Software Infrastructure for Sustained Innovation (SI²)
Grand Challenges in the Chemical Sciences

PROGRAM SOLICITATION
NSF 12-576

National Science Foundation

Directorate for Mathematical & Physical Sciences
   Division of Chemistry
   Office of Multidisciplinary Activities

Office of Cyberinfrastructure

UK Engineering and Physical Science Research Council

Engineering and Physical Sciences Research Council

Preliminary Proposal Due Date(s) *(required)* (due by 5 p.m. proposer's local time)**:**

   August 27, 2012

Full Proposal Deadline(s) (due by 5 p.m. proposer's local time):

   September 27, 2012

IMPORTANT INFORMATION AND REVISION NOTES

This solicitation under the SI² program is limited to collaborative projects between US and UK researchers addressing software for grand challenges in the chemical sciences. Only SSI category awards will be made (SSI awards target large, interdisciplinary teams organized around the development and application of common software infrastructure aimed at solving common research problems. SSI awards will result in a sustainable community software framework serving a diverse community).

Prospective PIs are strongly encouraged to contact appropriate program directors to discuss the suitability of their proposed activities to the particular intent and programmatic scope of this SI² solicitation prior to preliminary proposal submission.

SUMMARY OF PROGRAM REQUIREMENTS

General Information

Program Title:

   Software Infrastructure for Sustained Innovation (SI²)
   Grand Challenges in the Chemical Sciences

Synopsis of Program:

   Software is an integral enabler of computation, experiment and theory and a primary modality for realizing the NSF's vision for a Cyberinfrastructure Framework for 21st Century Science and Engineering (CIF21) (http://www.nsf.gov/cif21). Scientific discovery and innovation are advancing along fundamentally new pathways opened by the development of increasingly sophisticated software. Software is also directly responsible for increased scientific productivity and significant enhancement of researchers' capabilities. In order to nurture, accelerate and sustain this critical mode of scientific progress, NSF established the multi-tiered *Software Infrastructure for Sustained Innovation (SI²)* program, with the overarching goal of transforming innovations in research and education into sustained software resources that are an integral part of the cyberinfrastructure.

   Grand challenges in the chemical sciences will be advanced through the provision of enabling and sustainable software that allows researchers to flexibly and rapidly prototype and test new algorithms or methods; leverage new heterogeneous architectures; and explore new data-enabled scenarios. The NSF seeks to encourage collaborative software activities with foreign investigators which advance software innovation, capabilities, support and sustainability. This SI² solicitation is for international software collaborations addressing grand challenges in the chemical sciences, in partnership with the EPSRC in the United Kingdom.

Cognizant Program Officer(s):

Please note that the following information is current at the time of publishing. See program website for any updates to the points of contact.

- Evelyn Goldfield, Program Director, MPS/CHE, telephone: (703) 292-2173, email: egoldfie@nsf.gov

- Gabrielle Allen, Program Director, OD/OCI, telephone: (703) 292-2598, email: gdallen@nsf.gov

- Daniel S. Katz, Program Director, OD/OCI, telephone: (703) 292-2254, email: dkatz@nsf.gov

- Edward Clarke, Senior Manager, International Programs, EPSRC, telephone: +44 1793 444438, email: Edward.Clarke@epsrc.ac.uk

- Bruce Johnson, Program Director, MPS/CHE, telephone: (703) 292-2698, email: brjohnso@nsf.gov

- Sharon Neal, Program Director, MPS/CHE, telephone: (703) 292-4952, email: shneal@nsf.gov

Applicable Catalog of Federal Domestic Assistance (CFDA) Number(s):

- 47.049 --- Mathematical and Physical Sciences
- 47.080 --- Office of Cyberinfrastructure

Award Information

Anticipated Type of Award: Standard Grant or Continuing Grant

Estimated Number of Awards: 3 to 9

Anticipated Funding Amount: $4,500,000 pending availability of funds. The expected funding from the EPSRC for the UK component of US-UK collaborative projects will be a maximum of £3,000,000.

Eligibility Information

Organization Limit:

Proposals may only be submitted by the following:

- Universities and Colleges - Universities and two- and four-year colleges (including community colleges) accredited in, and having a campus located in the US, acting on behalf of their faculty members. Such organizations also are referred to as academic institutions.
- Non-profit, non-academic organizations: Independent museums, observatories, research labs, professional societies and similar organizations in the U.S. associated with educational or research activities.

PI Limit:

None Specified

Limit on Number of Proposals per Organization:

None Specified

Limit on Number of Proposals per PI: 1

An individual may participate as Principal Investigator, co-Principal Investigator or other Senior Personnel in at most one full proposal in this competition. Any individual whose biographical sketch is provided as part of the proposal will be considered as Senior Personnel in the proposed activity, with or without financial support from the project. After the proposal submission deadline, if a person appears on more than one full proposal both proposals will be returned without review. For this purpose, a multi-institution collaborative project is treated as one proposal that is considered submitted when the last component proposal is submitted.

Proposal Preparation and Submission Instructions

A. Proposal Preparation Instructions

- **Letters of Intent:** Not Applicable

- **Preliminary Proposals:** Submission of Preliminary Proposals is required. Please see the full text of this solicitation for further information.

- **Full Proposals:**
  - Full Proposals submitted via FastLane: NSF Proposal and Award Policies and Procedures Guide, Part I: Grant Proposal Guide (GPG) Guidelines apply. The complete text of the GPG is available electronically on the NSF website at: http://www.nsf.gov/publications/pub_summ.jsp?ods_key=gpg.
  - Full Proposals submitted via Grants.gov: NSF Grants.gov Application Guide: A Guide for the Preparation and Submission of NSF Applications via Grants.gov Guidelines apply (Note: The NSF Grants.gov Application Guide is available on the Grants.gov website and on the NSF website at: http://www.nsf.gov/publications/pub_summ.jsp?ods_key=grantsgovguide)

B. Budgetary Information

- **Cost Sharing Requirements:** Inclusion of voluntary committed cost sharing is prohibited.

