Program Announcement
To DOE National Laboratories

LAB 12-698

Office of Science

Office of Advanced Scientific Computing Research (ASCR)

2012 Mathematical Multifaceted Integrated Capability Centers (MMICCs)

GENERAL INQUIRIES ABOUT THIS LAB ANNOUNCEMENT SHOULD BE DIRECTED TO:

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SUMMARY:

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby invites proposals for basic research that addresses grand challenges of increasing complexity within DOE's mission areas of energy, environment and security, from a mathematical perspective that require new integrated, iterative processes across multiple mathematical disciplines. This Program Announcement will holistically address mathematics for increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment – this will be achieved through *Mathematical Multifaceted Integrated Capability Centers* (MMICCs).

This Program Announcement is ***seeking proposals for Mathematical Multifaceted Integrated Capability Centers addressing the long-term mathematical challenges*** for one or more DOE grand challenges of increasing complexity. These science and engineering challenges must be abstracted into an interrelated set of mathematical research challenges that require new integrated, iterative processes across multiple mathematical disciplines. Proposals focused on solution of a specific application problem will be considered outside the scope of this Program Announcement.

These MMICCs will enable applied mathematics researchers to work together in large, collaborative teams to more effectively address DOE grand challenge problems from a mathematical perspective much earlier in the problem solving process. The MMICCs allow researchers to take a broader view of the problem as a whole, and devise solution strategies that attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools. The MMICCs will have the flexibility and technical expertise to simultaneously consider all aspects of the problem-solving process ranging from the mathematical formulation to the development, analysis, and integration of appropriate models and methods to the demonstration of results and capabilities. The goal is to determine the most effective combination of the various mathematical components, as such, an iterative process will be necessary. These Centers will help serve as entry points for applied mathematicians and other researchers to more readily understand the mathematical challenges of DOE-relevant problems.

More specific information is included under SUPPLEMENTARY INFORMATION below.

A companion Funding Opportunity Announcement (FOA) DE-FOA-0000698 will also be posted at grants.gov and on the SC Grants and Contracts web site at: http://www.science.doe.gov/grants.

1. Pre-Proposal.

PRE-PROPOSAL DUE DATE: April 30, 2012

Pre-proposals are **REQUIRED** and must be submitted by April 30, 2012, 11:59 PM Eastern Time.

Failure to submit a pre-proposal by a proposer will preclude the full proposal from due consideration. Only the Lead institution of a Center should submit the pre-proposal. Pre-proposals referencing Program Announcement LAB 12-698 should be submitted electronically by E-mail to Sandy.Landsberg@science.doe.gov . **No FAX or mail submission of pre-proposals will be accepted.**

The pre-proposal will be reviewed for conformance with the guidelines presented in this Program Announcement and suitability in the technical areas specified in this Program Announcement. A response to the pre-proposal encouraging or discouraging formal proposals will be communicated to the proposers by **May 4, 2012**. Proposers who have not received a response regarding the status of their pre-proposal by this date are responsible for contacting the program to confirm this status.

Only those pre-proposals that receive notification from DOE encouraging a formal proposal may submit full proposals. **No other formal proposals will be considered.**

The intent in requesting a pre-proposal is to save the time and effort of proposers in preparing and submitting a formal project proposal that may be inappropriate for the program. Pre-proposals will be reviewed relative to the scope and research needs as outlined in the summary paragraph and in the SUPPLEMENTARY INFORMATION. The pre-proposal should contain (1) a cover sheet and (2) a technical narrative.

The cover sheet identifies the name, institutional affiliation, e-mail address, and telephone number of the Center Director, Senior/Key personnel expected to be involved in the planned proposal, and an estimated amount of funding requested for each year for the project for each funded institution. No biographical data need be included. Since among the purposes of the pre-proposal is to facilitate ASCR in planning the merit review and the selection of peer-reviewers without conflicts of interest, it is important that proposers ensure their list of supported or unsupported participants is as comprehensive as possible.

The technical narrative should be no more than three pages in length and briefly discuss one or more scientific or engineering grand challenges and identify an interrelated set of mathematics research challenges that represent abstractions of the grand challenges. These abstractions would then be optimally addressed through a multifaceted, integrated approach. The narrative should also include a brief summary of the multifaceted, integrated approach, the proposed team members, and their expertise.

