

# **U.S. Department of Energy**

# **REQUEST FOR PRE-APPLICATIONS NO. NEUP-001-12**

For Nuclear Energy R&D Proposals

By Battelle Energy Alliance (BEA) on behalf of the Department of Energy, Office of Nuclear Energy

ISSUE DATE: September 28, 2011

PRE-APPLICATION DUE DATE: October 27, 2011 SUBCONTRACT ADMINISTRATOR: Val Seeley

TELEPHONE NO.: (208) 526-0830 FACSIMILE NO.: (208) 526-8076

E-MAIL: neup@inl.gov

#### 1 Introduction

This solicitation is the fiscal year (FY) 2012 Request for Pre-Applications (RPA) for nuclear energy-related research and development (R&D) for the United States Department of Energy's (DOE) Office of Nuclear Energy's (NE) Nuclear Energy University Programs (NEUP). This RPA supports the NE and NEUP missions and goals described below:

The primary mission of the Office of Nuclear Energy is to advance nuclear power as a resource capable of meeting the Nation's energy, environmental, and national security needs by resolving technical, cost, safety, proliferation resistance, and security barriers through research, development, and demonstrations as appropriate.

The Nuclear Energy University Programs mission is to engage the U.S. university community to conduct program directed, program supporting, and mission supporting research and development, related infrastructure improvements, and student education support to build world class nuclear energy and workforce capability as an integral component of the Office of Nuclear Energy.

The goal of NEUP is to support outstanding, cutting-edge, and innovative research at U.S. universities through the following:

- ◆ Administering NEUP R&D awards to support NE's goal of integrating R&D at universities, national laboratories, and industry to revitalize nuclear education and support NE's R&D program objectives as defined in the NE R&D Roadmap
- ♦ Attracting the brightest students to the nuclear professions and supporting the Nation's intellectual capital in Nuclear Engineering and relevant Nuclear Science, such as Health Physics, Nuclear Materials Science, Radiochemistry, and Applied Nuclear Physics
- ♦ Improving relevant university and college infrastructures for conducting R&D and educating students
- Supporting NE's goal of facilitating the transfer of knowledge from the aging nuclear workforce to the next generation of workers

This RPA includes mandatory requirements and evaluation criteria that will be used to select a set of applications whose applicants will be invited to submit full proposals in response to a subsequent Call for Proposals (CFP).

The primary point of contact for questions regarding this solicitation is <u>Dr. Marsha Lambregts</u> from the NEUP Integration Office. However, all technical scope questions must be submitted through the question and answer feature on the RPA website accessible via the NEUP website: <u>www.neup.gov</u>.

A NEUP workshop was held on August 9-10, 2011, in Chicago, Illinois, to assist in the preparation of this R&D RPA. Workshop outcomes were captured as proceedings and are available via the NEUP website: <a href="www.neup.gov">www.neup.gov</a>.

This workshop product is an important source of background information on the R&D areas that are included in this solicitation. Applicants are encouraged to familiarize themselves with these documents, review the information posted at <a href="https://www.neup.gov">www.neup.gov</a> under the "**Proposal Writing Tips for Success**" tab, and communicate with technical points of contact as described in Section 6 of this RPA before responding to the solicitation or entering the proposal submittal system (online).

A stand-alone pre-application is required for each scope of work of interest. Applicants can collaborate on no more than **six** pre-applications and only **three** of those submissions can be as the lead principal investigator (PI). Availability of funding, technical merit, and program relevancy will factor into the determination of the final number of proposals selected for each technical area.

**NOTE:** All information and instructions required to respond to this solicitation are accessible via the NEUP website: <a href="www.neup.gov">www.neup.gov</a>. Applicants may request login credentials at <a href="www.neup.gov">www.neup.gov</a> beginning at 8 a.m. September 28, 2011 MDT. Applicants MUST submit their responses electronically. NO hard copy responses will be accepted.

## 2 RESEARCH AREAS OF INTEREST

NEUP will fund R&D that facilitates meeting NE's programmatic objectives. NE's strategic goals for nuclear energy are clearly defined within the <u>Nuclear Energy Research and Development Roadmap</u> (http://nuclear.gov/pdfFiles/NuclearEnergy\_Roadmap\_Final.pdf).

#### 2.1 NE ROADMAP OBJECTIVES

- ♦ R&D Objective 1: Develop Technologies and Other Solutions that Can Improve the Reliability, Sustain the Safety, and Extend the Life of Current Reactors
- ♦ R&D Objective 2: Develop Improvements in the Affordability of New Reactors to Enable Nuclear Energy to Help Meet the Administration's Energy Security and Climate Change Goals
- ◆ R&D Objective 3: Develop Sustainable Nuclear Fuel Cycles
- ◆ R&D Objective 4: Understand and Minimize the Risks of Nuclear Proliferation and Terrorism

NEUP components covered by this RPA are *Program Supporting* and *Mission Supporting* R&D in Fuel Cycle Research and Development, Reactor Concepts Research, Development and Demonstration, and Nuclear Energy Advanced Modeling and Simulation.

**Program Supporting R&D** is focused more directly on programmatic needs and defined by the scope statements issued by the responsible programs. This work should be focused and responsive to the representative scope. The scope statements are not prescriptive to a discipline, but can be limiting as defined by scope objective.

Mission Supporting R&D is considered creative, innovative, and transformative (blue-sky), but must also support the NE mission. Mission-supporting activities that could produce breakthroughs in nuclear technology are also invited to this solicitation. This includes research in the fields or disciplines of nuclear science and engineering that are relevant to NE's mission though may not fully align with the specific initiatives and programs identified in this solicitation. This includes, but is not limited to, Nuclear Engineering, Nuclear Physics, Health Physics, Radiochemistry, Nuclear Materials Science, or Nuclear Chemistry. Examples of topics of interest are new reactor designs and technologies, advanced nuclear fuels and resource utilization, instrumentation and control/human factors, radiochemistry, fundamental nuclear science, and quantification of proliferation risk and creative solutions for the management of used nuclear fuel.

Program supporting research requested by this solicitation is detailed as discreet workscopes in Appendix A. The information is organized by program area with each specified workscope providing the basis for a stand-alone R&D pre-application submittal.

Follow-on R&D work from previous projects may be submitted as new proposals for consideration under this RPA. All proposals submitted under this RPA will be considered equally.

#### 2.2 Major NE Funded Programs

**Fuel Cycle Research and Development (FCR&D) Program.** The mission of the FCR&D program is to research, develop, and demonstrate options to the current U.S. commercial fuel cycle to enable the safe, secure, economic, and sustainable expansion of nuclear energy while minimizing proliferation and terrorism risks.

In the near term, the goal for FCR&D is to define and analyze fuel cycle technologies to develop options that increase the sustainability of nuclear energy. In the medium term, the goal is to select a preferred fuel cycle option for further development and by 2050 deploy the preferred fuel cycle.

Current challenges include the development of high burnup fuel and cladding materials to withstand irradiation for longer periods of time with improved accident tolerance; the development of simplified separations, waste management (including storage, transportation, and disposal) and proliferation risk reduction methods; and development of processes and tools to evaluate sustainable fuel cycle system options and to effectively communicate the results of the evaluation to stakeholders.