- **Indirect Cost (F&A) Limitations:** Not Applicable

Other Budgetary Limitations: Not Applicable

C. Due Dates

- **Preliminary Proposal Due Date(s)** *(required)* (due by 5 p.m. proposer's local time)**:**

    August 27, 2012

- **Full Proposal Deadline(s)** (due by 5 p.m. proposer's local time):

    September 27, 2012

Proposal Review Information Criteria

Merit Review Criteria: National Science Board approved criteria. Additional merit review considerations apply. Please see the full text of this solicitation for further information.

Award Administration Information

Award Conditions: Additional award conditions apply. Please see the full text of this solicitation for further information.

Reporting Requirements: Standard NSF reporting requirements apply.

TABLE OF CONTENTS

I. INTRODUCTION

Software is a primary modality through which innovation and discovery will be realized as part of NSF's vision for a Cyberinfrastructure Framework for 21st Century Science and Engineering. Software permeates all aspects and layers of cyberinfrastructure (from application codes and frameworks, programming systems, libraries and system software, to middleware, operating systems, networking and the low-level drivers). CIF21 envisions a linked cyberinfrastructure architecture that integrates large-scale computing, high-speed networks, massive data archives, instruments and major facilities, observatories, experiments, and embedded sensors and actuators, across the nation and the world.

The CIF21 software infrastructure should address the complexity of this cyberinfrastructure, accommodating disruptive hardware trends, ever-increasing data volumes, complex application structures and behaviors and emerging concerns such as fault-tolerance and energy efficiency. The software should be continually refined, at one end, to support these new trends and requirements. At the other end, the software should support new advances in the disciplines and their computational methodologies. Across the spectrum, attention should be paid to reducing complexity so that software can be easily used. There is also a new sense of urgency and opportunity for such an investment driven in part by the confluence of various stresses, including disruptive hardware trends, new technologies, new application formulations, emerging new and diverse collections of data, and community readiness. Education is an important element needed to sustain this vision and to propagate through time a vital and responsive cyberinfrastructure -- one that

builds upon the most crucial existing cyberinfrastructure elements and one that innovatively creates needed new elements. SI^2 will contribute to an able workforce capable of exploiting the full capability of the cyberinfrastructure and the promise for innovation in

science and engineering.

Grand Challenges in the Chemical Sciences

Grand challenges in the chemical sciences will be advanced through the provision of enabling and sustainable software that allows researchers to flexibly and rapidly prototype and test new algorithms or methods; leverage new heterogeneous architectures; and explore new data-enabled scenarios. Recognizing the potential for international collaboration to advance research and development in software infrastructure for the chemical sciences, NSF has partnered with the Engineering and Physical Research Council (EPSRC) of the United Kingdom.

II. PROGRAM DESCRIPTION

Grand Challenge areas of interest include but are not limited to:

- **Exploring the chemical roots of biological complexity:** Computation geared toward modeling and simulation across multiple length scales to describe the emergence of complex structures from basic interactions of smaller units.

- **Identifying fundamental sustainable chemistry that addresses the critical needs of society:** Computation geared toward enabling fundamental scientific advances in utilizing new non-petroleum sources of raw materials, in enabling use of cheap non-toxic earth-abundant chemicals and materials, in economically recycling such things as rare-earth elements and phosphorus, and in devising environmentally friendly chemical reactions.

- **Understanding and predicting energy landscapes of reactive systems:** Computation geared toward predicting synthetic chemical routes, product branching ratios, reaction rates, energy costs, and other dynamic and kinetic quantities.

- **Molecular-scale tailoring of meso- and macro-scale properties:** Computation geared toward predicting macroscopic properties starting from atoms and molecules. Design of materials with sophisticated properties also requires theoretical understanding of how to control the self-assembly of matter, particularly how to control large numbers of weak interactions.

- **Harnessing light energy to bring about chemical change or for generating electricity:** Computation geared toward modeling and simulation methods to describe transport of energy and electrons in electronically excited states of complex systems.

- **Exploring the role of quantum effects in the dynamics of complex and condensed phase systems:** Computations geared toward understanding and predicting tunneling, long-lived coherences, and electronically non-adiabatic interactions, as well as the spectroscopic signatures of these processes.

Software used to address these grand challenge problems may include

Electronic structure/quantum chemistry codes, modeling tools for condensed phase systems including incorporation of quantum effects; multi-scale, multi-physics modeling platforms, advances in simulation software, including more sophisticated, accurate physics-based force fields, more effective phase-space sampling and efficient time-evolution methods. Innovative and forward-looking approaches to software design and generation are encouraged. Software features of interest may include code that is highly scalable on advanced computer architectures, architecture-agnostic code, scalable, portable and optimized libraries, frameworks that enable interoperability or plug and play capabilities, capabilities for managing, utilizing and analyzing large volumes of data, automatic code generation.

Sustainable Software

The goal of the SI^2 program is to create a software ecosystem that scales from individual or small groups of software innovators to large hubs of software excellence. The overall program includes three classes of awards: (1) Scientific Software Elements (SSE); (2) Scientific Software Integration (SSI); (3) Scientific Software Innovation Institutes (S2I2).

This solicitation is limited to SSI awards for collaborative partnerships between USA and UK that address grand challenges in the chemical sciences.

The SI^2 program envisions an integrated software infrastructure composed of interlocking and cooperating projects from the different classes of awards made through the overall program. It is expected that each SSI group will develop meaningful affiliations with SSE (Scientific Software Element) awardees, and that they will affiliate with one or more S2I2 institutes as they come online.

A **competitive** SI^2 proposal will:

- Describe application areas in science or engineering where the identified software is needed and describe how the use of the identified software will have a significant impact on science and engineering research;
- Describe the targeted user communities of the proposed software and how they will be engaged; and
- Provide a compelling discussion of the software's potential use by a wider audience and its contribution to a national cyberinfrastructure.

SSI awards target larger, interdisciplinary teams organized around the development and application of common software infrastructure that addresses shared research needs. SSI awards will result in a sustainable community software framework serving a diverse community or communities. These awards will focus on software architectures, processes that explicitly address issues of sustainability, manageability, usability, composability and interoperability, as well as environments (e.g., code repository, build and test framework, reporting mechanisms, etc.) that are meaningful for the targeted science community. Well thought-out dissemination

and outreach mechanisms, pathways for integration of community software elements (such as those developed by SSE teams) into the developed framework, as well as support structures, will be an integral part of these awards. When appropriate, involvement with industry and government laboratories, and partnering with international efforts are encouraged.