PROPOSAL DUE DATE:

Formal proposals submitted in response to this Program Announcement must be submitted from the Laboratory to the site office through Searchable FWP by **June 1, 2012, 11:59 p.m. Eastern Time**, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2012. <u>**Each proposal should be in a single PDF file. The first few pages of the PDF should be the Field Work Proposal followed in the same PDF by the full technical proposal.**</u> **You are encouraged to transmit your proposal well before the deadline. PROPOSALS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

SUBMISSION INSTRUCTIONS:

LAB administrators should submit the entire LAB proposal and Field Work Proposal (FWP) via Searchable FWP (https://www.osti.gov/fwp). Questions regarding the appropriate LAB administrator or other questions regarding submission procedures can be addressed to the Searchable FWP Support Center. All submission and inquiries about this Program Announcement must reference Program Announcement LAB 12-698.

SUPPLEMENTARY INFORMATION:

Mathematical Multifaceted Integrated Capability Centers

The "Grand Challenges" were U.S. policy terms set in the 1980's as goals for funding high-performance computing and communications research in response to foreign competition. They were described as "fundamental problems of science and engineering, with broad applications, whose solution would be enabled by high-performance computing resources…" Grand Challenges today are interpreted in a much broader sense with the realization that they cannot be solved by advances in high performance computing alone; they also require breakthroughs in computational models, algorithms, data and visualization technologies, software and collaborative organizations uniting diverse disciplines.

This Program Announcement is seeking proposals that address grand challenges of increasing complexity within DOE's mission areas of energy, environment and security, from a mathematical perspective that require new integrated, iterative processes across multiple mathematical disciplines. This new paradigm will holistically address mathematics for increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment – this will be achieved through *Mathematical Multifaceted Integrated Capability Centers* (MMICCs). These MMICCs will enable applied mathematics researchers to work together in large, collaborative teams to more effectively address grand challenge problems from a mathematical perspective much earlier in the problem solving process. The MMICCs allow researchers to take a broader view of the problem as a whole, and devise solution strategies that attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools. The MMICCs will have the flexibility and technical expertise to simultaneously consider all aspects of the problem-solving process ranging from the mathematical formulation to the development, analysis, and integration of appropriate models and methods to the demonstration of results and capabilities. The goal is to determine the most effective combination of the various mathematical components, as such, an iterative process will be necessary. These Centers will help serve as entry points for applied mathematicians and other researchers to more readily understand the mathematical challenges of DOE-relevant problems.

The DOE Applied Math Summit [1], the DOE ASCR 2012 Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems [2], and workshop report, *A Multifaceted Mathematical Approach for Complex Systems* [3] all concluded that future DOE challenges will require the ability to model systems of unprecedented complexity. Dealing with these increasingly complex systems will require new types of models that couple a broad array of diverse processes spanning a wide range of spatial and temporal scales. The models will likely combine both deterministic and stochastic elements; they are likely to have multiple representations; and they are likely to have dynamic properties. The goal is not to simply produce a simulation of the system, or couple existing models and methods, but rather to answer difficult questions regarding design, risk analysis, or optimization, while quantifying errors and uncertainties. These types of highly complex systems cannot be analyzed at the required fidelity with monolithic mathematical models. Effective models will be hierarchical and include multiple sub-models that represent different phenomena with vastly differing scales. These models can range from the representation of detailed physical processes to the description of complex engineered systems that must be optimized to obtain desired performance. This will require new approaches for understanding the impact on system behavior based on the interplay between sub-models at different physical resolutions or between decision points in an engineered system. Answering key questions about these systems may also require a much tighter coupling between data and simulation, and require new approaches to aggregate information from multiple sources.

The goal is to have researchers simultaneously examine, in an integrated form, all of the mathematical elements needed to make significant advances in the analysis, simulation, and optimization of a complex system. This holistic approach to problem solving is not a linear process of working from formulation to discretization to algorithm but rather an iterative one considering all aspects of the solution process. It is through this iteration that researchers will arrive at the combination of formulation, discretization, and solution methodologies that will enable the most effective combination of the various mathematical components to construct the tools needed to answer important questions about systems of increasing complexity while making efficient use of emerging computer architectures.

