category of reactions induced by neutrons with incident energies ranging from thermal to approximately 20 MeV. This broad range of energies will involve many nuclear processes, ranging from capture to neutron-induced fission. Neutron-induced reactions are quite complex and require new theoretical approaches for a successful description:

- **Optical Potential.** The optical potential is required to estimate the cross section for forming the compound nucleus as well as the transmission probabilities for particle emission. Present applications are excellent examples of empirical tools lacking a microscopic foundation, and hence predictive power when applied to nuclei away from region of normalization. This is a significant weakness because applications to exotic nuclei introduce significant uncertainties. At higher energy (> 50-100 MeV), microscopic formulations based on nucleon-nucleon interactions have been fairly successful. Microscopic formulations require detailed structure input with coupled channels, which has inhibited applications. The coupled channels problem involves iterative solutions to a large set of coupled integro-differential equations [26].

- **Statistical Decay.** Following the formation of the compound nucleus, depending on the open channels, the system decays by emission of particles and photons. For nuclei away from the drip line, the density of states is high enough that the decay path is statistical and is governed by transmission probabilities for particle emission, density of states l, and the gamma-strength function. The last two entries require detailed input from nuclear structure. As the system cools (or for compound systems near the drip line), rather than being statistical, the gamma decay-path is completely determined by nuclear structure. In many cases of interest, there are several isomeric states, whose population probabilities are due to explicit properties of the nucleus. The population and properties of these isomers are important because they themselves may act as a target for subsequent neutron reactions. The fact they have different properties than the ground state influences the reaction network and information inferred from the radio-chemical experiment. Complex structure models need to be developed and applied in order to predict (1) level densities (through Monte Carlo and other statistical approaches [27]), (2) gamma strength functions for statistical decays, and (3) decay paths for gammas at low excitation energy. Reaction networks also involve the solution of large sets of coupled differential equations.

- **Pre-equilibrium Reactions.** At higher incident neutron energies (>8 MeV) there is a significant chance that the system will decay by neutron emission before "thermalizing" into the compound system. This has important consequences because following pre-equilibrium emission the nucleus has less energy and less angular momentum transferred to it. This can affect isomer production and fission probabilities. In addition, the neutron emission spectrum is harder, that is, composed of higher energy neutrons. Most models do not include many microscopic effects and again utilize empirical components that inhibit predictive power. Microscopic models, for example those of Feshbach, Kerman and Koonin [28], Tamura, Udagawa, and Lenske [29], or Nishioka, Weidenmuller, and Yoshida [30], are complex and computationally intensive and need to be fully developed and integrated into the complete reaction formalism.

- **Fission.** No predictive model for fission exists. Simple models based on barrier penetration can be successful but lack predictive power. Basically, they can be tuned to reproduce known data, and hence be applied to model another channel. Here, a dynamical model describing the large-amplitude collective motion leading to fission that relies on microscopic structure for the energy surfaces and dynamical mass needs to be developed and applied. Microscopic models based on static or time-dependent generator coordinate (GCM and TDGCM [31]) methods might be promising. These methods, however, are computationally intensive. They will require realistic nuclear density functional calculations in three-dimensions as well as couplings with at least one-particle, one-hole excited states. Furthermore, the GCM equations need to be solved in several dimensions

for the collective coordinates involved in fission. Once again, iterative solutions of nonlinear coupled differential equations are required for numerical implementation. Good progress is being made on predictions of fission barriers and should continue to be pursued [32].

- **Direct, Nonstatistical Reactions**. For light nuclei and those near the neutron drip line, or shell closures, the density of states near the neutron-separation energy is low and the compound nucleus hypothesis is not valid. In this case, inelastic reactions occur through a more direct process, in which explicit properties of the target are probed and excited. A more comprehensive coupled-channels (coupled nonlinear integrodifferential equations) approach where the potential is derived from the nuclear densities and an effective NN interaction needs to be employed. Once again, detailed information about the structure of the individual states is required. Computationally, this area requires the solution of large eigenvalue problems.

