	Request for Proposals: Research in Computational Science
Directorate for Computer & Information Science & Engineering (CISE)	**Directorate for Education & Human Resources (EHR)**

Letter of Intent Due Date(s) (required) (due by 5 p.m. proposer's local time):

  March 4, 2022

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

  March 25, 20212

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

  April 20, 2022

SUMMARY OF PROGRAM REQUIREMENTS

Program Title: Research in Computational Science

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Synopsis of Program:

   Through the Research in Computational Science program, NSF seeks to understand the application of the technologies, techniques and tools of computational science (also known as modeling and simulation, high performance computing, and scientific computing) across a wide variety of disciplines. Disciplines include the natural and physical sciences, pure and applied mathematics, the social sciences, economics, and all health-related fields.   NSF specifically wants to:

     * better understand how people conduct research with computational science technology and how technology can be used productively to help people create knowledge, through individual use and/or through collaborations mediated by technology;

     * better use technology for creating, collecting, analyzing, sharing, and managing data to shed light on one or more aspects of a particular area of scientific study; and

     * design new technologies for these purposes, and advance understanding of how to use those technologies and integrate them into research environments so that their potential is fulfilled.

Cognizant Program Officer(s):

   * Robert Gotwals, CISE, BR239, telephone: (919) 452-8120, email: gotwals@ncssm.edu

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

   * 47.070 --- Computer and Information Science and Engineering
   * 47.076 --- Education and Human Resources

Award Information

       Anticipated Type of Award: Continuing Grant, duration two trimesters and one semester.

       Estimated Number of Awards: 6 to 10 awards will be made, contingent on the availability of space and funds.

       Anticipated Funding Amount: $2,500 Contingent upon availability of funds, up to $1250 will be available in FY 2022 combined to fund proposals submitted in response to this solicitation.

P**roposal Preparation and Submission Instructions**

A. Proposal Preparation Instructions

   * Letter of Intent (LOI): Submission of Letter of Intent is required.

   * Preliminary Proposal Submission: Submission of Preliminary Proposal is required.

   * Full Proposals: Full Proposals submitted via Moodle using Mathematica formatted documents

B. Budgetary Information

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

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

C. Due Dates

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Proposal Review Information Criteria

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 judgements.

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? To what extent will it enhance the infrastructure for research, 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.

Award Administration Information

Award Conditions: Standard NSF award conditions apply. Awards are made on a trimester by trimester basis. Failure to demonstrate satisfactory **documented progress** will result in the termination of the award.

Reporting Requirements: Standard NSF reporting requirements apply. Research notebooks are mandatory. At the end of each award period, a complete progress report must be provided to the Program Officer using an MMA template form. Research notebooks must also be submitted as a part of the reporting requirements.

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I. INTRODUCTION

Research supported by the Research in Computational Science program will explore the opportunities for pure and applied scientific research made possible by existing and emerging computational technologies. The program will help scientists capitalize on those opportunities, develop new practices that are made possible by computing technologies, and explore ways of using technology to promote deep and lasting study of a wide variety of disciplines, broadly defined. Research in Computational Science projects will marry the fields of science, mathematics and computing to shed light on interesting and complex problems of interest to the scientific community <u>or</u> develop new algorithms, computing technologies

(including computer programs), and other applicable tools that might be then used by other researchers to study research questions computationally.

II. PROJECT CLASSES

Awards will be made in two categories:

   * **Computational (Science Research) (C/SR)** projects apply the technologies, techniques and tools of computational science to one or more scientific questions. In this category, the computer and the associated software resources are the <u>means</u> by which the scientific problem is addressed. The over-reaching goal in this category is the accumulation, analysis, and/or visualization of scientific data that expressly provides insight into the research question. In the majority of cases, this category takes advantage of <u>existing</u> software tools (stand-alone and/or web-based software programs) to address the research question. For example, researchers in this category might use the Molegro software to study protein-ligand binding in drug design chemistry, the MOPAC or Gaussian programs to study quantum chemical phenomenon, or Paraview to create high-end data visualizations of large datasets. Researchers might also use general purpose tools such as Mathematica, MatLab, STELLA, and/or Excel to implement existing algorithms in a computational environment.