Proposals for a Mathematical Multifaceted Integrated Capability Center must:

1. Advance multifaceted, integrated mathematics that spans, as appropriate, novel formulations, discretizations, algorithm development, data analysis techniques, uncertainty quantification methodologies, optimization techniques, and other mathematical approaches;
2. Address one or more Grand Challenge problems with clear relevance and impact to the DOE; and
3. Advance the field of applied and computational mathematics.

This Program Announcement includes four illustrative DOE examples for MMICCs and the organizational structure and management plan of a MMICC.

Four Illustrative DOE Examples for MMICCs

Grand Challenges for MMICCs include defining one or more DOE-relevant scientific or engineering challenges; these are then abstracted into an interrelated set of mathematical research challenges that must be addressed through an integrated, iterative process. MMICC grand challenges are multifaceted: they may involve complex continuous and discrete phenomena with both stochastic and deterministic elements; they may involve coupled models from multiple scientific disciplines; they may require integration of simulation and data; and they may be characterized by pervasive uncertainties. The multifaceted nature of these problems demands a new mode of operation for applied mathematicians; researchers are going to have to cut across the boundaries of traditional development of mathematical methods and tools. To contribute towards solving problems of major importance to DOE, applied mathematics researchers must consider new research directions not just within traditional mathematical topic areas such as modeling, discretizations, linear algebra, optimization, stochastics, and data analysis, but how these interact in an overall integrated problem-solving process.

The MMICCs will provide an opportunity to enhance the impact of applied mathematics on solving problems of critical importance to the DOE. These centers will also produce high-impact, lasting contributions to applied mathematics. The process of developing integrated problem-solving strategies for complex systems will lead to the creation of a far richer, deeper set of mathematical tools in areas ranging from basic analysis to software development. These tools will, in turn, lead to improved theoretical understanding and computational methodologies for systems of increasing complexity.

One of the goals of the MMICCs is to have some level of buy-in from DOE application domains. A letter of endorsement is not required; however, a clear explanation of long-term potential impact to DOE is required. The proposal will need to discuss one or more scientific or engineering grand challenges and identify an interrelated set of mathematics research challenges that represent abstractions of the grand challenges. These abstractions would then be optimally addressed through a multifaceted, integrated approach. The results of MMICC research should have potential impact to the DOE mission in the 5-10+ year timeframe by transitioning to SciDAC Partnerships, SciDAC Institutes, Co-Design Centers, and/or directly to DOE application scientists. Application drivers of importance for MMICCs are:

I. Mathematical Challenges from Materials and Chemistry for Energy Applications

These long-term mathematical challenges potentially include bridging multiple scales, incorporating theory and experimental data, characterizing and propagating uncertainty, validation, and optimizing material design. The development of new models, methods, and computational approaches will dramatically accelerate the discovery of new materials and processes as well as provide fundamental understanding and improvement of current materials and processes. A series of workshops and reports discuss many of the associated challenges [4-6]. Most recently, the *Materials Genome Initiative for Global Competitiveness* [7] was announced. The long-term goal is to generate computational methods and tools that enable real-world materials development, that optimize or minimize traditional experimental testing, and that predict materials performance under diverse product conditions. One challenge is that current predictive algorithms do not have the ability to model behavior and properties across multiple spatial and temporal scales.

Another illustrative example is understanding and predicting the properties of catalysts and designing them for achieving the full potential of novel fuels [3,10]. Modeling and simulation built upon multifaceted integrated mathematics can help assess the technological feasibility of the resulting catalyst, has the potential of incorporating data from high-resolution experimental capabilities, and to significantly enhance predictability on multiple coupled scales. Mathematically this may include, but is not limited to, research in dynamical systems, partial differential and integral operators; optimization methods for inverse problems and energy minimization; and data analysis techniques.

II. Mathematical Challenges from Complex Engineered Systems for Energy Applications

These long-term mathematical challenges potentially include, but are not limited to, new algorithms that are scalable and robust for solving large nonlinear mixed-integer optimization problems and methods for efficiently solving, in real-time, large sets of differential equations with constraints, parameter uncertainties, and incorporating sensor data. One illustrative example is the US electricity grid which is the world's largest engineered system. It consists of a dynamic collection of interacting components, operated under an enormous range of physical, reliability, economic, social, and political constraints that need to be satisfied over time scales ranging from seconds for relay-action and closed-loop control to decades for transmission siting and construction. Fundamental advances are needed in the areas of algorithms, computer networking and architecture, data analysis, simulation and modeling, and computational security [9]. Novel mathematics is necessary for characterizing uncertainty in information created from large volumes of data as well as for characterizing uncertainty in models used for prediction. A MMICC may develop and analyze the coupling of new multiscale models of the components of the grid, allow for treatment and mitigation of uncertainties in the system, and provide mathematical analysis and insight into the interaction effects for better understanding of this complex system. These mathematical foundations support the DOE's goal of moving from a reactive environment to a real-time predictive one.