Clearly, a number of areas in the field of nuclear structure and reaction theory require both theoretical and numerical developments to make progress. The benefits to the AFC program and nuclear theory generally will be substantial. Today, much of reaction theory rests on empirical data fitting and consequently lacks predictive power.
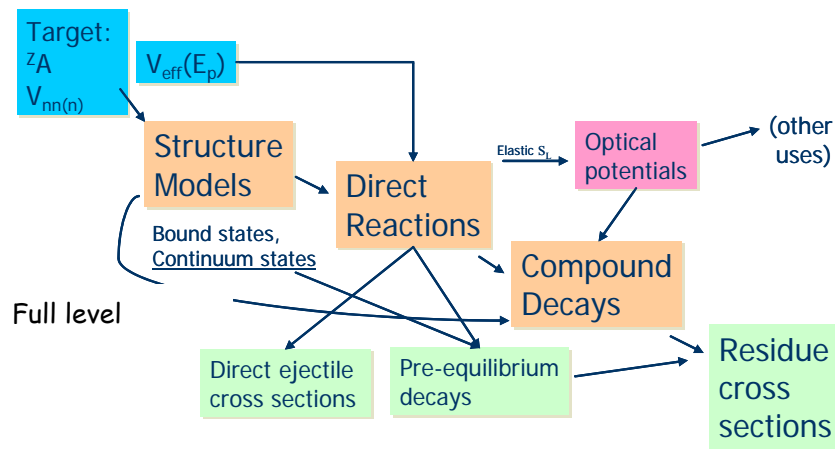
Fig. 12. Computational calculations and various connections among various reaction channels (supplied by I. Thompson, LLNL)

Development of the next generation of reaction theory will seek to overcome this limitation. The requirements for success include developments of a new generation of theoretical tools and several new computational codes developed for modern computational platforms. Figure 12 indicates how the theoretical tools need to be developed in order to successfully predict cross sections. One begins with information on the desired target and energy range, calculates the necessary nuclear structure information, feeds that into both direct and compound reaction models, and develops from the structure calculations both level density and optical potential information. Various aspects of this information are then used as input to the compound decay calculations. The final result is information on the cross section for a given reaction.

Computationally, three major thrusts are involved in this figure. The first involves solving the nuclear density functional equations including pairing correlations. Excellent codes exist that already break symmetries and can be used to generate structure information [33]. One area of research is to fine-tune the nuclear energy density functional. Optimization of the functional, including tensor and terms, will require substantial calculations across the chart of nuclei. These calculations are naturally parallel and will require several million processor hours over the next few years in order to optimize the energy density functional, which will also include time-odd terms associated with odd-mass nuclei. Through constrained calculations, one can use such codes to predict relative fission barriers.

Computation of the nuclear optical potential based on the energy density functional and including correlations beyond the mean-field level will require a solution of a Lipmann-Schwinger equation that includes appropriate boundary conditions on the scattering wave functions. Physics beyond the mean field will come into play through particle-hole excitations from mean-field solutions. The solution of such equations requires Krylov space implementations for Hamiltonian diagonalization to obtain the appropriate particle-hole states. One might also envision performing small-amplitude perturbations of the mean-field to obtain the one-particle-one-hole solutions although at higher energies, multiparticle-multihole excitations also play a role. Other extensions might be in the direction of coupled-cluster implementations of scattering. Initial work using complex basis states in shell-model diagonalization codes shows promise for expansions to calculations of doorway states and other inputs that will enable improvements of nuclear optical potentials and coupled-channel reactions calculations. Current Gamow shell model technology adapted to parallel computational platforms would be a viable avenue to incorporate such door-way states into calculations of the optical potential. Any of the methods that require solution to an eigenvalue problem should be able to take advantage of emerging parallel architectures, although to date parallel codes have only been built that solve the bound nuclear structure problem (in a standard nuclear shell-model format with Hermitian interactions).

The level density is another input to cross-section calculations. Quantum Monte Carlo algorithms have been developed to calculate the nuclear level density for a given Hamiltonian. The auxiliary field Monte Carlo (AFMC) approach readily yields the energy of the system as a function of temperature in the canonical ensemble. One then computes the level density by use of either the saddle-point approximation or maximum-entropy reconstruction methods. Projection of symmetries such as parity, angular momentum, partial densities, and isospin can also be achieved in the AFMC method [34,35,36]. A limitation of the AFMC method is the fermionic sign problem, and first studies will be limited semi-realistic pairing plus multipole-multipole interactions [37] that are free from this problem. Calculations of level densities require several thousand processors and several hours to obtain enough statistics for a reasonable description of the level density for a particular nucleus. Projection techniques (to obtain parity and/or angular-momentum projected states) increase the needed cycles modestly. The per-processor memory requirement of the AFMC code is less than two gigabytes for nuclei of AFC interest.