US-UK Collaborative Projects

Recognizing the potential for international collaboration to advance research, development and support of sustainable software infrastructure, NSF has partnered for this solicitation with the Engineering and Physical Research Council (EPSRC) of the UK. This partnership will catalyze new international collaborations and facilitate coordinated funding of U.S. and U.K. research collaborations. The U.K. component of the Collaborative proposal must fit within EPSRC's remit. The U.S. component of the Collaborative proposal must be responsive to scientific priorities in the involved NSF units.

U.K. researchers must meet EPSRC eligibility requirements and must apply through an institution eligible to receive EPSRC's funding rules. Please see EPSRC Funding Guide at www.epsrc.ac.uk. Individuals considering submitting a proposal to this solicitation are strongly encouraged to contact the relevant Cognizant Program Officer to confirm that the UK component fits EPSRC's requirements. Applications with non-eligible UK partners will not be considered for funding under this solicitation.

Industry and International Participation in SI^2: NSF encourages participation by industry and international collaborators in all classes of SI^2 awards where it clearly strengthens the proposed activity (e.g., involvement of specific and unique expertise or resources or addressing sustainability). This solicitation provides specific collaboration opportunities with the UK, however this specific activity does not preclude additional international collaborations.

- International participants are encouraged to seek support from their funding organizations. NSF funds may not be used to support the expenses of international researchers at their home institution. However, NSF funds may be used for travel expenses for US scientists and students in exchange integral to the project, or for international collaborators to participate in activities in the US. For those who plan to submit a proposal with international counterparts, please consult NSF Policies and Practices for International Engagements.
- The SI2 program recognizes that software is a fundamental infrastructure that cross-cuts academic, government, civic, and commercial organizations. The program encourages proposals to explore novel partnerships beyond academe wherever beneficial and permissible within the guidelines of the NSF GPG.

III. AWARD INFORMATION

Estimated program budget, number of awards and average award size/duration are subject to the availability of funds.

Awards are anticipated to total between $500,000 and $1,500,000 with an award duration of three or four years. Additional funding for the UK component has a maximum total (for all years) award size of £1 million and maximum award duration of four years. The total expected funding available is $4.5 million from NSF and £3 million from EPSRC (which reflects 80% of full economic costs in the U.K.).

The U.K. component of the collaboration will be awarded through the EPSRC in accordance with its policies. All applications selected for funding will be required to submit the costs for the UK element of the proposal via the RCUK's Je-S application submission system before final sign-off. UK collaborators should therefore ensure they are registered Je-S users before the proposal is submitted.

IV. ELIGIBILITY INFORMATION

Organization Limit:

Proposals may only be submitted by the following:

- Universities and Colleges - Universities and two- and four-year colleges (including community colleges) accredited in, and having a campus located in the US, acting on behalf of their faculty members. Such organizations also are referred to as academic institutions.
- Non-profit, non-academic organizations: Independent museums, observatories, research labs, professional societies and similar organizations in the U.S. associated with educational or research activities.

PI Limit:

None Specified

Limit on Number of Proposals per Organization:

None Specified

Limit on Number of Proposals per PI: 1

An individual may participate as Principal Investigator, co-Principal Investigator or other Senior Personnel in at most one full proposal in this competition. Any individual whose biographical sketch is provided as part of the proposal will be considered as Senior Personnel in the proposed activity, with or without financial support from the project. After the proposal submission deadline, if a person appears on more than one full proposal both proposals will be returned without review. For this purpose, a multi-institution collaborative project is treated as one proposal that is considered submitted when the last component proposal is submitted.

V. PROPOSAL PREPARATION AND SUBMISSION INSTRUCTIONS

A. Proposal Preparation Instructions

Preliminary Proposals *(required)*: Preliminary proposals are required and must be submitted via the NSF FastLane system, even if full proposals will be submitted via Grants.gov.

Preliminary proposals must be submitted to NSF by the US investigator. Preliminary proposals must adhere to the general guidelines described in the NSF's Grant Proposal Guide (GPG), except as specified below. One preliminary proposal per project should be submitted.

Cover Sheet: The title of the proposal to NSF should begin with "SI2-CHE:". In addition the US PI should check the box,"International Cooperative Activities" listed under Other Information and list the appropriate countries involved. The PI must select the option indicating that this is a preliminary proposal. For correct FastLane processing, enter $2 as the requested amount.

Project Summary:

The one page project summary should clearly state: (1) the grand challenge or challenges in the chemical sciences which would be advanced through this software activity; (2) the motivation for an international collaboration; (3) the intellectual merit; (4) the broader impacts.

Project Description:

The project description must be no more than four pages and should include just the following sections:

Section 1: List the names, affiliations and e-mail addresses of all PIs, Co-PIs, and other senior personnel, including foreign participants. For each senior personnel indicate their expertise and their role in the project.

Section 2: Describe the grand challenge problem or problems in the chemical sciences which this activity will advance.

Section 3: Describe the proposed software project including expected outcomes and products, key preliminary activities, and an outline of the research and development plan.

Section 4: Describe the motivation and justification for the international collaborative activity, summarize the collaborative approaches and software development mechanisms which will be used. In particular state the mechanisms which will be used for distributing software (e.g. open source license).

References Cited may contain up to one page of references to provide context for the proposed activities. The reference section will not count against the page limit of the preliminary proposal project description.

For the US investigators, **Biographical Sketches** should be submitted using the NSF standard format specified in the GPG. Biographical sketches for foreign investigators should be limited to 2 pages each and be part of a FastLane supplementary document.

For the US investigators, **Current and Pending support** statements should be submitted using the NSF standard format specified in the GPG. For the foreign investigator the information about current and pending support should be part of a FastLane supplementary document.

The remaining standard proposal sections (Budget, Budget Justification, Facilities and Equipment) are not required in this preliminary proposal. Other supporting documentation (including preprints, letters or support or collaboration) are not permitted in this preliminary proposal.