Reactor Concepts (RC) Research, Development and Demonstration Program. The mission of the RC Research, Development and Demonstration program is to develop new and advanced reactor designs and technologies that broaden the applicability, improve the competitiveness, and ensure the lasting contribution toward meeting our Nation's energy and environmental challenges. Research activities are designed to address the technical, cost, safety, and security issues associated with various reactor concepts. The four technical areas are Light Water Reactor Sustainability (LWRS), Small Modular Reactors (SMR), Next Generation Nuclear Plant Demonstration Project (NGNP), and Advanced Reactor Concepts (ARC). In addition, another

area of R&D supported through the Space and Defense Infrastructure Program, is the manufacturing of radioisotope power systems for national security and space exploration missions. In support of mission and function, Space and Defense Infrastructure Program is requesting mission supporting proposals under RC Research, Development and Demonstration.

Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program. The mission of the NEAMS program is to set computer modeling of nuclear energy systems on a modern footing simulating nuclear systems with much higher fidelity and well-defined and validated prediction capabilities. Current generation nuclear modeling and simulation tools are empirically based and are reliable for interpolation within the experimental regime used to calibrate them but have questionable reliability for extrapolating beyond. New tools are needed to inform the design, implementation, and safe operation of advanced nuclear energy systems.

Systems to be modeled include reactors, fuel fabrication plants, used-fuel processing plants, and waste disposition systems during normal and off-normal conditions. This will be achieved by employing advanced software environments and modern high-performance computers, to create a set of engineering-level codes in which fuels and materials continuum properties are informed by first-principles modeling of materials at the atomistic and meso scale. A set of simulation tools will be developed that promote interoperability of codes with respect to spatial meshing, materials and fuels models, and achieve a common "look and feel" for setting up problems and displaying results. The tool set to be developed aims to achieve scalability in terms of computing power and the types and couplings of the physics that dominates the system behavior.

#### 3 ESTIMATED FUNDING

Given the extreme uncertainty of the FY 2012 Budget, DOE is not providing funding estimates at this time. However, technical workscopes based on programmatic needs are provided in Appendix A and form the basis for the FY 2012 RPA.

#### 4 ELIGIBILITY INFORMATION

The lead applicant must be a U.S. university or college. Collaborations between universities and industry or national laboratories are permitted. A maximum of 20 percent of an award can be awarded to industry and national laboratories. Note that funding is for U.S. based researchers only. Although collaborations with foreign organizations are encouraged if their role is focused on fundamental research and they are not a denied party or a party that requires an export license, such participants are not eligible for U.S. government funding. Universities that partner with a National Laboratory, Underrepresented Groups, Minority-Serving Institutions, International partners, or Industry may receive additional points during proposal evaluation (see Section 11). The following link provides the list of minority-serving institutions; http://www.ed.gov/about/offices/list/ocr/edlite-minorityinst.html.

#### 5 CONTENT OF R&D PRE-APPLICATION AND BASIS FOR AWARD

#### 5.1 SUBMITTAL CONTENT AND FORMAT

Each applicant's R&D pre-application shall include the items found in Table 1. Applicants may input these pre-application elements on the NEUP R&D pre-application form provided at the RPA website. Access instructions are available at <a href="https://www.neup.gov">www.neup.gov</a>.

**Table 1: Submittal Content and Format** 

Item	Description	Page Limit
Pre-Application Narrative	Size 11 Times New Roman font minimum; Three single-spaced pages maximum; One-inch margins all around minimum.	3
Benefit of Collaborations	Size 11 Times New Roman font minimum; Two single-spaced pages maximum; One-inch margins all around minimum.	2
Principal Investigator Vita	Size 11 Times New Roman font minimum; Two single-spaced pages maximum; One-inch margins all around minimum.	2
Quality Assurance Requirements	Terms and Conditions check box at the bottom of the pre-application form.	N/A
Mandatory Requirements	Terms and Conditions check box at the bottom of the pre-application form.	N/A
Commitment of Partner(s)	Terms and Conditions check box at the bottom of the pre-application form.	N/A

#### 5.2 PRE-APPLICATION NARRATIVE

Applicant shall provide a narrative that addresses the specific information below:

- ♦ Title of Project
- ◆ Technical Work Scope Identifier No. (enter the number that appears in the Technical Work Scope Table)
- ♦ Name of Project Director/Principal Investigator(s) and associated organization(s)
- ♦ A summary of the proposed project, including a description of the project and a clear explanation of its importance and relevance to the objectives covered by this RPA
- ♦ Explanation of the importance and relevance of the proposed work to the objectives covered by this workscope area

- ♦ Logical path to work accomplishment
- ♦ Deliverables and outcomes the R&D will produce
- ◆ Timeframe for execution of proposed scope (specify if the R&D is for a one-, two-, or three-year period; see below discussion of project length limitations)
- ♦ For **Program Supporting** research, estimated cost of proposal (order of magnitude); applicants shall not propose costs of more than \$300,000/year and \$900,000/contract for contracts generally up to 3 years (no cost extensions up to 4 years must be approved by sponsoring R&D program office in consultation with NEUP).
- ♦ For **Mission Supporting** research, estimated cost of proposal (order of magnitude); applicants shall not propose costs of more than \$150,000/year and \$450,000/contract for contracts generally up to 3 years (no cost extensions up to 4 years must be approved by sponsoring R&D program office in consultation with NEUP).

#### 5.3 BENEFIT OF COLLABORATIONS

This document will contain an explanation of the contribution that will be made by the collaborating organizations and/or facilities to be utilized. It can contain brief biographies of collaborators and descriptions of the facilities wherein the research will be conducted. Please indicate within this section if this proposal has benefit or influence on other ongoing or proposed NEUP projects (e.g. modeling and simulation in one proposal and effect validation in a separate proposal).

## 5.4 PRINCIPAL INVESTIGATOR (PI) VITA

A two-page vita shall be provided for the PI from the lead college or university. It should include his/her relevant credentials, experience, and five most recent publications or commensurate accomplishments.

# 5.5 QUALITY ASSURANCE REQUIREMENTS

Institutions will be expected to follow quality assurance (QA) principles and requirements in conducting R&D activities. The integrity of R&D products and their usability by NE is predicated on meeting QA requirements as they apply to a specific scope of work and associated deliverables. In most cases, an institution's process for peer review in support of publishing research results will serve as a basis for QA requirements; however, there may be some instances where additional QA requirements are specified.

While QA requirements are not new to universities and colleges, it is recognized that familiarity with NE programmatic-specific QA requirements will vary; therefore, during the CFP process, the NEUP Integration Office will provide assistance, as needed, in understanding possible QA requirements for a specific workscope and in developing options to meet those QA requirements. Examples of typical implementation documents which meet the QA requirements are posted on the NEUP website. Acceptance of these requirements is indicated by the lead applicant checking the Terms and Conditions box at the bottom of the application form.