Another very important aspect of a theoretical reactions project is to create an integrated set of code tools for the description of neutron-nucleus cross sections. At the present time no such package exists. It would be important to create, following Figure 14, a computational framework (a COMPUtational Nuclear EnvironmenT, or COMPUNET) that would provide a common, integrated toolset for use by other communities involved in the AFC project that have an interest in calculating theoretical nuclear cross-sections. Such an effort could be built on the Common Component Architecture [38] with appropriate additional infrastructure for this community.

Important computer science contributions to this process will include the development of parallel eigenvalue solvers for low-memory/processor machines (such as the Blue Gene/P), uncertainty

propagation through large systems of ordinary differential equations, and scalable sparse linear system solves (e.g., conjuagant gradient methods for neutronics). These needs are also cross cutting and have representation within the current ASCR SciDAC programs.

4.2 Scientific Opportunities

The key feature of a relevant nuclear theory effort that will enhance AFC, NNSA, and basic studies of nuclei involves removing empiricism from current nuclear structure and reaction models. The result will be a theoretical capability that has predictive power and that enables one to make a reasonable assessment of the range and validity of these calculations. In most instances today, very crude models are all we have, with myriad adjustable parameters that lose meaning when one is in regions where sufficient data (or sufficiently constrained data) do not exist. A 5–10 year rebuilding of the nuclear reaction theory in the U.S. is foreseen that will address the needs of AFC encompassed in the five areas discussed above. While some of these efforts are being addressed elsewhere, there are clearly very significant gaps in both theoretical and computational developments. Two areas of agreement resulted from discussion. The first area calls for enhancing advanced nuclear theory training, akin to the proposal presented from the measurements working group (Appendix 7):

- Establishment of a graduate fellowship program specifically to train the next generation of students in computational nuclear science. This program would be in collaboration with ASCR and should combine training in computational sciences and nuclear reaction theory. Such expertise is lacking today and needs to be developed through graduate student training.

- Establishment of postdoctoral fellowship grants to address specific areas of reaction theory discussed above. Initially, two such grant awards per year would be appropriate. Such grants would also include standard summer support for university professors (or a small FTE support for Laboratory staff). These competitively awarded grants would be targeted toward theoretical developments and calculations of nuclear reaction cross sections relevant to the AFC program as outlined above.

- Enhanced funding in the NP theory base funding for nuclear structure and reaction theory development. Currently, reaction theory that would be relevant to AFC is not well funded under the base NP theory program. A concerted effort is needed to address this issue in order to have a sustainable program in nuclear reactions relevant to the AFC.

The second area calls for a cross-cutting effort between the nuclear science and engineering communities and computational scientists:

- Formulation of a framework approach that will bring together all reaction-code components (as outlined in Figure 12) under one computational umbrella. This would enable the group of scientists who will utilize these codes to map a strategy for common input and output data files, common language interfaces, and common algorithms. This framework may primarily need ASCR funding in order to be implemented, with some effort coming from nuclear theory to define the appropriate interfaces.

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Acronym List

ABTR	Advanced Burner Test Reactor
AFC	Advanced fuel cycle
AFCI	Advanced Fuel Cycle Initiative
AFMC	Auxiliary field Monte Carlo
ASCR	Advanced Scientific Computing Research
BUC	Burnup credit
CSEWG	Cross Section Evaluation Working Group
DOE	Department of Energy
ENDF	Evaluated Nuclear Data File
FP	Fission product
GNDI	Global Nuclear Data Initiative
GNEP	Global Nuclear Energy Partnership
IAEA	International Atomic Energy Agency (Vienna)
ICSBEP	International Criticality Safety Benchmark Experiments Project
INL	Idaho National Laboratory
IPNS	Intense Pulsed Neutron Source
JAEA	Japan Atomic Energy Agency
NE	Nuclear Energy
NEA	Nuclear Energy Agency (Vienna)
NNDC	National Nuclear Data Center (Brookhaven)
OECD	Organization for Economic and Cooperative Development
R&D	Research and Development
RIPL	Reference Input Parameter Library
RPI	Rensselaer Polytechnic Institute
SBSS	Science-Based Stockpile Stewardship
SNF	Spent nuclear fuel
TA	Transactinide
TPC	Time propagation chamber
WPEC	Working Party on International Nuclear Data Evaluation Cooperation

Appendixes

Appendix 1. Charge to the Workshop

Dr. Lee Schroeder
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Dear Dr. Schroeder and Dr. Lusk:

Thank you for agreeing to organize and co-chair a workshop on "Nuclear Physics and Related Computational Science R&D Research Contributions to for Advanced Fuel Cycles the Global Nuclear Energy PartnershipAdvanced Fuel Cycle Initiative. (AFCI) R&D Program" As you may know, the President's Nuclear Physics Budget for FY 2007 contains funding to support research efforts that are also relevant to the design of next generation nuclear reactors. This research can help to provide the nuclear data and knowledge required for advanced nuclear fuel cycles, and the related modeling and computing efforts. Funding has been provided in both the Low Energy subprogram and the Nuclear Data programs within the Office of Nuclear Physics (NP), and in the Office of Advanced Scientific Computing Research (ASCR). The development of advanced fuel cycles (AFCC) is a high priority within the President's budget and we believe ONP and OASCR Nuclear Physics have important roles in this effort.