Preliminary Proposal Review Procedure

The preliminary proposals will be reviewed by NSF and the EPSRC. At NSF, the preliminary proposals will be reviewed programmatically for their fit to NSF and specifically to the NSF Division of Chemistry in terms of scientific content. The Division of Chemistry will only encourage proposals involving software that specifically enables and advances the science supported by its programs: Chemical Synthesis; Chemical Catalysis; Chemical Theory, Models and Computational Methods; Chemical Imaging and Measurement; Chemical Structure, Dynamics and Mechanisms; Macromolecular Supramolecular and Nanochemistry; Environmental Chemical Sciences or Chemistry of Life Process. A detailed description of these programs can be found at: http://www.nsf.gov/div/index.jsp?div=CHE

The preliminary proposals will also be reviewed to ensure that the proposed projects do not significantly overlap projects that are already funded by NSF or other US funding agencies. Submission of full proposals that represent an incremental advance over currently funded work will be discouraged. Preliminary proposals must demonstrate a clear need for the international collaboration and provide an explicit statement of the intellectual contribution of both the U.S. and the U.K. contributors. **Upon completion of the review of the preliminary proposals, NSF and EPSRC will make a joint decision whether to encourage or discourage submission of full proposals to the program. Investigators will be notified of the decision 60 days prior to the full proposal submission deadline whenever possible**.

Full Proposal Preparation Instructions: Proposers may opt to submit proposals in response to this Program Solicitation via Grants.gov or via the NSF FastLane system.

- Full proposals submitted via FastLane: Proposals submitted in response to this program solicitation should be prepared and submitted in accordance with the general guidelines contained in the NSF Grant Proposal Guide (GPG). The complete text of the GPG is available electronically on the NSF website at: http://www.nsf.gov/publications/pub_summ.jsp?ods_key=gpg. Paper copies of the GPG may be obtained from the NSF Publications Clearinghouse, telephone (703) 292-7827 or by e-mail from nsfpubs@nsf.gov. Proposers are reminded to identify this program solicitation number in the program solicitation block on the NSF Cover Sheet For Proposal to the National Science Foundation. Compliance with this requirement is critical to determining the relevant proposal processing guidelines. Failure to submit this information may delay processing.

- Full proposals submitted via Grants.gov: Proposals submitted in response to this program solicitation via Grants.gov should be prepared and submitted in accordance with the NSF Grants.gov Application Guide: A Guide for the Preparation and Submission of NSF Applications via Grants.gov. The complete text of the NSF Grants.gov Application Guide is available on

the Grants.gov website and on the NSF website at: (http://www.nsf.gov/publications/pub_summ.jsp?
ods_key=grantsgovguide). To obtain copies of the Application Guide and Application Forms Package, click on the Apply tab
on the Grants.gov site, then click on the Apply Step 1: Download a Grant Application Package and Application Instructions
link and enter the funding opportunity number, (the program solicitation number without the NSF prefix) and press the
Download Package button. Paper copies of the Grants.gov Application Guide also may be obtained from the NSF
Publications Clearinghouse, telephone (703) 292-7827 or by e-mail from nsfpubs@nsf.gov.

In determining which method to utilize in the electronic preparation and submission of the proposal, please note the following:

Collaborative Proposals. All collaborative proposals submitted as separate submissions from multiple organizations must be
submitted via the NSF FastLane system. Chapter II, Section D.4 of the Grant Proposal Guide provides additional information on
collaborative proposals.

Cover Sheet: Provide a short informative title for the proposed SI^2 project. Full proposal titles should begin with "SI2-CHE:". The
system allows one PI and at most four Co-PIs to be designated for each proposal. Check the international activities box and list the
United Kingdom and any other countries involved. If needed, additional lead personnel should be designated as non co-PI, Senior
Personnel on the Budget form.

Project Summary (1-page limit): At the top of this page enter the title of the SI^2 project, beginning with "SI2-CHE:", the name
of the PI and the lead institution. Provide a summary description of the SI^2 project, including its transformative research and
education goals, the innovative software infrastructure being proposed, and the community (communities) that will be impacted, and
the motivation for and nature of the international collaboration. In separate statements, provide a succinct summary of the intellectual
merit and broader impacts of the proposed project. *Full proposals that do not address the intellectual merit and broader impacts of
the proposed project in separate statements will be returned without review.*

Project Description (15-page limit): The project description should explicitly address the following additional items:

- Define a research and development agenda that will lead to robust and sustainable software for grand challenges in the
  chemical sciences.
- Discuss how the proposed software will fill a recognized need and advance research capability.
- Provide a clear description of how the proposed software compares to alternative or existing elements (including other
  commercial and research solutions) and what are the limitations of these existing elements. Proposals that could be
  supported by other programs at NSF or at other agencies should be submitted to those programs, and possibly related
  programs should be explicitly identified and reasoned as to why the proposal is not appropriate for those opportunities.
  Investigators are encouraged to contact the program with questions about appropriateness for this program prior to sending
  in a proposal.
- Provide an explicit description of the engineering process to be used for the design, development, and release of the
  software, its deployments and associated outreach to the end user community, its interoperability with widely used tools by
  the community, and an evaluation plan that involves end users.
- Include a project plan, including user interactions and a community-driven approach, and provide a timeline including a
  proof-of-concept demonstration of the key software components. The proposal must include a list of tangible metrics, with
  end user involvement, to be used to measure the success of the software element developed, especially the quantitative
  and qualitative definition of a "working prototype" against which that milestone is judged, and the steps necessary to
  take the software element from prototype to dissemination into the community as reusable software resources.
- Provide a compelling discussion of the software's potential use by broader communities, preferably via use cases developed
  in concert with relevant domain scientists.
- Describe the extent to which issues of sustainability, manageability, usability and composability/interoperability will be
  addressed and integrated into the proposed software system.
- Provide an explicit outreach and education plan to allow additional end user groups to take advantage of the proposed work.
- Describe a sustainability plan for the developed software beyond the lifetime of the award. Identify the open source license
  to be used.
- The project description should clearly state the need and anticipated benefits of the proposed international collaboration and
  clearly describe the contribution of each collaborator to the proposed project.

