# Network for Computational Nanotechnology (NCN) Supporting the Next Phase of NCN Nodes Programs

# PROGRAM SOLICITATION

NSF 16-593



### **National Science Foundation**

Directorate for Engineering
Division of Chemical, Bioengineering, Environmental, and Transport Systems
Division of Civil, Mechanical and Manufacturing Innovation
Division of Electrical, Communications and Cyber Systems
Engineering Education and Centers

Directorate for Computer & Information Science & Engineering Division of Advanced Cyberinfrastructure

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

November 03, 2016

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

December 02, 2016

# **IMPORTANT INFORMATION AND REVISION NOTES**

Letter of intent and full proposals. Submission of a letter of intent is required for submission of a full proposal.

Any proposal submitted in response to this solicitation should be submitted in accordance with the revised NSF Proposal & Award Policies & Procedures Guide (PAPPG) (NSF 16-1), which is effective for proposals submitted, or due, on or after January 25, 2016.

# **SUMMARY OF PROGRAM REQUIREMENTS**

### General Information

# Program Title:

Network for Computational Nanotechnology (NCN) Supporting the Next Phase of NCN Nodes Programs

# Synopsis of Program:

The goals of the Network for Computational Nanotechnology (NCN) are to: 1) accelerate the transformation of nanoscience to nanotechnology through the integration of simulation with experimentation; 2) engage an ever-larger and more diverse cyber community sharing novel, high-quality nanoscale computation and simulation research and educational resources; 3) develop open-access, open-source software to stimulate data sharing; and 4) inspire and educate the next-generation workforce. The NCN consists of a stand-alone Cyber Platform, which provides computation, simulation, and education services to over 330,000 researchers, educators, students, and industry members of the nanoscience and engineering community annually worldwide; and Nodes, which develop compelling new computational and simulation tools to disseminate through Cyber Platform (nanoHUB.org) and cultivate communities of users in emerging areas of nanoscale science and engineering. For more information on NCN, please see http://nanohub.org/about#funding .

This solicitation will support the next phase of NCN Nodes Programs. Current awards for existing NCN Nodes expire in September 2017. Those who submit proposals in response to this solicitation will need to address the following questions:

- 1. What compelling new nanoscience modeling and computational tool(s) will be developed and how will it advance nanotechnology to meet critical national needs?
- 2. What will the Node undertake to nucleate a community of academic and industry users engaged in the new tool(s) and increase quality and quantity of nanoHUB tools, resources, and usage?
- 3. How will the Node interact productively with the Cyber Platform and other Nodes to augment existing capabilities and ensure seamless and complementary advancement of the NCN's goals?

Content areas of the three new Nodes will be:

**Engineered nanoBIO** - Create integrated computational tools that support new understanding and simulation of biological phenomena from the nanoscale across length scales for the design of devices and systems;

**Hierarchical nanoMFG** - Computation and simulation software to address the challenges of hierarchical nanomanufacturing processes from nanoscale components to devices and systems, and their scale up;

Nano-Engineered Electronic Device and Module Application Node (NEEDMA) - Develop computation and simulation tools that can be employed for turning nanoscale science and engineering into applications through the discovery and development of nanoelectronic-based devices and modules with impact on circuit and systems responding to grand challenges.

Proposals will be accepted only for the above Node content areas. A proposal for another Node content area will be returned without review.

### 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.

- Eduardo A. Misawa, ENG/EEC, telephone: (703) 292-5353, email: emisawa@nsf.gov
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- William Olbricht, ENG/CBET, telephone: (703) 292-2563, email: wolbrich@nsf.gov
- Dimitri Pavlidis, ENG/ECCS, telephone: (703) 292-2216, email: dpavlidi@nsf.gov
- Rajiv Ramnath, CISE/ACI, telephone: (703) 292-4776, email: rramnath@nsf.gov

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

- 47.041 --- Engineering
  47.070 --- Computer and Information Science and Engineering

# **Award Information**

Anticipated Type of Award: Cooperative Agreement

**Estimated Number of Awards: 3** 

Three Node awards

Anticipated Funding Amount: \$2,500,000

This support is provided by the NSF Directorate for Engineering (ENG) and the Directorate for Computer & Information Science & Engineering (CISE). The individual new Nodes will be funded at up to \$800,000 each per year for up to five years, pending quality of the Node activities and availability of funds. The Node awards are not renewable.

# **Eligibility Information**

### Who May Submit Proposals:

Proposals may only be submitted by the following:

. Only U.S. universities with Ph.D. degree granting programs in science and engineering may serve as the lead institution for each award. For Node proposals, a lead university may be joined by a small number of partner domestic universities/institutions (e.g., federal labs) but may not be joined by foreign universities/institutions. However, a multi -university configuration is not required [1]. If a multi -university proposal is submitted, the lead university must submit the proposal with subawards to collaborators. Separately submitted collaborative proposals are not acceptable and will be returned without review.

[1] If a partner is a Federal lab, NSF funds cannot be used to support the laboratory.

# Who May Serve as PI:

The PI of each respective Node proposal must be a tenured faculty member at the lead university of the proposal.

The PI and co-PI(s) on the full proposal must be the same as those named in the Letter of Intent.

# Limit on Number of Proposals per Organization: 3

A university may submit only one proposal per Node content area in this solicitation. Therefore, one university might submit up to three separate Node proposals, but only one to each Node content area.

# Limit on Number of Proposals per PI or Co-PI: 1

An investigator may serve as PI or co-PI on only one Node proposal.

# **Proposal Preparation and Submission Instructions**

### A. Proposal Preparation Instructions

- Letters of Intent: Submission of Letters of Intent is required. Please see the full text of this solicitation for further information.
- Preliminary Proposal Submission: Not required
- 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

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

November 03, 2016

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December 02, 2016

# 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**

**Summary of Program Requirements** 

- I. Introduction
- **II. Program Description**
- **III. Award Information**
- IV. Eligibility Information
- V. Proposal Preparation and Submission Instructions
  - A. Proposal Preparation Instructions
  - B. Budgetary Information
  - C. Due Dates
  - D. FastLane/Grants.gov Requirements

# VI. NSF Proposal Processing and Review Procedures

- A. Merit Review Principles and Criteria
- B. Review and Selection Process

# VII. Award Administration Information

- A. Notification of the Award
- **B.** Award Conditions
- C. Reporting Requirements
- VIII. Agency Contacts
- IX. Other Information

# I. INTRODUCTION

NSF established the Network for Computational Nanotechnology (NCN) in 2002 at Purdue University as part of the National Nanotechnology Initiative (NNI). In 2012, the NCN was reconfigured to include a stand-alone Cyber Platform, which provides computation, simulation, and education services to the nanoscience and engineering communities, and new Nodes in nano-engineered electronic device simulation (NEEDS) and nanoBIO areas. The Nodes develop new tools and content disseminated worldwide via the Cyber Platform. This reconfiguration supported expansion of NCN Cyber Platform (nanoHUB.org) as a gateway to the worldwide nanoscience and nanoengineering community for over 330,000 researchers, educators, students, industry users, and other professionals annually worldwide.