The purposes of the Workshop are to determine what nuclear physics R&D is needed for the AFC, to determine whether and how those needs can be met within our existing programs, to determine what facilities are appropriate for this research, and to identify the computing resources required for modeling and simulation. It is anticipated that the workshop will provide some overview of the overall AFC research. Thus, time should be allowed for general presentations of the AFC research and of the overall R&D needs of the program. We believe the Workshop should cover at least the primary areas of: AFC overview, nuclear data, nuclear measurements, and and nuclear theory and computing, as they apply to the AFC R&D needs.

We request that a written report be prepared by the co-chairs and a panel of several nuclear physics researchers, and reactor scientists and those utilizing computers for modeling and simulation in the nuclear physics arena. The report should address the four areas noted above along with guidance for implementation of the R&D program and answer such questions as: what are the specific needs of the AFC I for nuclear physics R&D, does the nuclear physics program have the tools needed to properly address the perceived R&D needs, is the existing nuclear data program database adequate for the AFC needs, what computational effort should be undertaken to provide theoretical and calculational support for the measurements, and are additional investments in existing nuclear physics facilities needed to carry out the R&D?

The workshop will be held August 10-12, 2006 at the Hyatt Regency Hotel in Bethesda, MD. Gene Henry (gene.henry@science.doe.gov), Division Director for Physics Research and Gary Johnson (gary.johnsonn@science.doe.gov), Program Manager for Advanced Scientific Computing Research will be the contacts in our office to work with you to provide support for the organization of the workshop as necessary.

We believe the workshop is an important step in our efforts to provide fundamental nuclear physics support to an important new energy initiative. Thank you again for agreeing to help.

Sincerely,

Dennis Kovar   Michael Strayer

Appendix 2: Agenda for the Plenary Sessions of the Workshop

Thursday August 10, 2006 (Day 1—Plenary Session, Haverford/Baccarat Ballroom)

7:30 a.m.   Registration and Continental Breakfast (outside Ballroom)

8:30 a.m.   Welcome/Introduction— Lee Schroeder (LBNL) and Ewing Lusk (ANL)

8:45 a.m.   Goals of the Workshop—DOE

                   Dennis Kovar (Office of Nuclear Physics)
                   Michael Strayer (Office of Advanced Scientific Computing Research)
                   Kirk Levedahl (Office Nuclear Energy and Technology)

OVERVIEW TALKS

9:15 a.m.   The Global Nuclear Energy Partnership—David Hill (INL) [35+10]

10:00 a.m.   BREAK

10:30 a.m.   Advanced Fuel Cycles and R&D Needs—Massimo Salvatores (ANL)
                   [45+15]

11:30 p.m.   Nuclear Measurements—Tony Hill (LANL) [22+8]

12:00 p.m.   LUNCH

CONTINUE OVERVIEW TALKS

1:30 p.m.   Nuclear Facilities and Instrumentation—Paul Koehler (ORNL) [22+8]

2:00 p.m.   Nuclear Data—[45+15]
                     Part 1: New ENDF/B-VII Library—Pavel Oblozinsky (BNL)
                     Part 2: Actinides, convariances, neutronics—Mark Chadwick (LANL)

3:00 p.m.   Perspectives from DOE—Ray Orbach (Under Secretary for
                   Science and Director of the Office of Science)

3:30 p.m.   BREAK

4:00 p.m.   Sensitivity/Uncertainty Methods for Fuel Cycle Analysis—Mark
                   Williams (ORNL) [22+8]

4:30 p.m.   Aspects of Nuclear Theory for AFC—David Dean (ORNL) [22+8]

5:00 p.m.   Computational Resources for AFC—Ewing Lusk/Andrew Siegel (ANL)
                   [22+8]

END OF FORMAL PRESENTATIONS

5:30 p.m.   'Open Mike'—Participant Comments

6:15 p.m.   Charge to working groups (co-chairs + panel members)