Budget: The NSF awardees are expected to participate in an Annual PI meeting with travel costs supported by the award. These
travel costs should be included in the FastLane budget.

Supplementary Documents: In addition to *Data Management Plan* and the *Postdoctoral Research Mentoring Plan*, the
following items are the only items permitted as supplementary documentation or appendices. Supplementary documentation should
be saved and uploaded as a single Portable Document Format (PDF) file.

Management and Coordination Plan (3-page limit): Each full proposal must contain a clearly labeled management and
coordination plan, which includes: 1) the specific roles of the PI, co-PIs, other senior personnel and paid consultants at all
institutions involved, 2) how the project will be managed across institutions and disciplines, 3) identification of the specific
coordination mechanisms that will enable cross-institution and/or cross-discipline scientific integration (e.g., yearly workshops,
graduate student exchange, project meetings at conferences, use of videoconferences, use of common software repositories, build
process and/or test suites, etc.), and 4) pointers to the budget line items that support these management and coordination
mechanisms.

**Project Personnel (a text-searchable single PDF document, in FastLane, under Additional Single Copy
Documents).** List all Senior Personnel in the project. For each person, provide the last name, first name, and
institution/organization. In the main body of the proposal, a corresponding biographical sketch should be provided for all individuals
included on this list, as instructed in Section II.C.2.f of the Grant Proposal Guide.

**Collaborators/Individuals with Conflicts of Interest (a text-searchable single PDF document, in FastLane,
under Additional Single Copy Documents).** Provide a single list, alphabetically ordered by last name and including
institutional affiliation, of potential conflicts of interest, as specified in NSF's Grant Proposal Guide, for each PI, Co-PI and other
Senior Personnel. Include all co-authors/editors and collaborators (within the past 48 months), all graduate advisors and advisees,
and any other individuals or institutions with which the investigator has financial ties (please specify type). In addition, list all sub-
awardees who would receive funds through the SI^2 award.

US-UK Collaborator Information

Information for the UK portion of the US-UK Collaborative Proposal should be included as Supplementary Documents. That
information should include the following:

1. **Biographical sketches of UK senior personnel:** Those biographical sketches must conform to NSF format and

limitations.

2. **UK budget:** Costs for the UK component of the project should be entered onto the Je-S system but the completed form SHOULD NOT be submitted electronically to EPSRC at this stage. Instead a PDF version of the form should be saved and sent to the US lead PI for inclusion as a supplementary document in the proposal. Also an electronic copy of this document should be sent to the EPSRC Cognizant Program Officer at NSFSoftware@epsrc.ac.uk before C.O.P. on September 24th 2012. Full details on what is required can be obtained at http://www.epsrc.ac.uk/funding/apprev/fundingguide/Pages/default.aspx. Applicants should ensure that they contact the EPSRC Cognizant Program Officer at EPSRC to discuss the remit of their proposal and to confirm whether they should complete a EPSRC Je-S form.

3. **Letters of collaboration:** Letters of collaboration from UK scientists are required. These letters must be restricted to a statement of intent to collaborate only. Additional information on the nature of the collaboration and the roles of the investigators should be included in the Project Description.

4. **Institutional endorsement:** An institutional certification of the submission must be a signed letter from an authorized U.K. institutional representative with the following text: "I confirm on behalf of [insert name of institution] that the U.S.-U.K. Collaborative proposal between [insert name of US PI and institution] and [insert name of UK PI] is endorsed and has been submitted by [name of Research Office]."

Electronic Document. In addition to the above PDF document, proposers must send the following document immediately after submission of the proposal.

"List of Personnel, Collaborators and Affiliates": After receipt of the proposal number from FastLane, send an e-mail to si2@nsf.gov. The subject heading of the e-mail should note the proposal number and the lead institution. Attach a file in CSV "flat text" format (e.g., by saving an Excel spreadsheet as a CSV file), which lists the full names and institutional affiliations of all people having conflicts of interest (COI) with any PIs, Co-PIs, and other senior personnel (SP). The columns of the spreadsheet should be "proposal number", "PI/SP Last Name", "PI/SP First Name", "PI/SP Institution", "COI Last Name", "COI First Name", "COI Institution". This list will be used by NSF to check for conflicts of interest in assembling the review community. The filename should be the submitted proposal number followed by the three characters "coi" (for example, for a proposal number 1223456, this file name will be 1223456coi.csv). The 7-digit proposal number should appear in every row of the file. Each project participant should be listed (repeatedly) in all rows that name his/her conflicted individuals.

(There is redundancy between the Additional Single Copy Documents, which become part of the FastLane proposal file, and the Electronic Document, which is used for automated data handling. At present, it is not technically possible for one document to perform both functions.)

NOTE: Full proposals that fail to provide the above listed electronic documents with proper information and according to the required format will be returned without review.

Letters of Commitment (Optional): Include only official letters of commitment with specific commitments of resources from participating institutions or organizations anticipated to receive subawards, or from organizations that will provide resources for the project. Scan your signed letters and upload them into the Supplementary Documents section of Fastlane or Grants.gov, but do not send originals. Do not submit letters of support, which do not provide specific commitments of resources. For example, letters of endorsement and letters of a laudatory nature for the proposed project are not acceptable.

No other items or appendices are to be included. *Full proposals containing items other than those required above or by the Grant Proposal Guide (GPG) will not be reviewed.*

Proposers are reminded to identify the program solicitation number in the program solicitation block on the NSF Cover Sheet For Proposal to the National Science Foundation. Compliance with this requirement is critical to determining the relevant proposal processing guidelines. Failure to submit this information may delay processing.

B. Budgetary Information

Cost Sharing: Inclusion of voluntary committed cost sharing is prohibited

Budget Preparation Instructions:

Awardees are expected to participate in an Annual PI meeting with travel costs supported by the award. These travel costs should be included in the FastLane budget.