This solicitation will support one Node in each of three content areas that address the three overarching questions. These Nodes will interact with and be supported by the Cyber Platform. The Cyber Platform, which maintains nanoHUB.org, is designed to join the nanoscience and engineering theory, simulation, experimentation and educational communities together through advanced computation and simulation in nanoscience and nanoengineering fields and to enrich the nano educational materials available to a broader spectrum of students, faculty, industry, and communities.

NCN is part of one of the Signature Initiatives of the National Nanotechnology Initiative (NNI) (http://www.nano.gov/initiatives/government/signature). Complementary NNI activities are identified at http://www.nano.gov/grants. Dissemination through the NCN of modeling, simulation, and data outputs from participants in the National Nanotechnology Coordinated Infrastructure (NNCI) and Nanosystem Engineering Research Centers (NERC) is critical to supporting NNI, its complementary activities, and other expanding nano communities of users.

# II. PROGRAM DESCRIPTION

The National Science Foundation (NSF), through its Directorate for Engineering (ENG) in partnership with the Directorate for Computer and Information Science and Engineering (CISE) plans to jointly support the Nodes in the Network for Computational Nanotechnology (NCN). The ENG Division of Engineering Education and Centers (EEC) leads the effort in the development of the solicitation, the review of proposals, and post-award oversight.

The purpose of the solicitation is to support the next phase of the NCN Nodes Programs. The new Nodes will, in their respective content areas, address the following overarching questions:

- 1. What compelling new nanoscience modeling and computational tool(s) will be developed and how will it advance nanotechnology to meet critical national needs?
- 2. What will the Node undertake to nucleate a community of academic and industry users engaged in the new tool(s) and increase quality and quantity of nanoHUB tools, resources, and usage?
- 3. How will the Node interact productively with the Cyber Platform and other Nodes to augment existing capabilities and ensure seamless and complementary advancement of the NCN's goals?

Simulation has proven to be a critical research methodology in the emerging fields of nanoscience and nanoengineering across fourteen years of support to the NCN. The current NCN Cyber Platform, nanoHUB.org, is an acknowledged leader in established an online science gateway which broadly engages researcher, educator, student, and industry participants in nanoscience and nanoengineering communities worldwide. Through this solicitation, NSF will expand this important service to the nanoscience and nanoengineering community for the next five years in three critical areas:

**Engineered nanoBIO** - Create integrated computational tools that support new understanding and simulation of biological phenomena from the nanoscale across length scales for the design of devices and systems;

Hierarchical nanoMFG - Computation and simulation software to address the challenges of hierarchical nanomanufacturing processes from nanoscale components to devices and systems, and their scale up; and

Nano-Engineered Electronic Device and Module Application Node (NEEDMA) - Develop computation and simulation tools that can be employed for turning nanoscale science and engineering into applications through the discovery and development of nanoelectronic -based devices and modules with impact on circuit and systems responding to grand challenges.

The construct of the NCN is as follows. The Cyber Platform, a part of the National Nanotechnology Initiative (NNI), provides ongoing support and development of nanoHUB.org, its open-access, open-source middleware, and its collection of tools, educational materials, and data. nanoHUB disseminates nanoscience tools and provides computation, simulation, and education services to over 330,000 researchers, educators, students, and industry members of the nanoscience and engineering community annually worldwide. The new Nodes develop new nanoscience modeling and computational tools to advance nanotechnology to meet national needs, and nucleate communities of academic and industry users to participate in development and use of the tools. The Cyber Platform and nodes interact via cooperative agreements to augment existing capabilities and to advance the NCN's goals to accelerate computation and simulation in nanoscience and nanoengineering fields and to enrich the nano educational materials available to a broader spectrum of students, faculty, industry, and communities.

Each of the three new content development Nodes will be separately funded, through separate cooperative agreements, and will be linked to the platform through requirements in their separate cooperative agreements. Each Node will be required to deliver user- tested content to the Cyber Platform. The Cyber Platform also will be responsible for determining areas where the content development Nodes could collaborate to improve the overall effectiveness of the NCN.

The three new Nodes will be funded for up to five years with no opportunity for renewal. Materials delivered to the NCN Cyber Platform by these Nodes will remain available to the community through the Cyber Platform once the Node awards expire.

### A. NCN Cyber Platform

Information about key features, goals, requirements, and deliverables of the NCN Cyber Platform is summarized here to support development of an approach to interact productively with the Cyber Platform which is an important aspect of the Node proposal.

# Key Features of the NCN Cyber Platform

The NCN Cyber Platform will continue its role in NCN, enabling broader use of modeling and simulation, joining theory with

experimentation through simulation to accelerate advances in the understanding of nanoscale phenomena and facilitate advances in technology and education. The Cyber Platform will continue to lower barriers to the pervasive use of simulation and maintain and create cyber communities united by common conceptual frameworks embodied in easily accessible simulation; modeling and design tools; educational modules; and information dissemination. Although simulation is especially effective when used in conjunction with experimentation, simulation is often challenged to keep up with the volume of data generated from large-scale experiments in fast moving, emerging fields of research. At the same time, it is further recognized that simulation plays an important role in education and business practice; especially since resource sharing lowers the cost of education and production in business.

### Cyber Platform Goals, Requirements, and Deliverables

### **Computation and Simulation Tools**

Cyber Platform will provide access to computation and simulation tools by the nanoHUB.org platform.

Cyber Platform through the nanoHUB.org platform will support computation and simulation tools developed from the new NCN Nodes: Engineered nanoBIO, Hierarchical nanoMFG, and NEEDMA.

Cyber Platform will support computation and simulation tools developed by other contributors.

#### Software

Cyber Platform will support software that provides access to core computational equipment and to other capabilities as needed to provide seamless computational and simulation service to the users.

Cyber Platform will provide ongoing analyses of middleware needs in light of current and future user needs and of cyberinfrastructure to support a software engineering and development plan that will include and/or enable the integration of relevant research activities, and ensure the software is responsive to new computing developments.

Cyber Platform will provide mechanisms for maintaining and periodically upgrading the platform to provide state-of-the-art services to the nano community, including metrics to measure the success of any software developed and the steps necessary to take the software from prototype to dissemination into the community as reusable software resources.