6:30 p.m.   Adjourn for Individual Dinners + 1st meeting of Working Groups

Friday August 11, 2006 (Day 2—Individual Working Group Meetings, Conference Level—individual meeting room TBA)

7:30 a.m.   Late Registration and Continental Breakfast (on Conference Level)

8:30 a.m.   Begin individual working groups (room assignments on Conference Level, see below)

- Group A—NP/ASCR Needs for AFC (Diplomat Room)
- Group B—Nuclear Measurements (Judiciary Suite)
- Group C—Nuclear Data (Congressional Room)
- Group D—Nuclear Theory/Computations (Ambassador Room)

10:30 a.m.   Break (all groups)

11:00 a.m.   Continue Working Groups

12:00 p.m.   Lunch

1:00 p.m.   Continue Working Groups

3:00 p.m.   Break

3:00 p.m. to 6:15 p.m. (Plenary Session—WG Reports, Haverford/Baccarat Ballroom)

- Report from Needs Working Group (A)
- Report from Nuclear Measurements Working Group (B)
- Report from Nuclear Data Working Group (C)
- Report from Nuclear Theory/Computations Working Group (D)
- Final Comments (co-chairs) and end of general workshop

Saturday August 12, 2006, (Day 3—Draft Writing and Close Out, Congressional Room on Conference Level)

8:30 a.m.   Further discussions with panel leaders, including comments/questions on charge from DOE

8:45 a.m.   Panel leaders prepare draft report on their working area

11:00 a.m.   Close out discussions with DOE

12:00 p.m.   End and Close Out

Appendix 3: Agendas of the Parallel Working Groups

Group A: R&D Needs of the AFC

ABTR Core Design Summary, M. Cappiello
Sensitivity and uncertainty analysis with the ERANOS code system, M. Salvatores
Overview of TSUNAMI, Mike Dunn
Data Needs to Support the Development of Fuel and Materials Performance Modeling and Simulation, Mike Todosow
Material Accounting Challenges for the Advanced Fuel Cycle, Potential Nuclear Measurements and Attendant Data Needs, Alan Hunt

Group B: Measurements

Thursday August 10, 2006
6:00 – 7:00 pm   Informal working group meeting to discuss general
                           organization—same ballroom as plenary session

Friday, August 11, 2006   Room will be announced at workshop

8:30   Introductory Remarks and Working Group Objectives—**Mike Dunn (ORNL)**

8:35   Advanced Fuel Cycle Data Needs
             • **Lead Speaker: Eric Pitcher (LANL)**—15 minutes
             • Group Discussion—10 minutes

9:00   Measurement Facility Review
             • **Lead Speaker: Paul Koehler (ORNL)**—5 minutes
             • Group discussion—5 minutes

9:10   Direct neutron measurements—Techniques/Instrumentation
             • **Lead Speaker: Tony Hill (LANL)**—10 minutes
             • Jerry Cole (INL)—10 minutes
             • John Becker (LLNL)—10 minutes
             • Bob Block (RPI)—10 minutes
             • Klaus Guber (ORNL)—10 minutes
             • Tom Massey (Ohio University)—10 minutes
             • Jeff Vanhoy (US Naval Academy/University of Kentucky)—10 minutes
             • (TUNL)—10 minutes
             • Group discussion with AFC R&D recommendations—15 minutes

10:45   Coffee Break

11:00   Surrogate and other charged particle reaction measurements—
           Techniques/Instrumentation
             • **Lead Speaker: Jutta Escher (LLNL)**—20 minutes
             • Lee Bernstein (LLNL)—10 minutes
             • Jolie Cizewski (Rutgers University)—10 minutes
             • 1 additional speaker contribution from floor—10 minutes
             • Group discussion with AFC R&D recommendations—10 minutes

12:00   Lunch

1:00   Nuclear Reaction Models
- **Lead Speaker: Mark Chadwick (LANL)**—15 minutes
- Gary Mitchell (TUNL)—10 minutes
- Group discussion with AFC R&D recommendations—5 minutes

1:30   Structure and Decay Properties
- **Lead Speaker: Filip Kondev (ANL)**—20 minutes
- Alejandro Sonzogni (BNL)—10 minutes
- 2 additional speaker contributions from floor—20 minutes (10 minutes per speaker)
- Group discussion with AFC R&D recommendations—10 minutes

2:30   Wrap-up Panel Discussion and Summary of Recommendations

                Panel:
- **Mike Dunn (ORNL)**
- **Con Beausang (University of Richmond)**
- **Bob Haight (LANL)**

3:00   End Working Group Session

Group C: Nuclear Data

Friday, August 11

Note: Speakers should, where appropriate, include comments on how high-performance computing can open up new opportunities.