## 5.6 MANDATORY REQUIREMENTS

A mandatory set of requirements (go/no-go) is provided below as Table 2. The lead university or college is required to obtain its institutional commitment, as well as the commitment of each collaborating organization, to each of the specified mandatory requirements. Only preapplications that accept these mandatory requirements shall be eligible for continued evaluation. Acceptance of these requirements is indicated by the lead applicant checking the appropriate box on the application form.

**Table 2: Mandatory Requirements** 

Requirement	Description	Evaluation
Commitment to financial and administrative (overhead) guidance	All participating organizations' adders shall be in accordance with their current negotiated rate agreement with the Department of Health and Human Services or the Office of Naval Research.	Go/No-Go
Commitment to reporting and budget requirements	Commitment to submit quarterly billing. Commitment to submit quarterly reports through the NEUP website.  Reports approved by NE Program Management.	Go/No-Go
Commitment to comply with QA requirements	The college or university is required to acknowledge that it will comply with QA requirements. Additional explanation is provided below.	Go/No-Go

Note 1: If the lead institution has a current master blanket subcontract in place with BEA and is awarded a R&D subcontract in response to the CFP, then the NEUP R&D award will be added to the existing subcontract as a task release.

Note 2: If an applicant proposes workscope to be conducted at a DOE facility, the work performed at DOE facilities shall be conducted in accordance with 10 CFR 851, Worker Safety and Health Program requirements.

Note 3: Applicants that progress to the full proposal stage will be required to agree to the terms and conditions of the Standard Research Subcontract.

#### 5.7 COMMITMENT OF PARTNERS

Each institution identified in the RPA as a team member shall be identified in the preapplication, with their commitment made to collaborate in the RFP process, and their agreement with the mandatory requirements. Minor contributors—anyone not expected to materially participate in the proposal, such as consultants or national laboratory personnel, who are not to be allocated more than \$49,999 to participate in the project—should not be listed. Acceptance of these requirements is indicated by the lead applicant checking the appropriate box on the application form.

#### 6 PRE-APPLICATION INSTRUCTIONS

Submit, in writing (electronically), any administrative questions or requests for additional information on this solicitation to neup@inl.gov. Technical scope questions should be made using the question and answer feature on the NEUP website: <a href="www.neup.gov">www.neup.gov</a>. NEUP will provide a response to substantive inquiries by restating the question and furnishing a response to all potential applicants by posting the question and response on the RPA website. Points of contact (POC) for program areas are posted on the NEUP website. NEUP encourages applicants to contact these POC's as necessary.

Pre-applications that fail to provide ALL items and quantities specified in this RPA may be deemed non-responsive in their entirety and may not be invited to submit full applications in response to the subsequent CFP.

## 7 APPLICATION AND SUBMITTAL INFORMATION

NEUP reserves the right to amend the solicitation schedule as needed.

#### 7.1 APPROXIMATE SOLICITATION SCHEDULE

Table 3: R&D Schedule

Issue Request for Pre-Applications	September 28, 2011	
Pre-Applications Due	October 27, 2011	
Call for Proposals Released	December 20, 2011	
Full Proposals Due	January 24, 2012	
Selection Announced	April 30, 2012	
Awards Completed	August 31, 2012	

#### 7.2 PRE-APPLICATION DUE DATE

In accordance with the schedule above, pre-applications are due by 5:00 p.m. MDT on October 27, 2011. Submittals to the R&D solicitation MUST be made electronically by using the "Submit Pre-application for Review" option on the pre-application form. Please read the instructions on the form carefully. Pre-applications not submitted via this option will be treated as incomplete and will not be evaluated.

#### 7.3 LATE PRE-APPLICATIONS

Pre-applications received after the designated date and time, i.e., late, will be treated as nonresponsive and not evaluated. Extension of the R&D pre-application due dates shall be determined at the sole discretion of the NEUP Integration Office on behalf of NE.

## 8 WORKSCOPE DESCRIPTIONS

Appendix A contains detailed descriptions of research needs in support of each programmatic element for submission to the Program Supporting and Mission Supporting sectors of the call. It should be noted that for Mission Supporting proposals, the submission of novel and creative solutions to the research challenges is strongly encouraged beyond the detailed needs described in Appendix A.

#### 9 PROGRAM CONTACTS

The NEUP website, <u>www.neup.gov</u>, provides a list of technical contacts for each program who can be contacted for further information on their respective areas of work, as well as the programs' websites that also provide relevant technical information.

#### 10 SUBMITTAL LIMITATION

**NEW for FY 2012:** Applicants can collaborate on no more than **six** pre-applications and only **three** of those submissions can be as the lead principal investigator (PI).

#### 11 EVALUATION CRITERIA

Selection of universities and colleges to be invited to provide full applications in response to the subsequent CFP shall be based on how well the pre-applications meet or exceed the weighted evaluation criteria provided below in Table 4. After considering the evaluation criteria and available funding, NE will make a final determination of applicants who will be invited to provide full applications in response to the subsequent CFP.

All pre-applications submitted under this solicitation will be reviewed and scored by two different groups. First, a panel of programmatic experts will assess each pre-application's relevancy to NE's R&D mission or program objectives, as described below in Table 4. Scores

will be assigned on the subjective scale of Highly Relevant, Relevant, Low Relevance, and Not Relevant. Subjective criteria, such as the level of participation of a National Laboratory, Underrepresented Group, Minority-Serving Institution, International, or Industrial partner will be incorporated into the relevancy/technical quality evaluation(s). Proposals scored as "Not Relevant" will not be evaluated further because NE has received clear Congressional direction that in no instance can NE allocate funds to activities that are not relevant to its mission. Second, a separate panel of technical experts/peers will assess each application on its technical merit. Scores will be assigned on the subjective scale of High Merit, Moderate Merit, Low Merit, and No Merit.

The two scores will be weighted per Table 4 below. Pre-applications will be arranged within each Program Area and technical area using the ranked information. Then, after evaluating the recommendations of the reviewers, the Selection Official will determine which applicants will be invited to submit full proposals in response to the subsequent CFP.

**NOTE**: Applicants who are not specifically invited to submit full proposals may still do so at their own decision/risk. There is no guarantee that uninvited full applications will receive a full review; however, all full applications received in response to the subsequent CFP will be re-reviewed for relevancy. Only those uninvited full proposals that are scored as Highly Relevant will be forwarded for technical peer review during the CFP evaluation phase.

**Table 4: Weighting of Scores** 

Criterion	Description	Weight (Percent)
Scientific/Technical Merit <sup>1</sup>	<ul> <li>Program Supporting: Advances the state of knowledge in the selected program workscope;</li> <li>Practicality of scope with respect to the program workscope;</li> <li>Practicality of scope with respect to requested funding and period of performance;</li> <li>Logical path to work accomplishment; ability of team to perform work.</li> </ul>	65
	<ul> <li>Mission Supporting: Advances the state of knowledge in an area supporting the overall NE mission;</li> <li>Practicality of scope with respect to NE's mission;</li> <li>Practicality of scope with respect to requested funding and period of performance;</li> <li>Logical path to work accomplishment; ability of team to perform work.</li> </ul>	80
Relevance <sup>2</sup>	<ul> <li>Program Supporting: Aligned with, and directly relevant to, program objectives.</li> <li>Submission should define and describe the significance of the proposal to the needs described by program workscopes.</li> </ul>	35
	<ul> <li>Mission Supporting: Aligned with, and relevant to the overall NE mission.</li> <li>Submissions should sufficiently capture a clear and supportive connection to the NE mission.</li> </ul>	20

<sup>1.</sup> Scientific Technical Merit: The technical section of the application will clearly define the research being proposed and its relationship to the selected program workscopes. This criterion will consider the technical merit of the application, including proposed technical objectives and deliverables, as well as the likelihood of achieving them.