Cyber Platform will provide proof-of-concept demonstration of any key software elements that would be developed under the award, with metrics for success and milestones.

Cyber Platform will integrate sustainability, manageability, usability, and composability/interoperability into the software.

Cyber Platform will provide identity management system and trust fabric between providers and platform host.

Cyber Platform will plan to integrate content and tools so as not to preclude sharing and future porting without renegotiation of proprietary agreements.

Cyber Platform will plan to link to the NSF Computational Infrastructure for 21st Century Science and Engineering (CIF21) in the Division of Advanced Cyberinfrastructure (ACI) particularly the Software Infrastructure for Sustained Innovation (SI2) (http://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=503489&org=NSF&sel\_org=XCUT&from=fund) program and to SI2 awards, e.g., SI2 Institutes as they come on line including contributions to SI2 PI meetings with associated travel costs included in the budget.

### **Education and Workforce Training**

Cyber Platform will provide current nanotechnology education modules, courses, and other educational materials important for nanoscience and nanoengineering education at the pre-college, undergraduate, and graduate levels via its nanoHUB.org platform.

Cyber Platform will support new nanotechnology education modules, courses, and other educational materials important for nanoscience and nanoengineering education at the pre-college, undergraduate, and graduate and workforce levels developed by the new NCN Nodes.

Cyber Platform may develop specialized web-based learning tools based on the educational materials provided by the Nodes.

Cyber Platform will provide tool-powered curricula to augment existing courses and enhance student learning by using turnkey simulations to teach concepts, design, and optimization, without requiring extensive training or software installation.

Cyber Platform will provide virtual immersive environments for development of insights and intuition in the nanoworld.

Cyber Platform will provide telepresence and remote experimentation frameworks, e.g., for re-training of the professional workforce in nanotechnology for industry.

# **User Support**

Cyber Platform will provide the following user support elements:

- User-friendly tools developed from tools and content delivered by the NCN Nodes;
- A forum and platform for vetting the quality of tools and educational materials;
- Support for the established community of users, including developing user guides;
- Expansion of the involvement of users across a wide range of academic institutions and industry;
- A question and answer forum, as well as a forum for collecting wish lists for tool and educational module improvements;
- Specification of minimum quality and functionality requirements for acceptance to the site; and
- Assurance that computational capabilities are available to augment the computational capacity of the users.

# Assessment of User Needs and Service Quality

Cyber Platform will assess collections of data on platform usage by sector and by purpose and assess the quality and utility of services based on that data.

# Requirements and Deliverables

The NCN Cyber Platform is positioned to best serve the emerging needs of the nano community while leveraging ongoing developments in cyberinfrastructure (CI). The importance and immediacy of such a platform is accentuated by the current and future trends in CI (e.g., disruptive hardware trends such as hybrid many cores and accelerators, increasing data volumes, complex application structures and behaviors, and emerging first-order concerns such as fault-tolerance and energy efficiency). The Cyber

Platform evolves to meet expanding needs of the community as it develops richer tools with increasing data volumes and computational requirements.

The Cyber Platform is used to increase the use of modeling and simulation in both research and education across a diverse set of universities and other user communities. It provides online simulation capabilities and a broad range of tools to very large communities of users through browser-based portals. For example, nanoHUB currently supports over 330,000 users annually. While all of these tools appear to run as applets in the user's browser window, they are powered by a much more sophisticated middleware that lets the user transparently tap into university and national grid resources. The Cyber Platform has had an uptime of over 99.9999% over the last five years, exceeding efficiency of the initial nanoHUB.

Access to the Cyber Platform is through an identity management system that is based on the users' local identity, a trust fabric between the local resource provider and the Cyber Platform host, and attributes (student, classroom user, etc.) provided by the user. NCN Cyber Platform is a leader in supporting resource access in a federated identify setting mode, for example, by joining the In Commons federation. See <a href="http://www.incommonfederation.org/">http://www.incommonfederation.org/</a> It also incorporates capacities that leverage national scale cyberinfrastructure such as eXtreme Digital (XD), Open Science Grid (OSG), and commercial cloud services.

NCN Cyber Platform employs tangible metrics to measure success and failure and the tasks necessary to take the software from prototype to dissemination as a reusable software resource. Its strong software engineering and development plan includes the integration of relevant research activities to ensure the software is responsive to new computing development.

The NCN Cyber Platform links to the NSF Computational Infrastructure for 21st Century Science and Engineering (CIF21) in the Division of Advanced Cyberinfrastructure (ACI) which includes CDS&E in ENG, see <a href="http://www.nsf.gov/funding/pgm\_summ.jsp?">http://www.nsf.gov/funding/pgm\_summ.jsp?</a> pims id=504817, and awards and PI meetings of SI2.

# B. General Goals, Requirements, and Deliverables for the New Nodes

The following sections describe the general goals, requirements, and deliverables that are common to each of the required nodes.

### 1. Goals and Requirements for each new Node:

- Develop compelling new nanoscience modeling and computational tool(s) to advance nanotechnology to meet critical national needs:
- Nucleate a community of engaged academic, government laboratory and industrial personnel and other users of the novel
  tool(s) to address broad based user needs, including those of small businesses and to provide their tools and educational
  materials to the Node for delivery to the Cyber Platform. Means for nucleation could include discussion groups, electronic/print
  communication, workshops, conferences;
- Specify expected deliverables to the Cyber Platform, develop a strategic plan to achieve the deliverables, and provide a
  milestone chart showing the timing of the deliverables;
- Link theory to experimentation to improve these tools: provide some funding of experimentalists and link in a collaborative nonfunded mode to the already funded experimentalists in the area through connectivity with the National Nanotechnology
  Coordination Infrastructure (NNCI), the Nanosystems Engineering Research Centers (NERC), and relevant ongoing
  Engineering Research Centers (ERC), etc.;
- Deliver user-tested simulation tools to the Cyber Platform, where they will be made more user friendly (once released, the
  platform would let the "market place" vet the quality and relevance to user needs); and
- Develop educational materials that link nanoscience to nanotechnology applications which could include user-friendly modules
  to stimulate interest and access to these materials among high school, community college, and university students as well as
  industry and regulatory professionals.

# 2. In collaboration with the Cyber Platform, all Nodes will be expected to share relevant findings and organizational lessons learned across the other Nodes.