III. Mathematical Challenges from Subsurface Flow and Transport for Energy Applications

These long-term mathematical challenges potentially include, but are not limited to, multiscale/ multiphysics modeling, characterizing uncertainty, optimization, and data assimilation techniques. Accurate models for subsurface flow and transport are needed to design optimal and efficient remediation strategies [3] and address the challenges related to geological CO_2 sequestration [10]. There is a strong need for significant advances in multiscale/ multiphysics models for subsurface flow and transport. Subsurface modeling can be highly uncertain, and characterization of the uncertainty becomes a crucial issue for decision-making and risk analysis in the design of remediation strategies. New optimization techniques and data assimilation strategies may be needed to make optimal use of available information. This will enable more accurate subsurface flow and transport modeling to develop more effective remediation strategies.

Another illustrative example is from geologic sequestration of large volumes of carbon dioxide, the challenge is that the relevant physical and chemical interactions occur on spatial scales that range from those of atoms, molecules, and mineral surfaces, up to tens of kilometers, and time scales that range from picoseconds to millennia and longer. Fundamental advances in the ability to simulate multiscale systems that may be perturbed during sequestration activities and for very long times afterward are needed. In addition, improved capabilities are needed to monitor those systems in real time with increasing spatial and temporal resolution. This will enable accurately predicting the performance of the subsurface storage systems building confidence to meet design targets.

IV. Mathematical Challenges from Office of Science Facilities

There is a rich set of mathematical challenges that has not been articulated or applied to enhancing scientific discovery at DOE Office of Science Facilities. A recent workshop and report on *Data and Communications in Basic Energy Sciences* [11] focused on identifying opportunities and needs for data analysis, ownership, storage, mining, provenance and data transfer at light sources, neutron sources, microscopy centers and other facilities. A MMICC addressing the broader long-term mathematical challenges, which potentially include both experimental and simulation information, may enable better understanding of future DOE SC facility challenges.

Organizational Structure and Management Plan for MMICCs

Each MMICC will require expertise from a variety of different mathematical sub-disciplines. In addition, the MMICCs may require long-term engagement from problem inception to demonstration of results with domain scientists, computational scientists, and/or computer scientists in working towards the Grand Challenges. Proposals may include funding for domain scientists or other expertise; the level of involvement or commitment is to be determined by the Center. Each MMICC must identify an appropriate team and organizational structure that enables it to function efficiently in a collaborative manner to address the multifaceted integrated mathematical research challenges and the associated grand challenges. The MMICC Director ("Center Director") will serve as the primary contact responsible for communications with the DOE Program Office on behalf of all of the Principal Investigators in the MMICC. A lean management structure is sought; as such, it is expected that the Center Director will provide overall direction for the center ensuring internal coordination and collaboration as well as appropriate external outreach. The expectation is the Center Director will need to devote at least 33% of their time to the MMICC. The MMICC structure must be sufficiently flexible to adapt to changing technical challenges and scientific needs. In particular, it is expected that there will be changes in the multifaceted mathematics research plans as research progresses; equally likely are potential changes in the scientific challenges. Proposals should identify key senior personnel who will contribute in a substantive, measurable way to the scientific/technical development or execution of the project. It is acceptable to not explicitly name all junior staff; however, the proposal should include a discussion of how the center will be fully staffed. Given the diversity of the expertise required for a successful MMICC, it is expected that MMICCs will involve more than one institution. Multi-institutional collaborations should be identified in the proposal. The role of each institution should be discussed in terms of the contributions to the MMICC. Additional collaborations may form after an MMICC is established; proposals should include a discussion of how this may be accomplished.