08:30 – 10:30

1. Introductory comments
   - Comments by Chadwick, LANL, 5'
   - Comments by Oblozinsky, BNL, 5'

2. Neutron cross section data
   - Improved cross sections for major actinides, Chadwick, LANL, 20'
   - Reduced uncertainties for minor actinides, Kawano, LANL, 10'
   - Improved cross sections for other materials
     - Zr data: New capabilities and future needs, Herman, BNL, 10'

3. Covariance data
   - Covariance data in ENDF/B-VII, D. Smith, ANL, 10'
   - Covariance tools
     - Resonance region: ORNL method, Larson, ORNL, 10'
     - Resonance region: BNL-LANL method, Rochman, BNL, 10'
     - Fast neutron region: BNL-LANL method, Herman, BNL, 10'
   - International effort and covariance vision, Oblozinsky, BNL, 10'

11:00-12:00

4. Other data
   - Decay data library in ENDF/B-VII, Sonzogni, BNL, 15'
   - Post-scission fission physics data, prompt and delayed neutrons, gammas and fission products and their energies, Bonneau, LANL, 15'
   - Cross sections for gas production, recoils and damage, Haight, LANL, 10'

12:00-01:00 Lunch Break

01:00-03:00

5. Quality assurance, processing, dissemination
   - Integral validation and quality assurance, Kahler, LANL, 15'
   - Performance of ENDF/B-VIIb2 for a series of diverse ZPR/ZPPR assemblies, McKnight, ANL, 10'
   - Processing of covariances in the resonance region, Dunn, ORNL, 10'
   - Processing codes development, Kahler, LANL, 10'
   - Data dissemination, Sonzogni, BNL, 5'

6. Topics relevant for high-performance computing
   - Global Nuclear Data Initiative, Herman, BNL, 15'
   - Nuclear reaction model codes development, Kawano, LANL, 10'

7. Concluding discussion
   - Comments, all
   - Summary and conclusions, Chadwick, LANL, 5'

Group D: Nuclear Theory and Computations

8:30 Opening remarks for breakout session

8:45 Erich Ormand (LLNL) -- Hauser-Feshbach today: what it takes to calculate a cross section using current technology

9:15 Ian Thompson (LLNL) -- Specific improvements to reaction theory

9:45 Witek Nazarewicz (U. Tennessee): Modern approaches to fission

Break

11:00 Jean Ragusa (Texas A&M): Overview of reactor core neutron transport codes

11:30 Massimo Salvatores (ANL): Impact of cross-section uncertainties on reactor core calculations
12:00 Lunch

1:30 W. Shelton (ORNL): Computational DFT in atoms and molecules -- thoughts on large scale DFT computations

2:00 Discussion/Slide preparation

3:30 Adjourn

Appendix 4: List of Workshop Cochairs and Working Group Leaders

Workshop co-chairs: Lee Schroeder (Lawrence Berkeley National Laboratory) and Ewing Lusk (Argonne National Laboratory)

Group A: Michael Cappiello (Los Alamos National Laboratory), Thomas Downar (Purdue University), William Martin (University of Michigan), Max Salvatores (Argonne National Laboratory)

Group B: Con Beausang (University of Richmond), Michael Dunn (Oak Ridge National Laboratory), Robert Haight (Los Alamos National Laboratory)

Group C: Mark Chadwick (Los Alamos National Laboratory), Pavel Oblozinsky (Brookhaven National Laboratory)

Group D: David Dean (Oak Ridge National Laboratory), Andrew Siegel (Argonne National Laboratory)