NSF is committed to providing a seamless transition, so the user community experiences a net positive impact from the next phase of NCN Node programs. It is imperative that proposals outline a clear path for ensuring continuity of service. For example, proposers may consider initial use of NCN Node middleware platforms based on hubZERO, available at <a href="http://hubzero.org">http://hubzero.org</a>, Next-generation platforms to meet the evolving and expanding requirements of the respective Node communities may be proposed. There must be evidence that a proposed next-generation platform has sufficient computing resources to host envisioned tools and resources and improves upon the existing platform. The proposal must provide a clear interface and easy-to-use pathways for content population and maintenance.

Because community building is a key component of proposed Nodes, each proposing team must include plans to engage communities which interact with existing relevant Nodes. Existing nodes are funded through FY2017, providing support during a transition period. Part of this transition phase will include the existing awardee working with the Cyber Platform to adapt and port existing and developing sets of tools and other content to the nanoHUB for continued support. Node proposals must include support for Node leaders to participate in a transition meeting in FY2017 in which activities that support a seamless transition are evaluated for implementation.

For all proposing institutions, all content and tools must be integrated in a way that does not preclude their sharing and future porting and use across other platforms. Further, if a transition to a different platform becomes necessary in the future, the awardee will be responsible for making sure that all content and tools are fully transitioned to that platform without requiring any renegotiation of proprietary agreements.

# C. Node Overviews, Goals, and Requirements

The following sections describe the specific goals, requirements, and deliverables for the three node topic areas.

1. **Engineered nanoBIO Node** - Integrated computational tools that support new understanding and simulation of biological phenomena across length scales for the design of devices and systems.

Novel and impactful computational nano-bio tools are important across multiple scales ranging from biomolecules (nano) and microorganisms and cells (micro), to tissues (meso) and whole organisms (macro). Computational tools that incorporate structure-function-property-design relations at the nanoscale are desired to understand interactions between biological components and nanoscale devices and to support development of resilient and predictable acute and chronic biotic/abiotic interfaces. Such tools could improve synergies between simulation and experiments and help advance new scientific discovery and understanding of biology at the nanoscale. Engineered nano-bio tools are needed to bridge concurrent advances in theory, computation, experiment, and instrumentation. Multiscale computational modeling and simulation can predict quantities that are not directly accessible by experiment, creating new knowledge.

### Areas

Descriptions of key physicochemical, structural, mechanical, electrical, and statistical features by engineered nano-bio tools are needed

to advance engineering biology and sustainable agriculture; to develop neurotechnologies, personalized medicine, regenerative medicine, tissue electronics, and electroceuticals; to diagnose, prevent, and treat genetic, infectious, and pandemic disease; to support new health informatics technologies; and to meet other biological and health-related current and emerging national and global challenges. The tools and theory should cross scales (e.g., from the atomic level to the molecular, and cellular/device level). The focus of the node may include, but is not limited to, the areas listed below:

- The structure of nanoscale biological components and how structure changes as those components interact with a nanoscale device;
- The tailoring of complex material architecture to enhance the properties of biological materials;
- Mechanical features of a nanoscale bio-device system and mechanotransduction of signals between device and biological component; and
- Design/prediction of biological device function, interference with surrounding biological systems, and orthogonality of components.
- 2. **Hierarchical NanoMFG Node** Computation and simulation software to address the challenges of hierarchical nanomanufacturing from nanoscale components to devices and systems, and their scale up.

The nanomanufacturing field could benefit from a comprehensive approach involving advanced cyberinfrastructure tools to design integrated manufacturing facilities incorporating knowledge from the full spectrum of length scales, from the molecular to the enterprise-wide, using state-of-the-art theoretical (analytical) formulations and computational (numerical) techniques. This includes introducing novel abstract concepts and representations, mathematical algorithms and analysis methods, and bridging from the atomistic to continuum domains, inspired by or mimicking the multifaceted synthetic manufacturing aspects of the natural and engineered manufacturing enterprise. Challenges of incorporating data and information from the nano to the meso scales need to be addressed. Plans should incorporate continuous feedback loops among all the length scales and stages of the simulation using atomistic scale information to design and synthesize the nanoscale building-blocks, their assembly into higher order nanostructures and integration of these into components and devices and systems while simultaneously developing either batch or continuous global manufacturing schemes, products and services. Of particular interest is development of nanomanufacturing concepts for complex, hierarchical systems involving diverse material sets, including inorganic, organic and biomaterials.

### Areas

- The focus may include but is not limited to the areas listed below. Computational simulations for predictive modeling to advance nanomanufacturing processes, technologies and platforms should consider the following criteria:
- Scalability (producibility, predictability, productivity), especially via parallel processing and continuous manufacture and integration;
- Conversion of available raw materials to commercially important intermediates to final consumer products incorporating factors such as the availability of feedstock, manufacturing conditions such as local environmental, global markets and legal constraints:
- Simulations in space and time with multi-scale, multi-dimensional, and/or hybrid multi-disciplinary nature that cut across conventional mechanical, thermal, electrical, optical, chemical, and biological approaches;
- Multi-domain manufacture, involving deposition, removal and transformation of matter, information through combined bottomup and top-down pathways;
- Unconventional approaches, such as probabilistic versus deterministic constructions; and
- Hierarchical complexity and system-level architectures.
- Causal inversion of the modeling framework for control, optimization, and decision making in designing and manufacturing at the nanoscale, especially via:
- Nano- and multi-scale design environments and software tools for computer-aided design, manufacturing and engineering (nano-CAD/CAM/CAE);
- Systems engineering and operations research methodologies for nano-/micro-factory platforms including process planning, supply chain and industrial engineering aspects; and
- Cybermanufacturing systems approach to accelerate the creation of an interoperable, cross-process manufacturing service layer, building upon an app-based infrastructure for nanomanufacturing processes.
- Synergistic coupling of computation with experimental instrumentation and automation research in nanomanufacturing, such as:
- Hardware-software interfacing and reconstruction algorithms for sensing, imaging and metrology, as well as actuation, manipulation, and nanorobotic guidance and navigation;
- Experimental calibration, validation and verification of computational simulations, as well as computational design of experiment methods for nanomanufacturing;
- Software databasing of laboratory properties of elemental/composite nanomaterials in various shapes and aspect ratios ("periodic table" of nanomaterials for manufacturing);
- Knowledge-bases of manufacturing processes, platforms and technologies for virtual integration, benchmarking, and evaluation before industrial implementation; and
- Human-machine interfacing for nanomanufacturing operations and cognition.
- 3. Nano-Engineered Electronic Device and Module Application Node (NEEDMA) Computation and simulation tools that can be employed for turning nanoscale science and engineering into applications through the discovery and development of nanoelectronic-based devices, modules, and system application oriented simulation packages that impact circuits and systems in response to grand challenges.