Proposers should identify key milestones of the research plan, including interactions among researchers, key dependencies (internal or external), and level of risk. It is expected that the MMICC will have multiple levels of risk. The milestones should:

1. Advance multifaceted, integrated mathematics that spans, as appropriate, novel formulations, discretizations, algorithm development, data analysis techniques, uncertainty quantification methodologies, optimization techniques, and other mathematical approaches;
2. Address one or more Grand Challenge problems with clear relevance and impact to the DOE; and
3. Advance the field of applied and computational mathematics.

The proposal must include a concise management plan that addresses the organization, communications, and coordination of the collaborating researchers. This plan should include mitigation strategies for foreseeable risks and explain how the project will have sufficient flexibility to adapt to changing priorities, challenges, and resources. Centers will be reviewed annually; additional informal reviews and reports will be conducted throughout the year. The proposal must contain a plan to support technical and programmatic review of the Center.

References

1. DOE 2012 Applied Math Summit, http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/doe-applied-math-summit/
2. DOE ASCR 2012 Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems, http://www.orau.gov/mathworkshop2011/
3. DOE ASCR 2012 A Multifaceted Mathematical Approach for Complex Systems Report, http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Multifaceted_Mathematical_Approach_for_Complex_Systems.pdf
4. DOE Basic Energy Sciences: Basic Research Needs Reports, http://science.energy.gov/bes/besac/reports

5. DOE Basic Energy Sciences Report 2010: Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Bes_exascale_report.pdf
6. DOE Basic Energy Sciences Report 2011: Computational Materials Sciences and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science, http://science.energy.gov/~/media/bes/pdf/reports/files/cmsc_rpt.pdf
7. National Science and Technology Council, Committee on Technology, Materials Genome Initiative, 2011, http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf
8. DOE Basic Energy Sciences Workshop Report 2007: Basic Research Needs: Catalysis for Energy, http://science.energy.gov/~/media/bes/pdf/reports/files/cat_rpt.pdf
9. DOE Office of Electricity Delivery and Energy Reliability 2011 Report: Computational Needs for the Next Generation Electric Grid Proceedings, http://energy.gov/sites/prod/files/FINAL_CompNeeds_Proceedings2011.pdf
10. DOE Basic Energy Sciences Workshop Report: Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems. http://science.energy.gov/~/media/bes/pdf/reports/files/geo_rpt.pdf
11. DOE Basic Energy Sciences Data Workshop 2011, https://www.orau.gov/dataworkshop2011/default1.htm

Additional Proposal Requirements: We are seeking strong teams that address novel research requiring multifaceted, integrated mathematics. We will give priority to proposals that clearly discuss one or more scientific or engineering grand challenges, abstract an interrelated set of mathematics research challenges that are optimally addressed through a multifaceted, integrated approach and have potential DOE impact in the 5-10+ year timeframe. Organizationally, the proposal must identify the Center Director, key personnel who will make significant technical contributions to the proposed research, and key collaborations.

For official postings see the Office of Science Grants and Contracts web site, http://www.science.doe.gov/grants.

Collaborations: Collaborative research projects with other institutions, such as universities, industry, non- profit organizations, and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are strongly encouraged. Collaborative proposals submitted from different institutions should clearly indicate they are part of a proposed collaboration and contain the same title, abstract and narrative for that research project. In addition, such proposals must describe the work and the associated budget for the research effort being performed under the leadership of the Principal Investigator at that participating institution. These collaborative proposals should all have the same title as the Lead Institution.

Program Funding: Awards are expected to be made for a period of five years at a funding level of up to $9,000,000 per year to support multiple awards in Fiscal Year 2012, with out-year support contingent on the availability of appropriated funds and satisfactory progress. The award size will depend on the number of meritorious proposals and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from $2,000,000 to $3,500,000 per year.

DOE is under no obligation to pay for any costs associated with the preparation or submission of a proposal. DOE reserves the right to fund, in whole or in part, any, all, or none of the proposals submitted in response to this Program Announcement.

The instructions and format described below should be followed. You must reference Program Announcement LAB 12-698 on all submissions and inquiries about this program.