C. Due Dates

- **Preliminary Proposal Due Date(s)** *(required)* (due by 5 p.m. proposer's local time)*:*

    August 27, 2012

- **Full Proposal Deadline(s)** (due by 5 p.m. proposer's local time):

    September 27, 2012

D. FastLane/Grants.gov Requirements

- **For Proposals Submitted Via FastLane:**

    Detailed technical instructions regarding the technical aspects of preparation and submission via FastLane are available at: https://www.fastlane.nsf.gov/a1/newstan.htm. For FastLane user support, call the FastLane Help Desk at 1-800-673-6188 or e-mail fastlane@nsf.gov. The FastLane Help Desk answers general technical questions related to the use of the FastLane system. Specific questions related to this program solicitation should be referred to the NSF program staff contact(s) listed in Section VIII of this funding opportunity.

    Submission of Electronically Signed Cover Sheets. The Authorized Organizational Representative (AOR) must

electronically sign the proposal Cover Sheet to submit the required proposal certifications (see Chapter II, Section C of the Grant Proposal Guide for a listing of the certifications). The AOR must provide the required electronic certifications within five working days following the electronic submission of the proposal. Further instructions regarding this process are available on the FastLane Website at: https://www.fastlane.nsf.gov/fastlane.jsp.

- **For Proposals Submitted Via Grants.gov:**

  Before using Grants.gov for the first time, each organization must register to create an institutional profile. Once registered, the applicant's organization can then apply for any federal grant on the Grants.gov website. Comprehensive information about using Grants.gov is available on the Grants.gov Applicant Resources webpage: http://www07.grants.gov/applicants/app_help_reso.jsp. In addition, the NSF Grants.gov Application Guide provides additional technical guidance regarding preparation of proposals via Grants.gov. For Grants.gov user support, contact the Grants.gov Contact Center at 1-800-518-4726 or by email: support@grants.gov. The Grants.gov Contact Center answers general technical questions related to the use of Grants.gov. Specific questions related to this program solicitation should be referred to the NSF program staff contact(s) listed in Section VIII of this solicitation.

  Submitting the Proposal: Once all documents have been completed, the Authorized Organizational Representative (AOR) must submit the application to Grants.gov and verify the desired funding opportunity and agency to which the application is submitted. The AOR must then sign and submit the application to Grants.gov. The completed application will be transferred to the NSF FastLane system for further processing.

VI. NSF PROPOSAL PROCESSING AND REVIEW PROCEDURES

Proposals received by NSF are assigned to the appropriate NSF program where they will be reviewed if they meet NSF proposal preparation requirements. All proposals are carefully reviewed by a scientist, engineer, or educator serving as an NSF Program Officer, and usually by three to ten other persons outside NSF who are experts in the particular fields represented by the proposal. These reviewers are selected by Program Officers charged with the oversight of the review process. Proposers are invited to suggest names of persons they believe are especially well qualified to review the proposal and/or persons they would prefer not review the proposal. These suggestions may serve as one source in the reviewer selection process at the Program Officer's discretion. Submission of such names, however, is optional. Care is taken to ensure that reviewers have no conflicts of interest with the proposal.

A. NSF Merit Review Criteria

All NSF proposals are evaluated through use of the two National Science Board (NSB)-approved merit review criteria: intellectual merit and the broader impacts of the proposed effort. In some instances, however, NSF will employ additional criteria as required to highlight the specific objectives of certain programs and activities.

The two NSB-approved merit review criteria are listed below. The criteria include considerations that help define them. These considerations are suggestions and not all will apply to any given proposal. While proposers must address both merit review criteria, reviewers will be asked to address only those considerations that are relevant to the proposal being considered and for which the reviewer is qualified to make judgments.

What is the intellectual merit of the proposed activity?
How important is the proposed activity to advancing knowledge and understanding within its own field or across different fields? How well qualified is the proposer (individual or team) to conduct the project? (If appropriate, the reviewer will comment on the quality of the prior work.) To what extent does the proposed activity suggest and explore creative, original, or potentially transformative concepts? How well conceived and organized is the proposed activity? Is there sufficient access to resources?

What are the broader impacts of the proposed activity?
How well does the activity advance discovery and understanding while promoting teaching, training, and learning? How well does the proposed activity broaden the participation of underrepresented groups (e.g., gender, ethnicity, disability, geographic, etc.)? To what extent will it enhance the infrastructure for research and education, such as facilities, instrumentation, networks, and partnerships? Will the results be disseminated broadly to enhance scientific and technological understanding? What may be the benefits of the proposed activity to society?

Examples illustrating activities likely to demonstrate broader impacts are available electronically on the NSF website at: http://www.nsf.gov/pubs/gpg/broaderimpacts.pdf.

Mentoring activities provided to postdoctoral researchers supported on the project, as described in a one-page supplementary document, will be evaluated under the Broader Impacts criterion.

Additional Solicitation Specific Review Criteria

- Does the proposal discuss how the proposed software will fill a recognized need and advance research capability for grand challenges in the chemical sciences?
- Does the proposal provide a project plan and timeline including a proof-of-concept demonstration of any key software element that may be developed? Are tangible metrics described to measure the success of any software that may be developed, and the steps necessary presented to take the software from prototype to dissemination into the community as reusable software resources?
- Does the software engineering and development plan include and/or enable the integration of relevant research activities to ensure the software is responsive to new computing developments?
- To what extent are issues of sustainability, manageability, usability and composability/interoperability addressed and integrated into the proposed software?
- Does the project plan include user interaction, a community-driven approach, and a timeline of new feature releases? Does it plan to extend the work to additional user communities?

These US-UK collaborative projects will also be reviewed with respect to the extent which they motivate and justify a beneficial and substantial collaboration between US and UK partners that enhances research and development of software for grand challenges in

the chemical sciences. The review will take into account the UK research context.

For all proposals involving international collaborations, reviewers will consider: mutual benefits, true intellectual collaboration with the foreign partner(s), benefits to be realized from the expertise and specialized skills, facilities, sites and/or resources of the international counterpart, and active engagement and training of US students and early-career researchers.

NSF staff also will give careful consideration to the following in making funding decisions:

> ### Integration of Research and Education
> One of the principal strategies in support of NSF's goals is to foster integration of research and education through the programs, projects, and activities it supports at academic and research institutions. These institutions provide abundant opportunities where individuals may concurrently assume responsibilities as researchers, educators, and students and where all can engage in joint efforts that infuse education with the excitement of discovery and enrich research through the diversity of learning perspectives.