   * (**Computational Science) Research) (CS/R)** projects look to develop new algorithms and/or computing tools for use by the computational science community. In these projects, the focus is on creating new tools from scratch, or improving the efficiency of one or more existing tools. For example, research in this category might look at ways to improve throughput in a multi-user computational chemistry environment such as is found on the North Carolina High School Computational Chemistry server (http://chemistry.ncssm.edu), or developing a new algorithm for predicting financial futures. In this category, the software tool or resource is the <u>end product</u> of the scientific research. In this category, the expectation is that the software/tool developer (i.e., the researcher in this category) will be able to address a clearly identified need in the computational science community.

III. IMPORTANT PROJECT CHARACTERISTICS

The critical project characteristic is the extent to which the researcher is able to intelligently and creatively bring the technologies, techniques, and tools of computational science to the investigation of one or more scientific problems, <u>or</u> to develop a new approach to computational science that has the potential to benefit a current or future computational scientist. Logistically, the project must delineate a clear research objective or question, provide a reasonable plan for how that objective will be accomplished, provide a sense of the type of data that might be obtained and how that data will be analyzed, and provide a reasonable sense of timeline, resource requirements (including funding required), and suggest possible endpoints for the research. Most importantly, the research proposal should attempt to answer the question: <u>what does success look like?</u> How will the researcher (and the program officer) know that the goals of this research have been accomplished? Are there identifiable breakpoints at which the researcher can conclude the research program? The researcher should keep in mind that research seldom proceeds as anticipated; however, the researcher should try to visualize the process and the end goal, and describe that in this proposal.

IV. PROPOSAL PREPARATION AND SUBMISSION INSTRUCTIONS

Letters of Intent (required): The LOI must contain (1) a proposed title; (2) the names of Principal Investigators and Co-Principal Investigators; (3) a brief synopsis (limited to 250 words) describing the proposed project in sufficient detail to permit selection of reviewers.   LOIs will not be used to encourage or discourage the submission of full proposals. They will be used only to help NSF plan for the merit review process, and are non-binding. Thus, changes may be made between the submission of the LOI and submission of the full proposal. LOIs are to be submitted using the LOI form in Microsoft Word.

Preliminary Proposal Preparation Instructions: Proposers must submit preliminary proposals using LaTeX format upload to Canvas by the proposal deadline. No proposals are accepted past the deadline. Proposals should be submitted in PDF format.

Full Proposal Preparation Instructions: Proposers must submit full proposals as a PDF document, preferably using LaTeX by the proposal deadline. No proposals are accepted past the deadline.

Proposal Titles: Proposal titles must begin with an acronym that indicates the categories in which proposals are being submitted, as follows

* Computational (Science Research) (C/SR)
* (Computational Science) Research) (CS/R)

The acronym should be followed with a colon, then the title of the proposed project. For example, the title of a proposal in computational (science research) would be C/SR: Project Title.

Project Summary: The Project Summary must include an explicit description of both the Intellectual Merit and Broader Impacts of the activities proposed, preferably in separate paragraphs titled "Intellectual Merit" and "Broader Impacts".   The Project Summary is limited to one page in length.

Project Description: Project Descriptions should include the following sections:

1. Vision and Goals.

Describe:
     * The overall research question and/or the anticipated end result of the research.
     * The specific aims of the project, including a description of potential products and/or other deliverables.

2. Review of the Literature

List and describe the relevant research and primary literature that addresses the relevant research question and research agenda for this work.

3. Research Plan and Methodology.

The researcher should provide a reasonably detailed description of the research plan and methodology, including a timeline (for example, a Gantt chart) for the researcher. The proposed methodology should be described by trimester to the extent possible. The research plan should provide a description of required resources (software, books/journals, other resources as appropriate).

4. Expected Outcomes

The researcher should endeavor to describe the expected outcomes, including the type and amount of data that might be collected, The potential end product should be described to the maximum extent possible. Most importantly, the researcher should provide a description of how success will be evaluated and measured.