Physics-based compact models have been developed in a Verilog-A compliant environment for emerging nanodevices. Compact models assist device development by complementing experimental efforts, supporting exploration of a larger space of operating conditions that increase their application potential and assisting in circuit implementation. Ideally, compact model development includes experimental validation (based on understanding material science, device physics and engineering as well as process technology and system architecture); translation for use in open source SPICE-compatible simulation platforms for use by experts and non-experts alike in design; going beyond Verilog-A to satisfy needs imposed by nanoscale devices; and establishment of components libraries to build compact models for advanced nano-devices. Applications include advanced transistors, memory devices, sensors, optical devices, spintronic devices, power and energy devices and MEM/NEM devices.

Expansion of compact model development and use beyond the device level could facilitate development of novel nanoelectronic-based circuits, modules and systems, while ensuring that currently explored nanoelectronic approaches are transitioned to practical systems. This requires expanding existing compact models by considering (i) experimentally observed nano-structure characteristics obtained both at the development stage as well as in more mature, industry level environments and (ii) physics properties that include among other transport properties, phase changes, topological, plasmonic, atomic level resolution, strain, polarization, and quantum effects. Developed methodologies at the nanoscale should support control of nanoscale device and module, system reproducibility and narrow the gap between research and product development. Basic 'nano' blocks should be configurable to develop more complex models and simulate complex systems with an assortment of nanocomponents. Teams with complementary expertise should (i) use synergistic approaches to address novel complex nanotechnology based modules and systems with new functionality and improved performance and (ii) use industry- and application-specific approaches to address advanced, mature techniques as well as new nanotechnology

concepts specified based on current and future user needs that are uniquely served by nanotechnology, with specific performance targets to be demonstrated within specified phases of the program.

#### Areas

The scope of the proposed NEEDMA Node should encompass, but not be limited to, the areas listed below.

- First-principles based simulations of nano-based components range from basic functions like switching, signal generation, and amplification to sophisticated modules that integrate such functions;
- Nanomodules that explore physics properties of nano-materials in their zero-, one-, two- and three-dimensional forms while
  maintaining the nanoscale properties of individual components; including consideration of compositional variations, electronic,
  photonic, biological and mechanical interactions between atoms, molecules and layered structures;
- Three dimensional analyses that includes the capability to incorporate heterogeneous layers of different nature and functionality and having electronic, thermal, photonic, magnetic and mechanical functionality;
- The range of materials used in fabricating nanodevices e.g., silicon, III-V, II-VI semiconductors, nanowires and nanospheres, carbon electronic, two-dimensional atomic lavers:
- DC, high-frequency, transient properties should be considered and operation should extend from DC to the THz and optical regime, perhaps with separate, interconnected modules;
- Operating-point solutions, transient analysis, various small- and large-signal analyses;
- Simultaneous consideration of fundamental and applied aspects, material, device, module, system and architecture aspects
  and their interactions in order to satisfactorily respond the system requirements;
- Effects of interconnects, parasitic elements and other factors that may influence the actual module and system performance;
- Characteristics of nanomodules, such as switches, amplifiers, signal sources, sensors, detectors, modulators, foldable components etc.: and
- · Visualization and user interfaces.

# III. AWARD INFORMATION

Anticipated Type of Award: Cooperative Agreement

**Estimated Number of Awards: 3** 

Three Node awards

Anticipated Funding Amount: \$2,500,000

This support is provided by the NSF Directorate for Engineering (ENG) and the Directorate for Computer & Information Science & Engineering (CISE). The individual new Nodes will be funded at up to \$800,000 each per year for up to five years, pending quality of the Node activities and availability of funds. The Node awards are not renewable.

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

# IV. ELIGIBILITY INFORMATION

### Who May Submit Proposals:

Proposals may only be submitted by the following:

Only U.S. universities with Ph.D. degree granting programs in science and engineering may serve as the lead institution for each award. For Node proposals, a lead university may be joined by a small number of partner domestic universities/institutions (e.g., federal labs) but may not be joined by foreign universities/institutions. However, a multi -university configuration is not required [1]. If a multi -university proposal is submitted, the lead university must submit the proposal with subawards to collaborators. Separately submitted collaborative proposals are not acceptable and will be returned without review.

[1] If a partner is a Federal lab, NSF funds cannot be used to support the laboratory.

### Who May Serve as PI:

The PI of each respective Node proposal must be a tenured faculty member at the lead university of the proposal.

The PI and co-PI(s) on the full proposal must be the same as those named in the Letter of Intent.

### Limit on Number of Proposals per Organization: 3

A university may submit only one proposal per Node content area in this solicitation. Therefore, one university might submit up to three separate Node proposals, but only one to each Node content area.

### Limit on Number of Proposals per PI or Co-PI: 1

An investigator may serve as PI or co-PI on only one Node proposal.

# V. PROPOSAL PREPARATION AND SUBMISSION INSTRUCTIONS

### A. Proposal Preparation Instructions

# Letters of Intent (required):

A Letter of Intent (LOI) is required to facilitate the NSF review process. The letter should be submitted via FastLane (not Grants.gov) no later than the LOI deadline date specified in this solicitation. The LOI allows NSF to screen the proposals with respect to eligibility requirements, to categorize the proposals, and identify conflicts -of-interest so as to prepare for the proposal review processes. Follow these steps for the LOI preparation and submission:

Submit information for your LOI through FastLane under these categories and only under these categories (note the character limits, which include spaces, as stated below):

Project Title: The project title should be: one of the following as appropriate

Network for Computational Nanotechnology - Engineered nanoBIO Node

Network for Computational Nanotechnology – Hierarchical nanoMFG Node

Network for Computational Nanotechnology - NEEDMA Node

Synopsis (max 2,500 characters in this section, including any spaces): Provide brief statements of the vision, goals, and features of the NCN Node at a sufficient level of detail to understand the Node.

Other Comments (max 2,500 characters including any blank spaces): Continue Synopsis as needed in this section.

Organizational Attribute: Select the appropriate organizational attribute for the lead university from the drop down list.

Key Academic Participants (max 255 characters including any blank spaces): In this section, identify the core academic participants (people). Include the titles/roles in the Node, and their departmental and institutional affiliations for the lead PI, co PIs and any other key academic faculty or staff.

**Key Academic Participants Continued (max 255 characters including any blank spaces):** Continue the list of "Key Academic Participants (people)" as needed.

Point of Contact for NSF Inquiries: Lead PI

Project PI Information: Lead PI's Contact Information

Submitter Information: This section does not require input from LOI author. FastLane automatically adds this information to the final LOI submission.