> ### Integrating Diversity into NSF Programs, Projects, and Activities
> Broadening opportunities and enabling the participation of all citizens -- women and men, underrepresented minorities, and persons with disabilities -- is essential to the health and vitality of science and engineering. NSF is committed to this principle of diversity and deems it central to the programs, projects, and activities it considers and supports.

B. Review and Selection Process

Proposals submitted in response to this program solicitation will be reviewed by Ad hoc Review and/or Panel Review.

Reviewers will be asked to formulate a recommendation to either support or decline each proposal. The Program Officer assigned to manage the proposal's review will consider the advice of reviewers and will formulate a recommendation.

After scientific, technical and programmatic review and consideration of appropriate factors, the NSF Program Officer recommends to the cognizant Division Director whether the proposal should be declined or recommended for award. NSF is striving to be able to tell applicants whether their proposals have been declined or recommended for funding within six months. The time interval begins on the deadline or target date, or receipt date, whichever is later. The interval ends when the Division Director accepts the Program Officer's recommendation.

A summary rating and accompanying narrative will be completed and submitted by each reviewer. In all cases, reviews are treated as confidential documents. Verbatim copies of reviews, excluding the names of the reviewers, are sent to the Principal Investigator/Project Director by the Program Officer. In addition, the proposer will receive an explanation of the decision to award or decline funding.

In all cases, after programmatic approval has been obtained, the proposals recommended for funding will be forwarded to the Division of Grants and Agreements for review of business, financial, and policy implications and the processing and issuance of a grant or other agreement. Proposers are cautioned that only a Grants and Agreements Officer may make commitments, obligations or awards on behalf of NSF or authorize the expenditure of funds. No commitment on the part of NSF should be inferred from technical or budgetary discussions with a NSF Program Officer. A Principal Investigator or organization that makes financial or personnel commitments in the absence of a grant or cooperative agreement signed by the NSF Grants and Agreements Officer does so at their own risk.

VII. AWARD ADMINISTRATION INFORMATION

A. Notification of the Award

Notification of the award is made to *the submitting organization* by a Grants Officer in the Division of Grants and Agreements. Organizations whose proposals are declined will be advised as promptly as possible by the cognizant NSF Program administering the program. Verbatim copies of reviews, not including the identity of the reviewer, will be provided automatically to the Principal Investigator. (See Section VI.B. for additional information on the review process.)

B. Award Conditions

An NSF award consists of: (1) the award letter, which includes any special provisions applicable to the award and any numbered amendments thereto; (2) the budget, which indicates the amounts, by categories of expense, on which NSF has based its support (or otherwise communicates any specific approvals or disapprovals of proposed expenditures); (3) the proposal referenced in the award letter; (4) the applicable award conditions, such as Grant General Conditions (GC-1); * or Research Terms and Conditions * and (5) any announcement or other NSF issuance that may be incorporated by reference in the award letter. Cooperative agreements also are administered in accordance with NSF Cooperative Agreement Financial and Administrative Terms and Conditions (CA-FATC) and the applicable Programmatic Terms and Conditions. NSF awards are electronically signed by an NSF Grants and Agreements Officer and transmitted electronically to the organization via e-mail.

*These documents may be accessed electronically on NSF's Website at http://www.nsf.gov/awards/managing/award_conditions.jsp?org=NSF. Paper copies may be obtained from the NSF Publications Clearinghouse, telephone (703) 292-7827 or by e-mail from nsfpubs@nsf.gov.

More comprehensive information on NSF Award Conditions and other important information on the administration of NSF awards is contained in the NSF *Award & Administration Guide* (AAG) Chapter II, available electronically on the NSF Website at http://www.nsf.gov/publications/pub_summ.jsp?ods_key=aag.

Special Award Conditions:

- All awardees are expected to participate in an Annual PI meeting with travel costs supported by the award.
- SSI awards are anticipated to be continuing awards and funds will be released annually subject to agreed-to milestones, and based on approval by NSF and the availability of funds.

C. Reporting Requirements

For all multi-year grants (including both standard and continuing grants), the Principal Investigator must submit an annual project report to the cognizant Program Officer at least 90 days before the end of the current budget period. (Some programs or awards require more frequent project reports). Within 90 days after expiration of a grant, the PI also is required to submit a final project report, and a project outcomes report for the general public.

Failure to provide the required annual or final project reports, or the project outcomes report will delay NSF review and processing of any future funding increments as well as any pending proposals for that PI. PIs should examine the formats of the required reports in advance to assure availability of required data.

PIs are required to use NSF's electronic project-reporting system, available through FastLane, for preparation and submission of annual and final project reports. Such reports provide information on activities and findings, project participants (individual and organizational), publications, and other specific products and contributions. PIs will not be required to re-enter information previously provided, either with a proposal or in earlier updates using the electronic system. Submission of the report via FastLane constitutes certification by the PI that the contents of the report are accurate and complete. The project outcomes report must be prepared and submitted using Research.gov. This report serves as a brief summary, prepared specifically for the public, of the nature and outcomes of the project. This report will be posted on the NSF website exactly as it is submitted by the PI.

More comprehensive information on NSF Reporting Requirements and other important information on the administration of NSF awards is contained in the NSF *Award & Administration Guide* (AAG) Chapter II, available electronically on the NSF Website at http://www.nsf.gov/publications/pub_summ.jsp?ods_key=aag.

VIII. AGENCY CONTACTS

Please note that the program contact information is current at the time of publishing. See program website for any updates to the points of contact.