<sup>2.</sup> Proposals must recognize work currently underway under earlier NERI and NEUP awards to ensure that the work is not duplicative of those already approved.

# 12 NEUP/ADVANCED TEST REACTOR NATIONAL SCIENTIFIC USER FACILITY RESEARCH COLLABORATION

In addition to NEUP projects, DOE-NE supports university research through the Advanced Test Reactor (ATR) National Scientific User Facility (NSUF), whose research awards provide funding to perform specific experiments in a test reactor or make use of other NSUF facilities. However, ATR NSUF research awards, like all DOE user facilities, only cover the cost of the facilities and associated staff support, not the university time needed to prepare the project and perform the research. In order to help address this issue and provide other benefits to the university community while enhancing nuclear research, NEUP and NSUF are collaborating to align certain projects, as appropriate and as described below.

**New in FY 2012:** University researchers may submit a single proposal to NEUP in response to this solicitation that also requires the capabilities of ATR NSUF. Proposals submitted through this joint solicitation will be reviewed and ranked by both organizations. As funding permits, proposals scored the highest by both NEUP and ATR NSUF will be awarded an NEUP research contract as well as access to required ATR NSUF capabilities.

**NOTE:** These projects must be mature projects that require immediate access to NSUF facilities. For example, if the project requires more than a year to develop the fuel or material before it is ready for reactor time, this joint type of proposal is not appropriate. For developmental proposals, an application solely to NEUP is appropriate. For those proposals that do not require NEUP dollars, an application through the NSUF system alone is appropriate.

As described in Sections 4 and 11, international partners are allowed and encouraged for NEUP projects, although no NEUP funding may be allocated to a non-US university. Similarly, the ATR NSUF interacts with non-US researchers as experimenters who may participate in projects as collaborators as long as the non-US researcher's salary is funded by their country. Alternatively, NSUF projects may include non-US organizations who work with NSUF on a cost sharing basis (e.g., joint sharing of facilities in both countries) or by directly funding work in ATR or other NSUF facilities.

# Appendix A Workscope Descriptions

#### SEPARATIONS AND WASTE FORMS

(FEDERAL POC – JIM BRESEE & TECHNICAL POC – TERRY TODD)

Separations and Waste Forms (FC-1) – The separations and waste forms campaign develops the next generation of fuel cycle and waste management technologies that enable a sustainable fuel cycle, with minimal processing, waste generation, and potential for material diversion. Today's technology challenges include the economical recovery of transuranic elements for recycle/transmutation; and minimizing waste generation (including both high level and low level waste). Priority research efforts revolve around achieving near-zero radioactive off-gas emissions; developing a simplified, single-step recovery of transuranic elements; and significantly lessening the process wastes. Exploratory paths include developing fundamental understanding of separation processes and waste form thermodynamics; understanding the underlying separation driving forces; exploiting thermodynamic properties to effect separations; elucidating microstructural waste form corrosion mechanisms; and developing improved sampling and process monitoring technologies. The results of this R&D should contribute to development of a predictive capability for separation and waste form performance over a broad range of operational conditions and novel separations technologies. Key university research needs for this activity include:

- Experimental collection of fundamental data to characterize and quantify chemical processes of aqueous or electrochemical separation, validation of modeling approaches as well as to develop a better understanding of electrochemical separation methods;
- Develop a fundamental understanding of interfacial electrochemistry of actinides and fission product elements important in the fuel treatment process;
- Development of novel transformational separation technologies that have the potential of significantly reducing cost of processing fuel while reducing proliferation risk and waste generation;
- Development of alternative waste forms that have the potential of significantly increased waste loading (of fission products) and durability over borosilicate glass;
- Investigation of novel volatilization methods for complete or partial recycle of used fuel components. Approaches could include oxidation/reduction methods, reactive gas reagents, or any combination of approaches to segregate used fuel components for recycle or disposal.

#### ADVANCED FUELS

(FEDERAL POC - FRANK GOLDNER & TECHNICAL POC - KEMAL PASAMEHMETOGLU)

Advanced Fuels (FC-2) – The advanced fuels program conducts research and development of innovative next generation LWR and transmutation fuel systems. The major areas of research include, for example, enhancing the accident tolerance of fuels and materials, improving the fuel system's ability to achieve significantly higher fuel and plant performance, and developing innovations that provide for major increases in burn-up and performance. The advanced fuels program is interested in advanced nuclear fuel and materials technologies that are robust, have high performance capability and are more tolerant to accident conditions than traditional fuel systems. Research and development in the areas of fabrication, characterization, and performance of advanced fuel, materials, and target systems are within the scope of this program element. Key university research needs for this activity include:

Advanced fabrication technology and research with potential for decreasing fabrication process

losses while increasing fuel quality and consistency;

- Fabrication process models, such as compaction and sintering models, fuel materials studies, and associated technology development that supports increased understanding of fuels performance;
- Supporting the development of predictive, physics-based fuels performance models at a microstructural level by developing and conducting separate effects tests to provide the required fundamental physical and chemical data;
- Development of in-pile instrumentation, novel characterization techniques and innovative out of pile testing that supports the goal of understanding the behavior of and predicting the performance of the nuclear fuel system at a microstructural level;
- Fuel related core materials tolerant to LWR beyond-design-basis events.

#### **NUCLEAR MATERIALS SAFEGUARDING AND INSTRUMENTATION**

(FEDERAL POC – DAN VEGA & TECHNICAL POC – MARK MULLEN)

Nuclear Materials Safeguarding and Instrumentation (FC-3) — This program element develops technologies and analysis tools to support next generation nuclear materials management and safeguards for future U.S. fuel cycles. This includes both extrinsic measures and safeguards over-laid on a nuclear energy system, as well as the intrinsic design features incorporated into system design. New technologies and approaches to in-facility accounting and safeguarding of nuclear materials will be pursued under this research area. This research topic will also pursue advanced measurement techniques that could complement the ongoing measurement program. In particular, fission multiplicity and fission neutron spectrum measurements as a function of incident neutron energy have been identified as important data in recent sensitivity analyses. Key university research needs for this activity include:

- New and improved detector systems and sensor materials that can be used to increase the accuracy, reliability, and efficiency of nuclear materials quantification and tracking from the perspective of the operator or state-level regulator. Such systems could include new neutron coincidence/anti-coincidence counting, spectroscopic analysis, chemical, calorimetric, or other non-nuclear methods, as well as any other novel methods with potential MC&A benefits;
- Methods for data integration and analysis, include cutting-edge work in multi-variant statistical
  techniques for process monitoring, risk assessment, plant-wide modeling & simulation directed at
  the accounting challenges of high-interest fuel cycle processes, including advanced separations
  processes;
- High-fidelity nuclear data measurements and associated technology that benefit MC&A
  effectiveness. Such proposals should include clear sensitivity analyses addressing the benefits of
  the evaluation of key nuclear parameters such as multiplicity, covariance data, and cross section
  refinement for isotopes of interest to the nuclear fuel cycle.