Appendix 5: Participant List

Last Name	First Name	Institution
Ahle	Larry	LLNL
Ai	Ho-Chiang	Yale U
Anitescu	Mihai	ANL
Aryaeinejad	Rahmat	INL
Baglin	Coral	Berkeley
Baktash	Cyrus	ORNL
Beausang	Con	U of Richmond
Beck	Sharon May-Tal	NRC-Negev, Israel
Becker	John	LLNL
Beise	Elizabeth	NSF
Bernholdt	David	ORNL
Bernstein	Lee	LLNL
Bertrand	Fred	DOE/NP
Bleuel	Darren	LBNL
Block	Robert	RPI
Boger	John	DOE/GNEP
Bonneau	Ludovic	LANL
Budnitz	Bob	LLNL
Burke	Jason	LLNL
Burrow	Richard	DOE/BES
Cappiello	Mike	LANL
Carlson	Donald	NRC
Chadwick	Mark	LANL
Cizewski	Jolie	Rutgers
Clark	Rod	Berkeley
Cole	Jerry	INL
Coon	Sidney A.	DOE/NP
Dean	David	ORNL
Diachin	Lori	LLNL
Downar	Tom	Purdue
Dunn	Mike	ORNL
Escher	Jutta	LLNL
Farkhondeh	Manouchehr	DOE/SC
Felty	James	DOE/NNSA
Geesaman	Donald	ANL
Goldner	Frank	DOE
Gomes	Itacil	I.C. Gomes Consulting
Greife	Uwe	CO School of Mines
Guber	Klaus	ORNL
Haight	Bob	LANL/LANSCE
Hartouni	Ed	LLNL
Henderson	Douglas	U of Wisconsin-Madison
Henry	Eugene	DOE/NP
Henshaw	Bill	LLNL
Herczeg	John	DOE/NE
Herman	Mike	BNL

Hill	Dave	INL
Hill	Tony	LANL
Hoole	Jeffrey	KAPL Inc.
Hough	Patricia	SNL
Howell	Calvin	TUNL/Duke U
Hunt	Alan	Idaho State U
Ingram	David	Ohio U
Ishikawa	Makoto	JAEA, Japan
Iverson	Erik	ORNL
Johnson	Gary	DOE/SC
Joo	Kyungseon	U of Connecticut
Kahler	Albert	LANL
Karwowski	Hugon	UNC
Kawano	Toshihiko	LANL
Kelley	John	NCSU/TUNL
Khan	Ehsan	DOE/SC
Kikuchi	Shin	Embassy of Japan
Koehler	Paul	ORNL
Kondev	Filip	ANL
Kouzes	Richard	PNNL
Kovar	Dennis	DOE/NP
Kreisman	Norman	DOE/SC
Kugo	Teruhiko	JAEA, Japan
Larson	Nancy	ORNL
Lee	John	U of Michigan
Lesher	Shelly	U. of Richmond
Levedahl	Kirk	DOE
Libby	Steve	LLNL
Lister	Kim	ANL
Lusk	Ewing (Rusty)	ANL
Mailhiot	Christian	LLNL
Martin	William	U of Michigan
Massey	Thomas	Ohio U
McKnight	Richard	ANL
Mitchell	Gary	NC State U
Morss	Lester	DOE/BES
Nazarewicz	Witold	U of Tennessee/ORNL
Mertyurek	Ugur	Global Nuclear Fuel, GE
Nigg	David	INL
Nitsche	Heino	UC Berkeley
Nolen	Jerry	ANL
Nowak	David	ANL
Oblozinsky	Pavel	BNL
Ormand	Erich	LLNL
Page	Philip	LANL
Parks	Cecil	ORNL
Perry	Dale	LBNL
Pierpoint	Lara	DOE/NE (Intern)
Petrovic	Bojan	Westinghouse Electric Co.
Pitcher	Eric	LANL

Raap	Michaele	PNL
Ragusa	Jean	Texas A&M
Rai	Gulshan	DOE/SC
Rearden	Brad	ORNL
Reed	Phillip	NRC
Roche	Kenneth	ORNL
Rochman	Dimitri	BNL
Rundberg	Robert	LANL
Saito	Earl	GE/Nuclear
Salvatores	Massimo	ANL
Sanchez	Lawrence	SNL
Savage	Buzz	DOE
Schröder	Udö	U of Rochester
Schroeder	Lee	LBNL
Shelton	William	ORNL
Siegel	Andrew	ANL
Smith	Donald	ANL
Sonzogni	Alejandro	BNL
Springer	Paul	LLNL
Strayer	Michael	DOE/SC
Symons	James	Berkeley
Thompson	Ian	Surrey (LLNL)
Tippens	Brad	DOE/SC
Todosow	Mike	BNL
Tulenko	James	Florida State
Turinsky	Paul	NCSU
Uddin	Rizwan	U of Illinois
Vanhoy	Jeffrey	US Naval Academy
Vetter	Jeff	ORNL
Ward	Thomas	Techsource Inc.
Wender	Stephen	LANL
Werner	Volker	Yale U
Westfall	Mike	ORNL
Williams	Mark	ORNL
Wilson	Paul	Wisconsin
Yedvab	Yanai	NRC - Israel
Young	Glenn	ORNL