General inquiries regarding this program should be made to:

- Evelyn Goldfield, Program Director, MPS/CHE, telephone: (703) 292-2173, email: egoldfie@nsf.gov

- Gabrielle Allen, Program Director, OD/OCI, telephone: (703) 292-2598, email: gdallen@nsf.gov

- Daniel S. Katz, Program Director, OD/OCI, telephone: (703) 292-2254, email: dkatz@nsf.gov

- Edward Clarke, Senior Manager, International Programs, EPSRC, telephone: +44 1793 444438, email: Edward.Clarke@epsrc.ac.uk

- Bruce Johnson, Program Director, MPS/CHE, telephone: (703) 292-2698, email: brjohnso@nsf.gov

- Sharon Neal, Program Director, MPS/CHE, telephone: (703) 292-4952, email: shneal@nsf.gov

For questions related to the use of FastLane, contact:

- FastLane Help Desk, telephone: 1-800-673-6188; e-mail: fastlane@nsf.gov.

For questions relating to Grants.gov contact:

- Grants.gov Contact Center: If the Authorized Organizational Representatives (AOR) has not received a confirmation message from Grants.gov within 48 hours of submission of application, please contact via telephone: 1-800-518-4726; e-mail: support@grants.gov.

IX. OTHER INFORMATION

The NSF Website provides the most comprehensive source of information on NSF Directorates (including contact information), programs and funding opportunities. Use of this Website by potential proposers is strongly encouraged. In addition, National Science Foundation Update is a free e-mail subscription service designed to keep potential proposers and other interested parties apprised of new NSF funding opportunities and publications, important changes in proposal and award policies and procedures, and upcoming NSF Regional Grants Conferences. Subscribers are informed through e-mail when new publications are issued that match their identified interests. Users can subscribe to this service by clicking the "Get NSF Updates by Email" link on the NSF web site.

Grants.gov provides an additional electronic capability to search for Federal government-wide grant opportunities. NSF funding opportunities may be accessed via this new mechanism. Further information on Grants.gov may be obtained at http://www.grants.gov.

ABOUT THE NATIONAL SCIENCE FOUNDATION

The National Science Foundation (NSF) is an independent Federal agency created by the National Science Foundation Act of 1950, as amended (42 USC 1861-75). The Act states the purpose of the NSF is "to promote the progress of science; [and] to advance the national health, prosperity, and welfare by supporting research and education in all fields of science and engineering."

NSF funds research and education in most fields of science and engineering. It does this through grants and cooperative agreements to more than 2,000 colleges, universities, K-12 school systems, businesses, informal science organizations and other research organizations throughout the US. The Foundation accounts for about one-fourth of Federal support to academic institutions for basic research.

NSF receives approximately 55,000 proposals each year for research, education and training projects, of which approximately 11,000 are funded. In addition, the Foundation receives several thousand applications for graduate and postdoctoral fellowships. The agency operates no laboratories itself but does support National Research Centers, user facilities, certain oceanographic vessels and Arctic and Antarctic research stations. The Foundation also supports cooperative research between universities and industry, US participation in international scientific and engineering efforts, and educational activities at every academic level.

Facilitation Awards for Scientists and Engineers with Disabilities provide funding for special assistance or equipment to enable persons with disabilities to work on NSF-supported projects. See Grant Proposal Guide Chapter II, Section D.2 for instructions regarding preparation of these types of proposals.

The National Science Foundation has Telephonic Device for the Deaf (TDD) and Federal Information Relay Service (FIRS) capabilities that enable individuals with hearing impairments to communicate with the Foundation about NSF programs, employment or general information. TDD may be accessed at (703) 292-5090 and (800) 281-8749, FIRS at (800) 877-8339.

The National Science Foundation Information Center may be reached at (703) 292-5111.

The National Science Foundation promotes and advances scientific progress in the United States by competitively awarding grants and cooperative agreements for research and education in the sciences, mathematics, and engineering.

To get the latest information about program deadlines, to download copies of NSF publications, and to access abstracts of awards, visit the NSF Website at http://www.nsf.gov

- **Location:** 4201 Wilson Blvd. Arlington, VA 22230

- **For General Information** (NSF Information Center)**:** (703) 292-5111

- **TDD (for the hearing-impaired):** (703) 292-5090

- **To Order Publications or Forms:**

  Send an e-mail to: nsfpubs@nsf.gov

  or telephone: (703) 292-7827

- **To Locate NSF Employees:** (703) 292-5111

PRIVACY ACT AND PUBLIC BURDEN STATEMENTS

The information requested on proposal forms and project reports is solicited under the authority of the National Science Foundation Act of 1950, as amended. The information on proposal forms will be used in connection with the selection of qualified proposals; and project reports submitted by awardees will be used for program evaluation and reporting within the Executive Branch and to Congress. The information requested may be disclosed to qualified reviewers and staff assistants as part of the proposal review process; to proposer institutions/grantees to provide or obtain data regarding the proposal review process, award decisions, or the administration of awards; to government contractors, experts, volunteers and researchers and educators as necessary to complete assigned work; to other government agencies or other entities needing information regarding applicants or nominees as part of a joint application review process, or in order to coordinate programs or policy; and to another Federal agency, court, or party in a court or Federal administrative proceeding if the government is a party. Information about Principal Investigators may be added to the Reviewer file and used to select potential candidates to serve as peer reviewers or advisory committee members. See Systems of Records, NSF-50, "Principal Investigator/Proposal File and Associated Records," 69 Federal Register 26410 (May 12, 2004), and NSF-51, "Reviewer/Proposal File and Associated Records," 69 Federal Register 26410 (May 12, 2004). Submission of the information is voluntary. Failure to provide full and complete information, however, may reduce the possibility of receiving an award.

An agency may not conduct or sponsor, and a person is not required to respond to, an information collection unless it displays a valid Office of Management and Budget (OMB) control number. The OMB control number for this collection is 3145-0058. Public reporting burden for this collection of information is estimated to average 120 hours per response, including the time for reviewing instructions. Send comments regarding the burden estimate and any other aspect of this collection of information, including suggestions for reducing this burden, to:

Suzanne H. Plimpton
Reports Clearance Officer
Division of Administrative Services
National Science Foundation
Arlington, VA 22230

Policies and Important Links | Privacy | FOIA | Help | Contact NSF | Contact Web Master | SiteMap

The National Science Foundation, 4201 Wilson Boulevard, Arlington, Virginia 22230, USA
Tel: (703) 292-5111, FIRS: (800) 877-8339 | TDD: (800) 281-8749

Last Updated:
11/07/06
Text Only