Senior Project Personnel (maximum of five official Co-Pls): In this section identify your PI and up to four additional Co-Pls. Include their names, universities, departments, and locations (city, state, country). Because the coversheet only allows a total of five PIs (the PI and up to four Co-Pls), any additional Co-Pls will be shown as "Senior Personnel" in any subsequent proposal and should be identified in the "Key Academic Participants" section above.

Participating Organizations: This section will list the lead and partner institutions for the Node proposal. In this section for each university include the name and location (city, state, and country), then the appropriate heading for each: 1) the lead university (LU) 2), partner university(ies) (PU), if any, and 3) other types of partner institutions. Each entry can have up to 76 characters (including any spaces) to show all of the information you are asked to provide (university name, city, state, country and abbreviation for type of partner, (i.e., LU). You can abbreviate information, as needed. You can also do a search for the organization and if FastLane finds it you can then add the additional text information asked for above (i.e., LU), after you have selected the searched organization.

# Letter of Intent Preparation Instructions:

When submitting a Letter of Intent through FastLane in response to this Program Solicitation please note the conditions outlined below:

- · Submission by an Authorized Organizational Representative (AOR) is required when submitting Letters of Intent.
- A Minimum of 1 and Maximum of 4 Other Senior Project Personnel are allowed
- A Minimum of 0 and Maximum of 20 Other Participating Organizations are allowed
- Key Academic Participants is required when submitting Letters of Intent
- Submission of multiple Letters of Intent is allowed

**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: <a href="http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=gpg">http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=gpg</a>. Paper copies of the GPG may be obtained from the NSF Publications Clearinghouse, telephone (703) 292-7827 or by e-mail from <a href="mailto:nsfpubs@nsf.gov">nsfpubs@nsf.gov</a>. 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.

See Chapter II.C.2 of the GPG for guidance on the required sections of a full research proposal submitted to NSF. Please note that the proposal preparation instructions provided in this program solicitation may deviate from the GPG instructions.

The text of the project description must follow the spacing, font and formatting requirements of the NSF Grant Proposal Guide (GPG). Tables and lists in the project description may be in smaller type but be sure the type is readable when the page is printed out. Both will include the items listed below in the order indicated.

If the proposal has a multi -university configuration (which is not required), the proposal must be submitted as an integrated proposal by the lead university, with proposed sub awards to the other partner institutions. Separate proposals from each partner will not be accepted since separately submitted collaborative proposals are not allowed.

Except as modified below, full proposals should be prepared in accordance with the guidelines in the Grant Proposal Guide or NSF Grants.gov Application Guide.

- 1. **Cover Sheet.** Select the NCN solicitation number from the pull down list. If submitting via Grants.gov, the program solicitation number will be prepopulated by Grants.gov on the NSF Application Cover Page. Where asked to identify the NSF Unit of Consideration, select the Division of Engineering Education and Centers. The proposal title should follow the guidance in the Letter of Intent instructions. For planning purposes, September 1, 2017 should be shown as the start date.
- 2. **Project Summary (three text boxes).** The summary should be written in the third person (i.e. the use of the pronoun "it" not "we") and should make a compelling case for the proposed Node. The summary should be informative to persons working in the same or related fields and, insofar as possible, understandable to a scientifically or technically literate lay reader.

In the "Overview" section include the proposal title, the lead PI's name, and the submitting university's name. Clearly summarize the vision, goals, and program of the proposed Node. In the "Intellectual Merit" and "Broader Impact" sections summarize features of the proposal relevant to NSF's Intellectual Merit and Broader Impacts review criteria, respectively.

### 3. Project Description.

The project description must contain sections 3.a and 3.b and is limited to 25 pages for full proposals, including all figures, tables, and charts. If the Project Description section exceeds these extended page limits, the proposal will be returned without review. The project description should be prepared with reference to the review criteria and the guidance provided in this and the preceding sections of this solicitation.

Please note that per guidance in the GPG, the Project Description must contain, as a separate section within the narrative, a section labeled "Broader Impacts of the Proposed Work." This section should provide a discussion of the broader impacts of the proposed activities. Pls can decide where to include this section within the Project Description.

### (3.a) Objectives and Plans of the NCN Node

Given the guidance and requirements for the Node chosen, develop the proposal narrative to provide the following information at a minimum:

- Articulation of a compelling new nanoscience modeling and computational tool(s) to advance nanotechnology to meet critical national needs
- Plans to nucleate a community of engaged academic, government laboratory and industrial personnel and other users of the
  novel tool(s) to address broad based user needs, including those of small businesses and to provide their tools and
  educational materials to the Node for delivery to the Cyber Platform;
- Expected deliverables to the Cyber Platform, strategic plan to achieve the deliverables and a milestone chart showing the timing of the deliverables;
- Plans to link theory to experimentation to improve these tools and to provide some funding of experimentalists and link in a
  collaborative non-funded mode to the already funded experimentalists in the area through connectivity with the National
  Nanotechnology Coordination Infrastructure Network (NNCI), the Nanosystems Engineering Research Centers (NERC), and
  relevant ongoing Engineering Research Centers (ERC), etc.;
- Methods to user-test simulation tools and educational materials to the Cyber Platform;

### (3.b) Infrastructure for the NCN Node

- A. Institutional Configuration
  - 1. Justify the institutional configuration of the Node given its goals and deliverables.
- B. Leadership and Team
  - Briefly discuss the background of the leaders, faculty and staff and justify the relevance of that background to the goals of the Node. Provide a table of the diversity of the proposed team.
- C. Organizational Structure and Management
  - Describe the proposed organizational structure and include an organization chart. If the proposal includes more than
    one university/institution discuss how the participants will be developed into a team to deliver the proposed
    goals/milestones. Discuss how the internal oversight system for the Cyber Platform or Node. Discuss how the project
    will be managed.
- D. Financial Support and Functional Allocation of Resources
  - Discuss how the funding will be allocated to the proposed tasks and provide a functional budget table, showing for year one how the funding will be distributed by major task, with a row for each major task, including overhead charges as the last row before the row showing the total.
- E. Headquarters and Equipment Infrastructure

Discuss the headquarters space for the Node, its size and functionality. Generally describe the equipment infrastructure supporting the Node, referring the reader to the required section of the FastLane proposal template on "Facilities, Equipment and Other Resources" for more detail.