#### USED NUCLEAR FUEL DISPOSITION

(FEDERAL POC – SYED BOKHARI & TECHNICAL POC – PETER SWIFT)

*Used Nuclear Fuel Disposition (FC-4)* – The used fuel disposition technical area develops technologies for storing, transporting, and disposing of used nuclear fuel and assessing performance of the waste forms in the associated storage and disposal environments. Key university research needs for the storage and transportation portion of this activity include:

• Innovative approaches to evaluating degradation and aging phenomena of fuel, cladding,

containers, and storage facilities including vertical over packs, horizontal bunkers and pads, relevant to extended interim storage;

- Development of superior concrete that could be used for extended storage;
- Materials research that would facilitate transportation of used nuclear fuel;
- Advanced modeling approaches for radiological consequence analyses of disruptive scenarios relevant to storage transportation;
- Data relevant to risk-informed cask qualification and the storage and transportation behavior of high-burnup and advanced fuels;
- Development of techniques to monitor and managing the aging of dry storage systems.

Assessments of waste form and disposal options start with the degradation of waste forms and consequent mobilization of radionuclides, reactive transport through the near field environment (waste package and engineered barriers), and transport into and through the geosphere. Research needs support the development of modeling tools or data relevant to permanent disposal of used nuclear fuel and high-level radioactive waste in a variety of generic disposal concepts, including mined repositories in clay/shale, salt, and crystalline rock, and deep boreholes in crystalline rocks.

Key university research needs for the disposal portion of this activity include:

- Improved understanding of the degradation processes (i.e., corrosion and leaching) for used nuclear fuel and waste forms that could be generated in advanced nuclear fuel cycles (i.e., glass, ceramic, metallic) in aqueous environments leading to the development of improved models to represent these degradation processes;
- Improved understanding of the degradation processes for engineered barrier materials (i.e., waste containers/packages, buffers, seals) and radionuclide transport processes through these materials leading to the development of improved models to represent these processes;
- Improved understanding of coupled thermal-mechanical-hydrologic-chemical processes in the near-field of relevant disposal model environments, leading to the development of improved models to represent these processes;
- Improved understanding of hydrologic and radionuclide transport processes in the geosphere of relevant disposal model environments, leading to the development of improved models to represent these processes;
- Systematic experiments under controlled conditions to obtain data regarding material properties, degradation processes, and radionuclide transport processes;
- Development of methods to upscale atomistic descriptions into continuum-scale models of barrier degradation and radionuclide transport processes;
- Aqueous speciation and surface sorption at temperatures and geochemical conditions relevant to the disposal environments being considered;
- Radiation and thermal effects on used fuel, waste forms, and engineered barrier materials.
- Consideration of how specific waste forms may perform in different disposal environments using theoretical approaches, models, and/or experiments, with quantitative evaluations of how the long-term performance of waste forms can be matched to different geologic media and disposal concepts.

#### FUEL CYCLE OPTION ANALYSIS

(FEDERAL POC - BRADLEY WILLIAMS & TECHNICAL POC - TEMI TAIWO)

Fuel Cycle Option Analysis (FC-5) – The Fuel Cycle Options campaign performs analysis and evaluates integrated fuel cycle systems with the purpose of identifying and exploring sustainable nuclear fuel cycles that are candidates for future deployment. Results of these studies and R&D activities must be effectively disseminated to program stakeholders and the public in an accurate, open, and simple manner. Initial efforts will support development of the understanding of what needs to be communicated and why, the audiences to reach, how best to communicate the messages, and the evaluation approach to measure effective communication. Of prime importance is the development of effective methods to communicate the potential benefits of alternative nuclear fuel cycle options and associated enabling technologies that could be developed in the future. Key university research needs for this activity include:

- Identify and develop the essential features and messages for effective communication of the fuel cycle program and its achievements;
- Develop any tools, processes, and products to improve communication of the progress and results of the program and campaigns;
- Interact with the public, stakeholders and other customers external to the program to develop understanding of communication needs and approaches;
- Develop methods to evaluate the effectiveness of program communications;
- Understanding the societal and public viewpoints associated with nuclear power and advanced nuclear fuel cycles.

# MISSION SUPPORTING TRANSFORMATIVE RESEARCH

#### FUEL CYCLE R&D

(FEDERAL POC - BRADLEY WILLIAMS & TECHNICAL POC - MIKE GOFF)

Fuel Cycle R&D (MS-FC) – Game-changing, innovative ideas will play an important role in developing revolutionary fuel cycle concepts of the future. Developing and defining these concepts can support the Fuel Cycle Research and Development (FCR&D) Program's mission to research, develop, and demonstrate alternatives to the current U.S. commercial fuel cycle to enable the safe, secure, economic, and sustainable expansion of nuclear energy while minimizing proliferation and terrorism risks. While proposals relevant to all fuel cycle R&D areas are sought, there is particular program interest in developing accident tolerant light water reactor fuel designs and concepts; and in analyzing extended dry storage of used nuclear fuel, including the subsequent transportation of used fuel (with particular interest on high burn up fuel). Project proposals should include a description of the concept, an analysis of technology risks and feasibility, and a technology roadmap describing how this concept can be further developed.

#### SMALL MODULAR REACTORS

(FEDERAL POC - TIM BEVILLE & TECHNICAL POC - DAN INGERSOLL)

Advanced Concepts (SMR-1) – SMR concepts offer the opportunity to expand nuclear energy to a broader range of customers and energy-intensive applications, including base-load electricity for remote communities or dedicated facilities, dispatchable electricity to stabilize local grids with high renewable fractions, process heat applications, etc. The more diverse customer base imposes new or enhanced requirements such as extreme reliability or power agility. Innovative concepts are sought that are designed from the outset to provide increased levels of safety and robustness and new functionalities while also maintaining or improving the operational and economic performance. The concepts may utilize advanced technologies or innovative engineering but should be viable for eventual commercial deployment. The scope of the proposed project should include: a thorough viability assessment of the advanced concept, a detailed technology gap analysis, and a comprehensive technology development roadmap.

Advanced Technologies and Analysis Methods (SMR-2) – Advanced technologies can enable new SMR concepts and designs to achieve even greater levels of safety and resilience, flexibility of use, sustainability and construction or operational affordability. For example, improved materials can provide additional core integrity in severe accident situations and advanced sensors and instrumentation can provide better knowledge of plant health during normal and upset conditions. Also, SMRs differ from large plants in their fundamental design features, which may require or benefit from new analysis methods to quantitatively characterize the performance and risk factors associated with SMRs. For example, modeling and simulation methods must accurately predict: radionuclide inventory and component integrity for non-traditional materials and components, different source term release and dispersion paths, extended refueling and maintenance cycles, and greater use of intrinsic safety and security features. Innovative technologies and analysis methods for extending and modeling unique SMR performance and safety factors are encouraged.