Appendix 6: Cross-Cutting Educational Proposal

A common theme in the working group discussions is the need for better connections between universities and national laboratories to train the next generation of nuclear scientists (nuclear and radiation chemists and nuclear physicists). It is alarming that universities keep having serious difficulties attracting students to the field of nuclear science.   The national laboratory representatives confirmed the university concern by noting that the best nuclear physics job candidates are often recruited from institutions outside the United States. As has been pointed out in the plenary session, because of the sustained difficulty to attract students to the field of nuclear science, the U.S. has already lost one generation of nuclear scientists. However, discussion at the workshop revealed a much deeper issue. The U.S. is also on the verge of losing the university faculty that would be able to train the next generation of nuclear scientists. Nuclear and radiation chemistry has essentially disappeared from U.S. university faculty ranks. Nuclear Physics is likely to follow the same path. The essentials of nuclear science are no longer taught in the undergraduate curriculum, and only a handful of graduate programs in nuclear science are left at U.S. universities.

Given these concerns, the university participants noted that U.S. universities need to be actively recruited to reestablish nuclear science programs. They will have to be convinced of the national necessity to attract new faculty who can train the next generation of nuclear scientists. Because of the vigorous competition for brainpower by fashionable fields associated with bio-oriented and material sciences, there needs to be an aggressive effort to establish scholarships and fellowships to support faculty and students, respectively, in nuclear science research areas. Such efforts are required to:

- Educate the next generation of nuclear scientists,
- Advance basic science R&D, and
- Sustain the AFC development.

Scholarships and fellowships should be available to both nuclear science and nuclear engineering students.

To address some of the nuclear science educational needs, Prof. Jolie Cizewski (Rutgers University) presented a proposal to establish a Prestigious Fellowship program for nuclear students that would have the following tenants:

- Targeted applicants
  - Senior undergraduates or first year graduate students
  - U.S. citizens or permanent residents
  - Applicants must demonstrate a commitment to the nuclear science or energy field
  -
- General program structure
  - 1st year of fellowship = 1st year of award (1st or 2nd year of Ph.D. studies)
  - In the first summer of fellowship, initiate research in basic nuclear science that could have importance to AFC
  - In 2nd year of the fellowship, the student could have the opportunity spend extended time (e.g., 6-12 months) performing research at a national laboratory
- Cost
  - 6 fellowships/year in steady state
  - $45k/fellow ($30k stipend; $15k educational expenses)
  - Total annual fellowship cost $270k/year

The proposed fellowship program would encourage students to perform research in the field of nuclear science and provide a mechanism to strengthen university and national laboratory collaborations.

One area of research that does attract students and that universities are trying to grow is nuclear astrophysics. Some of the oft-mentioned branch point nuclei in s-process astrophysics are also long-lived fission product, and their further reactions with neutrons can be important in reducing radioactive waste from nuclear energy. Neutron capture cross sections are almost always calculated for these nuclides because of the lack of experimental data. However, surrogate reactions as well as direct measurements, now possible with 4π γ-ray calorimeters (see figure below), open up new opportunities.
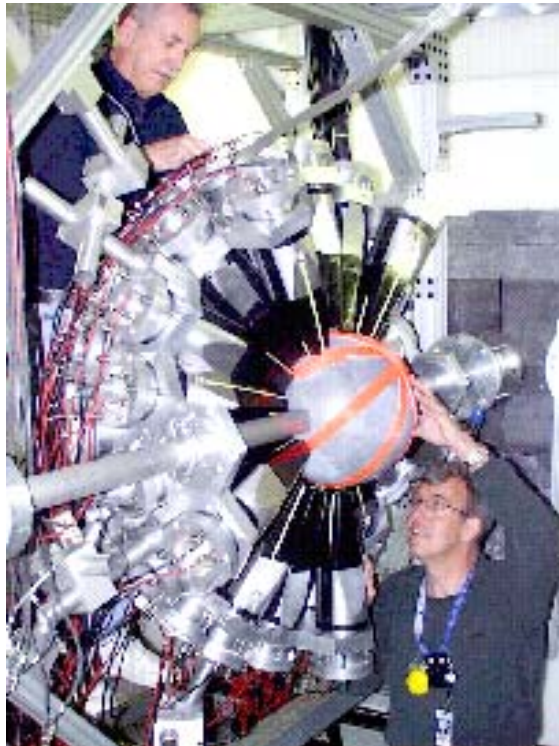
The DANCE 4π calorimeter at LANSCE is used to measure neutron capture cross sections on small samples including radioactive nuclides of importance to reactors and to s-process astrophysical nucleosynthesis. This instrument has already attracted several students from universities for their thesis research, some in nuclear astrophysics and others in the fundamental process of neutron capture.