Single Copy Document: In the Single Copy Documents section, upload the following:

(1) A list of Collaborators: In lieu of the instructions specified in the GPG, Collaborators and Other Affiliations Information should be submitted as follows. (Note: In collaborative proposals, the lead institution should assemble and provide this information for all participants in the collaborative group):

Provide current, accurate information for all active or recent collaborators of personnel and institutions involved in the project. NSF staff will use this information in the merit review process to manage conflicts of interest. This list is distinct from (1) below under Supplementary Documents in that it must include all active or recent Collaborators of all personnel involved with the proposed project. Collaborators include any individual with whom any member of the project team – including Pls, Co-Pls, Senior Personnel, paid/unpaid Consultants or Collaborators, Subawardees, Postdocs, and project-level advisory committee members – has collaborated on a project, book, article, report, or paper within the preceding 48 months; or co-edited a journal, compendium, or conference proceedings within the preceding 24 months. This list should be numbered and include (in this order) Full name and

Organization(s), with each item separated by a semi-colon. Each person listed should start a new numbered line.

- 1. Collaborators for Mary Smith; XYZ University; PI
  - a. Helen Gupta; ABC University
     b. John Jones; University of PQR

  - c. Fred Gonzales; DEF Corporation
    d. Susan White; DEF Corporation
- 2. Collaborators for John Jones; University of PQR; Senior Personnel
  - a. Tim Green; ZZZ University
  - b. Ping Chang, ZZZ University
  - c. Mary Smith; XYZ University
- 3. Collaborators for Jane Brown; XYZ University; Postdoc
  - a. Fred Gonzales; DEF Corporation
- 4. Collaborators for Bob Adams; ABC Community College; Paid Consultant
  - a. None
- 5. Collaborators for Susan White; Welldone Institution; Unpaid Collaborator
  - a. Mary Smith; XYZ University
  - b. Harry Nguyen; Welldone Institution
- 6. Collaborators for Tim Green; ZZZ University; Subawardee
  - a. John Jones; University of PQR

Supplementary Documents: In the Supplementary Documents section, upload the following information where relevant:

(1) A list of Project Personnel and Partner Institutions (Note: In separately-submitted collaborative proposals, only the lead institution should provide this information):

Provide current, accurate information for all personnel and institutions involved in the project. NSF staff will use this information in the merit review process to manage conflicts of interest. The list must include all PIs, Co-PIs, Senior Personnel, paid/unpaid Consultants or Collaborators, Subawardees, Postdocs, project-level advisory committee members, and writers of letters of support. This list should be numbered and include (in this order) Full name, Organization(s), and Role in the project, with each item separated by a semi-colon. Each person listed should start a new numbered line. For example:

- 1. Mary Smith; XYZ University; PI
- 2. John Jones; University of PQR; Senior Personnel
- 3. Jane Brown; XYZ University; Postdoc
- 4. Bob Adams; ABC Community College; Paid Consultant
- 5. Susan White; Welldone Institution; Unpaid Collaborator
- 6. Tim Green; ZZZ University; Subawardee

### (2) Collaboration Plan:

Since the success of collaborative research efforts are known to depend on thoughtful coordination mechanisms that regularly bring together the various participants of the project, a Collaboration Plan is required for all proposals. Up to 2 pages are allowed for Collaboration Plans. The length of and level of detail provided in the Collaboration Plan should be commensurate with the complexity of the proposed project. Where appropriate, the Collaboration Plan should include: 1) the specific roles of the project participants in all organizations involved; 2) information on how the project will be managed across all the investigators, institutions, and/or disciplines; 3) identification of the specific coordination mechanisms that will enable cross-investigator, cross-institution, and/or cross-discipline scientific integration (e.g., yearly workshops, graduate student exchange, project meetings at conferences, use of video-conferences, software repositories, etc.); and 4) specific references to the budget line items that support collaboration and coordination mechanisms. The Collaboration Plan should reference and support the project research plan, including key interdependencies between tasks for different PIs, outlined in the Project Description. However, note that the Collaboration Plan should not be used to expand discussions on proposed research activities; the activities themselves should be described within the Project Description section.

# If a proposal does not include a Collaboration Plan of up to 2 pages, then that proposal will be returned without review.

(3) Postdoctoral Researcher Mentoring Plan (if applicable):

Each proposal that requests funding to support postdoctoral researchers must include, as a supplementary document, a description of the mentoring activities that will be provided for such individuals. In no more than one page, the mentoring plan must describe the mentoring that will be provided to all postdoctoral researchers supported by the project, irrespective of whether they reside at the submitting organization, any subawardee organization, or at any organization participating in a simultaneously submitted collaborative project. Please be advised that if required, FastLane will not permit submission of a proposal that is missing a Postdoctoral Researcher Mentoring Plan. See Chapter II.C.2. of the GPG for further information about the implementation of this requirement.

(4) Data Management Plan (required):

Proposals must include a supplementary document of no more than two pages labeled "Data Management Plan." This supplementary document should describe how the proposal will conform to NSF policy on the dissemination and sharing of research results.

See Chapter II.C.2.j of the GPG for full policy implementation.

# B. Budgetary Information

### Cost Sharing:

Inclusion of voluntary committed cost sharing is prohibited.

# C. Due Dates

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

November 03 2016

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

# D. FastLane/Grants.gov Requirements

### For Proposals Submitted Via FastLane:

To prepare and submit a proposal via FastLane, see detailed technical instructions available at: <a href="https://www.fastlane.nsf.gov/a1/newstan.htm">https://www.fastlane.nsf.gov/a1/newstan.htm</a>. 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.

### 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: <a href="http://www.grants.gov/web/grants/applicants.html">http://www.grants.gov/web/grants/applicants.html</a>. In addition, the NSF Grants.gov Application Guide (see link in Section V.A) provides instructions regarding the technical 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: <a href="mailto:support@grants.gov">support@grants.gov</a>. 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.

Proposers that submitted via FastLane are strongly encouraged to use FastLane to verify the status of their submission to NSF. For proposers that submitted via Grants.gov, until an application has been received and validated by NSF, the Authorized Organizational Representative may check the status of an application on Grants.gov. After proposers have received an e-mail notification from NSF, Research.gov should be used to check the status of an application.

# VI. NSF PROPOSAL PROCESSING AND REVIEW PROCEDURES

Proposals received by NSF are assigned to the appropriate NSF program for acknowledgement and, if they meet NSF requirements, for review. 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 either as *ad hoc* reviewers, panelists, or both, who are experts in the particular fields represented by the proposal. These reviewers are selected by Program Officers charged with 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. In addition, Program Officers may obtain comments from site visits before recommending final action on proposals. Senior NSF staff further review recommendations for awards. A flowchart that depicts the entire NSF proposal and award process (and associated timeline) is included in the GPG as Exhibit III-1.

A comprehensive description of the Foundation's merit review process is available on the NSF website at: http://www.nsf.gov/bfa/dias/policy/merit\_review/.