#### **NEXT GENERATION NUCLEAR PLANT**

The NGNP is a high temperature helium-cooled, graphite moderated reactor with a core outlet temperature between 750 and 850°C. These reactors are well suited for the co-generation of process heat and electricity and for the production of hydrogen from water for industrial applications in the chemical and petrochemical sectors. NGNP is a part of the Office of Nuclear Energy's gas-cooled very high temperature reactor technologies research and development (R&D) program that has a long term goal of achieving outlet temperatures of 950°C. The NGNP R&D program is organized into the areas of: (a) materials, (b) fuels, (c) computational methodologies, and (d) heat transport, energy conversion, hydrogen and nuclear heat applications.

Focused materials research projects have already been initiated that focused on the development of graphite, ceramics, composites and high temperature structural materials, fundamental mechanisms of creep, creep-fatigue, dynamic strain aging, stress relaxation, and environmentally assisted crack growth in component alloys and pressure vessel steels. Ongoing research is studying graphite for fuel blocks and core structures, detecting small cracks in graphite, advanced carbon fiber carbon composite (CFC), silicon

carbide fiber composite (SiC/SiC), composites and ceramics for gas-cooled reactor ceramic components, and improved Non-Destructive Examination (NDE) techniques for predicting lifetimes for CFC, SiC/SiC, and composites. No materials-related proposals are sought at this time.

Fuel development and qualification activities are focused on producing robust fuel particles that can retain fission products during normal and accident conditions and have very low failure rates, as demonstrated by irradiation and accident safety testing programs. Tristructural-isotropic (TRISO) fuel designs for current pebble bed and prismatic gas-cooled reactors are based on historical designs that build upon large experimental fuel performance databases and historical fabrication methods, and ensure robust performance and fission product retention. The NGNP Advanced Gas Reactor TRISO Fuels program has developed novel TRISO fuel particle designs, fabrication methods, characterization techniques, and initiated research to evaluate radiation source term and fission product transport effects. No TRISO fuels-related proposals are sought at this time.

Proposals are being sought for the Computational Methodologies and Heat Transport, Energy Conversion, Hydrogen and Nuclear Heat Application areas that do not duplicate completed or currently funded NEUP grants and programmatic research activities:

Computational Methodologies (NGNP-1) — (FEDERAL POC – STEVE REEVES & TECHNICAL POC – HANS GOUGAR)

The computational methodologies R&D is focused on providing practical tools to analyze the reactor core neutronics/thermal-hydraulics, performance, and reactor gas-coolant helium thermal fluids behavior during normal operations, transient and accident scenarios, and safety evaluations for gas-cooled reactors and scaled experimental design. Research efforts have been initiated and/or completed in the areas of neutronics, thermal-hydraulics, and multiphysics, in terms of time-dependent coupled fuel/neutronic/thermal fluids modeling, reactor kinetics effects, and mechanical-neutronic-thermal fluid interactions during graphite dimensional changes under irradiation with thermal and neutronic feedback. Gas-cooled reactor plant simulation and safety analysis methods development has been initiated for uncertainty and sensitivity analysis for statistical importance ranking. Methodologies for determining credible fission product transport mechanisms that support the mechanistic source term approach for gas-cooled reactors under normal operating conditions, off-normal events, and accident conditions, including both air and/or moisture ingress events are under development.

Proposals related to gas-cooled reactors that have a special emphasis on experimental validation and uncertainty and sensitivity analysis to benchmark computer simulation methods are particularly encouraged. Proposals are particularly sought in the areas of: (a) Steam Ingress Flow and Chemistry, (b) Seismic Interactions Analysis of the reactor vessel, inlet/outlet vessel and steam generator/turbo-machinery, in a below-grade silo containment/confinement building structure, (c) impact of externally-initiated events and accident scenarios (e.g., seismic, flooding) on safety and risk analyses, and (d) methods that integrate externally initiated events (e.g. earthquake, flooding) and core/reactor dynamics and structures vibrations (e.g. graphite reflector and prismatic block movement). Proposals are sought that focus on conducting integral benchmark experiments for fission product/source term transport and dispersion, using non-radioactive surrogates, that investigate fission product release phenomena (i.e., aerosols, metallic and gaseous species plate-out, dust transport) inside the reactor vessel, turbo-machinery, piping systems during severe accident conditions, including benchmarks with historical gas-reactor tests (COMEDIE, KUFA, etc.), which could be used to benchmark computational fission

product/source term methods/algorithms compatible with NRC's MELCOR code methodology.

Heat Transport, Energy Conversion, Hydrogen, and Nuclear Heat Applications (NGNP-2) – (Federal POC – Carl Sink & Technical POC – MW "Mike" Patterson)

The Heat Transport, Energy Conversion, Hydrogen and Nuclear Heat Applications area focuses on the development of approaches to coupling gas-cooled reactors with the wide variety of process heat applications (co-generation, coal-to-liquids, chemical feedstocks).

Proposals are only sought in these areas: (a) dynamic simulation and control of Reactor-driven Process Heat Plants, including interactions of multiple modules and (b) simulation and analyses for the use of interactive and prognostic "intelligent control" systems and advanced instrumentation and control methods (e.g. adaptive controllers, "fuzzy logic", neural networks, genetic algorithms, etc.) to handle combined interactions between the heat transport, energy conversion plant and the reactor systems (core, reactor systems, turbo-machinery, steam generator, compressors) and balance-of-plant systems, during plant upsets, off-normal events, and accident conditions. No Hydrogen-related proposals are sought at this time.

#### LIGHT WATER REACTOR SUSTAINABILITY

Advanced Mitigation Strategies (LWRS-1) — (FEDERAL POC – RICH REISTER & TECHNICAL POC – JEREMY BUSBY)

Advanced mitigation strategies and techniques. Extended operating periods may reduce operating limits and safety margins of key components and systems. While component replacement is one option to overcome materials degradation, other methods (e.g. thermal annealing or water chemistry modification) may also be developed and utilized to ensure safe, long-term operation. Validation and/or development of techniques to reduce, mitigate, or overcome materials degradation of key LWR components are sought. Mitigation strategies for pressure vessel steels, core internals, weldments, or concrete are encouraged. Universities engaging in this effort will be expected to produce concepts, supporting data and/or model predictions demonstrating the viability of mitigation strategies for key LWR components.