OFFICE OF SCIENCE
GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS
TO BE SUBMITTED BY NATIONAL LABORATORIES

Proposals from DOE National Laboratories submitted to SC as a result of this Program Announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

Evaluation Criteria

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance. Included within each criterion are specific questions that the merit reviewers will be asked to consider:

1. **Scientific and/or Technical Merit of the Project**
    a. What compelling, scientific grand challenge problems are identified and to what extent are they relevant to the DOE mission? What is the potential long-term impact of the MMICC?
    b. What are the main technical challenges and how well does the proposal articulate the difficulties that bar scientific progress?
    c. What fundamental mathematical advances are needed to achieve the desired scientific discoveries and breakthroughs?
    d. What is the likelihood and to what extent can the proposed research overcome the main technical challenges to the scientific grand challenge problems?

2. **Appropriateness of the Proposed Method or Approach**
    a. How well does the proposal articulate a mathematical, multifaceted, integrated approach to addressing the scientific grand challenge problems?
    b. To what extent does the proposed research treat the grand challenges holistically and justify the choice of mathematical abstractions?
    c. To what extent does the proposed research identify novel mathematical models, methods and approaches of individual components as well as integrated approaches?
    d. How well does the research plan describe metrics that will allow research progress and contributions to be measured?
    e. To what extent does the proposal articulate a plan for effectively coordinating and managing the research activities of the Center?

3. **Competency of Applicant's Personnel and Adequacy of Proposed Resources**
    a. How well is the role of the Center Director articulated? What prior experience and success does the Center Director have in effectively managing collaborative teams?
    b. To what extent are the roles of key personnel adequately described? To what extent do key personnel have a proven record of success in delivering results in computational and applied mathematics?

c. To what extent do key personnel have extensive research and development experience in the mathematical sub-disciplines needed for the success of the Center?

4. **Reasonableness and Appropriateness of the Proposed Budget**
   a. To what extent is the overall requested budget appropriate for the scope of the work proposed?
   b. Is the requested budget and level of effort of the Center Director and key personnel sufficient and appropriate to achieve success?
   c. How well does the requested budget support the Center's management structure? What Center procedures, if any, will be used to permit flexibility in staffing and allow for additional future collaborations?
   d. What Center procedures, if any, will be used for reallocating funds to address changing priorities?

The selection official will also consider the following program policy and management factors in the selection process:

a. Potential impact of proposed research activities on DOE mission.
b. Potential for developing synergies and/or relation of the proposed research activities to other research efforts supported by ASCR, for example, other applied mathematics projects, SciDAC Institutes, and/or SciDAC Partnerships; and
c. Total amount of DOE funds available.

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the Program Announcement and the agency's programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

2. Summary of Proposal Contents

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page
- Table of Contents
- Budget (DOE Form 4620.1) and Budget Explanation
- Abstract (one page)
- Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel – 20-page limit
- Literature Cited
- Biographical Sketch(es)
- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

2.1 Submission Instructions

LAB administrators should submit the entire LAB proposal and FWP via Searchable FWP (https://www.osti.gov/fwp). Questions regarding the appropriate LAB administrator or other questions regarding submission procedures can be addressed to the Searchable FWP Support Center. All submission and inquiries about this Program Announcement must reference Program Announcement to DOE National Laboratories LAB 12-698. Full proposals submitted in response to this Program Announcement must be submitted to the searchable FWP database no later than **June 1, 2012,** 11:59 pm, Eastern Time. It is important that the entire peer reviewable proposal be submitted to the Searchable FWP system as a single PDF file attachment.

3. Detailed Contents of the Proposal

Adherence to type size and line spacing requirements is necessary for several reasons. No researcher should have the advantage, or by using small type, of providing more text in his or her proposal. Small type may also make it difficult for reviewers to read the proposal. Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher, but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

3.1 Field Work Proposal Format (Reference DOE Order 412.1A) (DOE ONLY)

The FWP is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review.

3.2 Proposal Cover Page

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project:
SC Program Announcement title and number: **2012 Mathematical Multifaceted Integrated Capability Centers (MMICCs) – LAB 12-698**
Name of laboratory:
Name of principal investigator (PI):
Position title of PI:
Mailing address of PI:
Telephone of PI:
Fax number of PI:
Electronic mail address of PI:
Name of official signing for laboratory*:
Title of official:
Fax number of official:
Telephone of official:
Electronic mail address of official:

Requested funding for each year; total request:
Use of human subjects in proposed project:
If activities involving human subjects are not planned at any time during the proposed project period, state "No"; otherwise state "Yes", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.
Use of vertebrate animals in proposed project:
If activities involving vertebrate animals are not planned at any time during this project, state "No"; otherwise state "Yes" and provide the IACUC Approval date and Animal Welfare Assurance number from NIH and include all necessary information with the proposal.
Signature of PI, date of signature:
Signature of official, date of signature*:

* The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

3.3 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages, and do not use suffices, such as 5a, 5b.