Risk-Informed Safety Margin Characterization (LWRS-2) — (FEDERAL POC – RICH REISTER & TECHNICAL POC – ROBERT YOUNGBLOOD)

R&D should address the Risk-Informed Safety Margin Characterization (RISMC) methodology. Areas of high priority include advanced modeling and simulation methods to support the development, verification, and validation of next-generation system safety codes that enable the nuclear power industry to perform analysis of a nuclear power plant's transients and accidents. An especially important need in this analysis is a very clear understanding of the real uncertainties in the analysis. This requires not just propagation of parameter uncertainty via sampling techniques, but also meaningful quantification of the underlying distributions, addressing not only epistemic uncertainty but also variability in phenomena, including variability in component behavior (variability in stroke times, pump head curves, heat transfer coefficients, and so on). Universities performing this research will be expected to produce results that integrate multiple mechanistic processes. Also of interest are advanced approaches to coarse-grained single-phase and two-phase thermal-hydraulics modeling and experimental validation, including coupling of models of different resolutions, for example, between one dimensional system thermal-hydraulics and

three dimensional Computational Fluid Dynamics-type models, and treatment of dynamic flow regimes.

Instrumentation and Control (LWRS-3) — (FEDERAL POC – RICH REISTER & TECHNICAL POC – BRUCE HALLBERT)

Digital instrumentation and control technologies for highly integrated control and display, improved monitoring and reliability. Research is needed to improve upon available methods for online monitoring of active and passive components to reduce demands for unnecessary surveillance, testing, and inspection and to minimize forced outages and to provide monitoring of physical performance of critical structures, systems, and components (SSCs). In addition, methods are needed to analyze the reliability of integrated hardware/software technologies that comprise digital systems. Research should investigate NDE technologies to characterize the performance of physical systems in order to monitor and manage the effects of aging on SSCs. High priority research areas include the following: 1) methods and technologies that can be deployed for monitoring nuclear plant systems, structures, and components, and that can be demonstrated in test bed environments representative of nuclear plant applications; and 2) methods for analyzing the dynamic reliability of digital systems, including hardware and software systems based on formal methods that can be demonstrated on systems that are proposed or representative of systems proposed for nuclear plant control and automation. This research is expected to support the development of methods and technologies to support digital instrumentation and control integration for monitoring and control as well as for noting areas of improved reliability and areas requiring further information and research. Universities performing this research will be expected to produce results that integrate multiple mechanistic processes.

Advanced LWR Nuclear Fuel (LWRS-4) — (Federal POC – Rich Reister & Technical POC – George Griffith)

The Light Water Reactor Sustainability program is conducting research and development on the use of silicon carbide ceramic matrix composite nuclear fuel cladding. The goal is to provide improved economic performance and a greater resistance to accident conditions than could be achieved with current zirconium based claddings. Areas of particular interest are the development of radiation resistant silicon carbide ceramic matrix composites, novel fabrication methods, and unique end plug to cladding tube connecting methods.

# ADVANCED REACTOR CONCEPTS (ARC)

Advanced Reactors Concept Development (ARC-1) — (FEDERAL POC – BRIAN ROBINSON & TECHNICAL POC – ROBERT HILL)

Development of new reactor concepts that use advanced technologies or innovative engineering is sought. The goals of the advanced reactor system should be to provide electricity at the same cost or lower than light water reactors with improved safety and system performance. This category could include the incorporation of advanced systems and components into existing reactor concepts or the inclusion of innovative design alternatives (e.g., new fuel type, coolant modifications, fuel handling strategy, etc.). Components within this scope include, but are not limited to innovative design for containment, seismic, fuel handling, pumps, safety systems, and instrumentation for both operations and maintenance. The scope of the proposed project should include a thorough viability and applicability assessment of the proposed reactor system, advanced systems and/or components, a detailed technology gap analysis, and a

comprehensive technology development roadmap.

Advanced Energy Conversion (ARC-2) – (FEDERAL POC – BRIAN ROBINSON & TECHNICAL POC – JIM SIENICKI)

Development of new energy conversion systems that use advanced technologies or innovative engineering is sought. Supercritical CO<sub>2</sub> shows promise as a working fluid suitable for fast and thermal reactors because of its compatibility with materials and thermodynamic properties. Basic R&D is needed in turbomachinery performance and loss mechanisms. System optimization requires a detailed modeling of the system components and their response to steady-state and off-normal conditions. The university participants could contribute detailed Computational Fluid Dynamics (CFD) modeling of key components, such as the main compressor, for comparison to one-dimensional system level models and experimental data from ongoing small-scale testing. Alternately, contributions could be made to the development of plant dynamics models and control strategies, including the investigation of alternative cycle layouts (e.g., having turbomachinery on multiple shafts). The efficiency of different power conversion cycles is degraded by leaks at component interfaces. R&D is needed to develop models and/or test beds to predict the performance of seals (labyrinth, dry liftoff seal, brush, etc.) and bearings. Another topic could be projects that explore coupling of the reactor heat source with diverse process heat applications (cogeneration, coal-to-liquids, chemical feedstocks) and/or other energy products with an emphasis on novel approaches that can greatly improve the ease of coupling, the operability of the combined system, and the ultimate economics. The scope of the proposed project should include a thorough viability assessment of the advanced energy conversion system, a detailed technology gap analysis, and a comprehensive technology development roadmap.

Advanced Structural Materials (ARC-3) — (FEDERAL POC – BRIAN ROBINSON & TECHNICAL POC – JEREMY BUSBY)

Development of new materials for advanced reactor systems is being sought for high temperature liquid metal, high temperature molten salt, and other advanced reactor applications. There are several key needs to support this effort.

- The microstructure stability of advanced structural materials must be validated at elevated temperatures and extended lifetimes under irradiation, elevated temperature and/or exposure to coolants. Novel test techniques and approaches to provide long-term performance data on key candidate-alloys and materials are sought. Such tests must be closely coordinated with advanced alloy development efforts in the supporting program.
- Semi-empirical modeling of material aging and irradiation degradation mechanisms need to be developed to predict neutron damage and temperature effects on bulk/macrostructural mechanical properties, including yield strength, creep, fatigue, ductility, etc. Such a model provides a near-term tool for future experiments by allowing interpolation and deeper understanding of the physical data and, in addition, provide a tool for designers to explore different operating conditions while having at least some understanding of the effects on materials performance, but is not expected to be atomic level detail. Such a model should be based on sound materials science and mechanistic understanding.

# MISSION SUPPORTING TRANSFORMATIVE RESEARCH

#### REACTOR CONCEPTS RD&D

Reactor Concepts RD&D (MS-RC1) — (FEDERAL POC – SAL GOLUB & TECHNICAL POC – ROBERT HILL)

Identification, investigation and development of revolutionary transformational advanced reactor system concepts having the potential to significantly improve performance in sustainability, safety, economics, performance, security or proliferation resistance. Such transformational advanced reactor concepts could include designs employing advanced coolants, fuel configurations and operational characteristics. Concepts could also include small modular reactors with unique capabilities to address operational missions other than the delivery of baseload electric power, such as industrial process heat or mobile reactors that can provide temporary power during emergency situations. The scope of the proposed project should include a thorough viability assessment of the concept, a detailed technology gap analysis and a comprehensive technology development roadmap that identifies research needed on key feasibility issues.