3.4 Budget and Budget Explanation

A detailed budget is required for the entire project period and for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site: http://www.science.doe.gov/grants/budgetform.pdf

3.5 Abstract

Summarize the proposal in one page. Give the project objectives (in broad scientific terms), the approach to be used, and what the research is intended to accomplish. State the hypotheses to be tested (if any). At the top of the abstract give the lead DOE National Laboratory, project title, names of all the investigators and their institutions, and contact information for the principal investigator, including e-mail address.

3.6 Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel).

The narrative comprises the research plan for the project and is limited to a **maximum of 20 pages**. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. It is important that the 20-page technical information section provide a complete description of the proposed work, because reviewers are not obliged to read the Appendices. Proposals exceeding these page limits may be rejected without review or the first 20 pages may be reviewed without regard to the remainder.

The page count of 20 does not include the Cover Page and Budget Pages, the Title Page, the biographical material and publication information, or any Appendices. However, it is important that the 20-page technical information section provide a complete description of the proposed work, since reviewers are not obliged to read the Appendices. <u>Please do not submit general letters of support as these are not used in making funding decisions and can interfere with the selection of peer reviewers</u>.

<u>Background</u>

Background – explanation of the importance and relevance of the proposed work.

<u>Proposed Research and Tasks</u>

In addition to the technical description of the proposed work and tasks, include a discussion of schedule, milestones, and deliverables.

Is this a Collaboration? If yes, please list Collaborating Institutions/PIs* and indicate which ones will also be submitting proposals. Also indicate the PI who will be the point of contact and coordinator for the combined research activity.

* Note that collaborating proposals must be submitted separately. However, if you are submitting as a Lead Institution, in addition to meeting all criteria for submitting a peer reviewable proposal, please provide the following information in the form of a table as shown below:

Sample Table for the Lead Institution ($ in thousands)

2012 MMICC	Year 1	Year 2	Year 3	Year 4	Year 5	Total
Name of the Center Director and Institution	$	$	$	$	$	$
Collaborating Institutions						**Total**
Name of Institution and Principal Investigator	$	$	$	$	$	$
Name of Institution and Principal Investigator	$	$	$	$	$	$
Name of Institution and Principal Investigator	$	$	$	$	$	$
TOTALS	$	$	$	$	$	$

3.7 Literature Cited

Give full bibliographic entries for each publication cited in the narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal.

3.8 Biographical Sketches

This information is required for senior personnel at the institution submitting the proposal and at all subcontracting institutions (if any). The biographical sketch is limited to a maximum of two pages for each investigator and must include:

Education and Training. Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

Research and Professional Experience. Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

Publications. Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.

Synergistic Activities. List no more than five professional and scholarly activities related to the effort proposed.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information must also be provided in each biographical sketch.

> *Collaborators and Co-editors:* A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co-authors with the investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, include those individuals who are currently or have been co-editors of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. Finally, list any individuals who are not listed in the previous categories with whom you are discussing future collaborations. If there are no collaborators or co-editors to report, this should be so indicated.
>
> *Graduate and Postdoctoral Advisors and Advisees:* A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations. A list of the names of the individual's graduate students and postdoctoral associates during the past five years, and their current organizational affiliations.

3.9 Description of Facilities and Resources

Facilities to be used for the conduct of the proposed research should be briefly described. Indicate the pertinent capabilities of the institution, including support facilities (such as machine shops), that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution (if any).

3.10 Other Support of Investigators

Other support is defined as all financial resources, whether Federal, non-Federal, commercial, or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort (months per year or percentage of the year) devoted to the project.

3.11 Appendix

Information not easily accessible to a reviewer may be included in an appendix, but **do not use the appendix to circumvent the page limitations of the proposal.** Reviewers are not required to consider information in an appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper.

The appendix may contain the following items: up to five publications, manuscripts accepted for publication, abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community. If letters of endorsement are included in a proposal, they will be removed before the proposal is submitted for review.

4. Detailed Instructions for the Budget (DOE Form 4620.1 "Budget Page" may be used).

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of $50,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off- the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.