Space and Defense RD&D – Radioisotope Thermal Generator (RTG) Technologies (MS-RC2) – (Federal POC – Wade Carroll & Technical POC – Stephen Johnson)

Space and Defense Power Systems program has designed, developed, built and delivered radioisotope thermal generators (RTG) for space and terrestrial applications for over fifty years. These systems apply the decay heat from plutonium-238 to the hot side of thermoelectric couples to induce direct current electricity flow. Materials used in the early designs for these systems are increasingly difficult to obtain. Proposals that identify more readily available materials that can perform effectively in the extreme environment of atmospheric re-entry are encouraged. Proposals for breakthrough thermoelectric couples that produce electricity more efficiently than current designs are also encouraged.

- **Replacement Materials.** Develop alternate materials for the aeroshell module that protects radioisotope power system fuel during potential atmospheric reentry events. The material will need ablation resistance, thermal conductivity, and structural strength (compressive and tensile) that meet minimum performance requirements.
- Ultra high efficiency Thermoelectric couples. Develop a thermoelectric couple (N and P legs) with a hot side temperature of 1000 C. The couple should demonstrate efficiency between 20-30% with stable properties providing for a minimum operable life of 10 years.

# NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

#### ADVANCED MODELING AND SIMULATION

Structural materials (and nuclear fuels) for future generation nuclear reactors (NEAMS-1) – (Federal POC – Jim Peltz & Technical POC – Xin Sun)

Degradation of structural components (and fuels) under the harsh operating environment of a nuclear power plant are important challenges for future generation nuclear power plants, as well as for the current reactor fleet. Accurate assessment of structural component performance using integrated reactor performance and safety codes will require science-based, validated materials models incorporating mechanical properties, degradation kinetics, and chemical evolution of the material constituents under severe thermal, mechanical, and radiation loads, and propagate these materials behaviors into continuum level descriptions of structural response. The research needs are the development of validated materials models and methods that lead to accurate continuum simulations of materials response, with appropriate quantitative consideration of uncertainties at every scale.

- Predictive Models for Material Degradation at Different Scales. Aging and degradation mechanisms of different structural materials under various thermal and irradiation environments need to be better understood, quantified, and validated. Key university research needs in this area include (1) Development of atomistic chemical kinetics parameters and upscaling into meso-scale models; (2) Meso-scale models of microstructural and chemical evolution (e.g., phase field, Potts model, kinetic Monte Carlo and rate theory) with extraction of physical parameters for continuum scale materials models; and (3) Validated prediction of physical/mechanical property degradation, i.e., thermal conductivity, yield strength, ductility and fracture toughness, creep resistance, etc., to populate continuum scale constitutive models.
- Small-Scale Separate Effects Experiments for Model Validation. This element calls for the linkage between model development and small-scale experiments. Small scale separate effect experiments are necessary specifically targeted to validate models for different phenomena at various scales. These small scale experiments are intended for materials relevant to current and future generations of fuel, cladding and reactor vessels; and the properties of interest include but are not limited to: grain-level, directional dependent thermal conductivity and thermal expansion coefficient measurements with irradiation induced defects; grain boundary strength measurement with defect evolution; effective properties for mass and heat transport; directional dependent stress vs. strain curves for irradiated materials with pre-characterized defect distributions.
- Methodology Development for Scale Bridging. Multi-scale approaches (from atomic-level to
  meso-scale to continuum, and from picoseconds to years) are needed. New algorithms to achieve
  upscaling are a key component to the development of integrated reactor performance and safety
  codes.

# NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

Model and method development to support current and future generation nuclear reactor performance and safety analyses (NEAMS-2) — (FEDERAL POC – ROB VERSLUIS & TECHNICAL POC – DAVE POINTER)

Concepts have been identified for future generation nuclear power plants that take advantage of safety phenomenon that are inherent to the design and do not rely on active engineering systems in order to function. These phenomena include natural convection cooling, thermal-mechanical feedback, and passive decay heat removal. In the past, large base-technology programs existed in order to mature the components and technologies that would be deployed in future plant designs. Future design concepts will rely more heavily on modeling and simulations that can better predict core, systems, and plant performance, thus reducing the need for a large base-technology program. Research needs to support the needed predictive performance and safety analysis capabilities include:

- Methods to perform probabilistic safety assessment of component or system performance weighted over a broad spectrum of anticipated component or inherent feature failure conditions.
- Methods to perform sensitivity studies to evaluate variability and/or flow dominance regimes during the initiating phases of natural convection cooling and relevant experimental data to support validation of new methods.
- Predictive methods for simulation of two-phase boiling and/or flashing flows in complex geometry and relevant experimental data to support validation of new methods.
- Predictive methods for simulation of fluid-structure interaction in components with complex mechanical structure and thermal energy distributions, such as reactor fuel assemblies, and relevant experimental data to support validation of new methods.
- Upscaling methods to enable reduced order modeling of long term transients and fuel cycle performance informed by a limited number of high resolution quasi-steady case studies are needed.
- Water coolant chemistry models to support simulation of steam generating fouling and in core applications are needed.
- Modular structural mechanics codes to understand all aspects of pressure boundary integrity (piping, vessels, steam generators, nozzles etc.) are also needed.
- Expanded visualization techniques to assess system-wide coupling impacts so that the impact of perturbations in one part of a system can be viewed on a system-wide domain.
- Development of a coolant properties code library that contains highly-detailed correlations and uncertainty quantification data on coolant properties in liquid, vapor, and supercritical phases. This library could act as a reference for benchmark and validation purposes.
- Multi-scale integration methods to enable development of virtual reactor simulations using multiple levels of resolution to represent a single physics (e.g., neutronics, fluid dynamics, heat transfer, etc.) and relevant experimental data to support validation of new methods.
- Efficient, scalable mesh generation methods to provide accurate descriptions of realistic nuclear reactor component geometries for high-fidelity finite element or finite volume simulations.

# NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

Development of phenomena-based methodology for uncertainty quantification (NEAMS-3) — (Federal POC – Jim Peltz & Technical POC – Jim Stewart)

To promote quantitative confidence in the results, explicit consideration of verification of simulation codes, validation of models for an intended application, and quantitative assessment of physical and computational uncertainties (VVUQ) are expected elements of all computational and experimental work proposed under this call. In addition to this routine application of good computational practices, there are needs for targeted university research in methods for data analysis and VVUQ in support of:

- Propagating uncertainties through inter-fidelity multiscale physics models—upscaling. The uncertainty associated with model prediction of material behaviors need to be mathematically propagated through different scales. Systematic approaches are needed for managing uncertainties stemming simultaneously from abstraction into reduced (compact) models and in populating parameters in those reduced models. Conversely, methods are needed to propagate solution sensitivities downward, to identify inadequacies in constitutive model formulations and prioritize important sub-scale phenomena.
- Evaluating parameter sensitivities and uncertainties in tightly-coupled multi-physics models. Improved methods for efficient evaluation of sensitivities and uncertainties are needed for intra-fidelity simulations of highly coupled, non-linear multiphysics (e.g., thermal-chemical-mechanical) phenomena.
- Interpretation of large experimental data sets. Advanced modeling and computer simulation methods are needed to process and extract information from large data sets obtained from NDE measurements, and to establish the relationships between microstructural evolution and measured properties.