Proposers should also be aware of core strategies that are essential to the fulfillment of NSF's mission, as articulated in *Investing in Science, Engineering, and Education for the Nation's Future: NSF Strategic Plan for 2014-2018.* These strategies are integrated in the program planning and implementation process, of which proposal review is one part. NSF's mission is particularly well-implemented through the integration of research and education and broadening participation in NSF programs, projects, and activities.

One of the strategic objectives in support of NSF's mission is to foster integration of research and education through the programs, projects, and activities it supports at academic and research institutions. These institutions must recruit, train, and prepare a diverse STEM workforce to advance the frontiers of science and participate in the U.S. technology-based economy. NSF's contribution to the national innovation ecosystem is to provide cutting-edge research under the guidance of the Nation's most creative scientists and engineers. NSF also supports development of a strong science, technology, engineering, and mathematics (STEM) workforce by investing in building the knowledge that informs improvements in STEM teaching and learning.

NSF's mission calls for the broadening of opportunities and expanding participation of groups, institutions, and geographic regions that are underrepresented in STEM disciplines, which 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.

# A. Merit Review Principles and Criteria

The National Science Foundation strives to invest in a robust and diverse portfolio of projects that creates new knowledge and enables breakthroughs in understanding across all areas of science and engineering research and education. To identify which projects to support, NSF relies on a merit review process that incorporates consideration of both the technical aspects of a proposed project and its potential to contribute more broadly to advancing NSF's mission "to promote the progress of science; to advance the national health, prosperity, and welfare; to secure the national defense; and for other purposes." NSF makes every effort to conduct a fair, competitive, transparent merit review process for the selection of projects.

# 1. Merit Review Principles

These principles are to be given due diligence by Pls and organizations when preparing proposals and managing projects, by reviewers when reading and evaluating proposals, and by NSF program staff when determining whether or not to recommend proposals for

funding and while overseeing awards. Given that NSF is the primary federal agency charged with nurturing and supporting excellence in basic research and education, the following three principles apply:

- All NSF projects should be of the highest quality and have the potential to advance, if not transform, the frontiers of knowledge.
- NSF projects, in the aggregate, should contribute more broadly to achieving societal goals. These "Broader Impacts" may be
  accomplished through the research itself, through activities that are directly related to specific research projects, or through
  activities that are supported by, but are complementary to, the project. The project activities may be based on previously
  established and/or innovative methods and approaches, but in either case must be well justified.
- Meaningful assessment and evaluation of NSF funded projects should be based on appropriate metrics, keeping in mind the
  likely correlation between the effect of broader impacts and the resources provided to implement projects. If the size of the
  activity is limited, evaluation of that activity in isolation is not likely to be meaningful. Thus, assessing the effectiveness of these
  activities may best be done at a higher, more aggregated, level than the individual project.

With respect to the third principle, even if assessment of Broader Impacts outcomes for particular projects is done at an aggregated level, PIs are expected to be accountable for carrying out the activities described in the funded project. Thus, individual projects should include clearly stated goals, specific descriptions of the activities that the PI intends to do, and a plan in place to document the outputs of those activities.

These three merit review principles provide the basis for the merit review criteria, as well as a context within which the users of the criteria can better understand their intent.

#### 2. Merit Review Criteria

All NSF proposals are evaluated through use of the two National Science Board approved merit review criteria. In some instances, however, NSF will employ additional criteria as required to highlight the specific objectives of certain programs and activities.

The two merit review criteria are listed below. **Both** criteria are to be given **full consideration** during the review and decision-making processes; each criterion is necessary but neither, by itself, is sufficient. Therefore, proposers must fully address both criteria. (GPG Chapter II.C.2.d.i. contains additional information for use by proposers in development of the Project Description section of the proposal.) Reviewers are strongly encouraged to review the criteria, including GPG Chapter II.C.2.d.i., prior to the review of a proposal.

When evaluating NSF proposals, reviewers will be asked to consider what the proposers want to do, why they want to do it, how they plan to do it, how they will know if they succeed, and what benefits could accrue if the project is successful. These issues apply both to the technical aspects of the proposal and the way in which the project may make broader contributions. To that end, reviewers will be asked to evaluate all proposals against two criteria:

- Intellectual Merit: The Intellectual Merit criterion encompasses the potential to advance knowledge; and
- Broader Impacts: The Broader Impacts criterion encompasses the potential to benefit society and contribute to the
  achievement of specific, desired societal outcomes.

The following elements should be considered in the review for both criteria:

- 1. What is the potential for the proposed activity to
  - a. Advance knowledge and understanding within its own field or across different fields (Intellectual Merit); and
  - b. Benefit society or advance desired societal outcomes (Broader Impacts)?
- 2. To what extent do the proposed activities suggest and explore creative, original, or potentially transformative concepts?
- 3. Is the plan for carrying out the proposed activities well-reasoned, well-organized, and based on a sound rationale? Does the plan incorporate a mechanism to assess success?
- 4. How well qualified is the individual, team, or organization to conduct the proposed activities?
- 5. Are there adequate resources available to the PI (either at the home organization or through collaborations) to carry out the proposed activities?

Broader impacts may be accomplished through the research itself, through the activities that are directly related to specific research projects, or through activities that are supported by, but are complementary to, the project. NSF values the advancement of scientific knowledge and activities that contribute to achievement of societally relevant outcomes. Such outcomes include, but are not limited to: full participation of women, persons with disabilities, and underrepresented minorities in science, technology, engineering, and mathematics (STEM); improved STEM education and educator development at any level; increased public scientific literacy and public engagement with science and technology; improved well-being of individuals in society; development of a diverse, globally competitive STEM workforce; increased partnerships between academia, industry, and others; improved national security; increased economic competitiveness of the United States; and enhanced infrastructure for research and education.

Proposers are reminded that reviewers will also be asked to review the Data Management Plan and the Postdoctoral Researcher Mentoring Plan, as appropriate.

# **Additional Solicitation Specific Review Criteria**

# **Node Review Criteria**

What compelling new nanoscience modeling and computational tool(s) will be developed and how will it advance nanotechnology to meet critical national needs?

What will the Node undertake to nucleate a community of academic and industry users engaged in the new tool(s) and increase quality and quantity of nanoHUB tools, resources, and usage?

How will the Node interact productively with the Cyber Platform and other Nodes to augment existing capabilities and ensure seamless and complementary advancement of the NCN's goals?

Are proposed objectives strongly relevant to the chosen Node description?

Are there strong plans to nucleate a community of engaged academic, government laboratory and industrial personnel and other users of the novel tool(s) to address broad based user needs, including those of small businesses and to provide their tools and educational materials to the Node for delivery to the Cyber Platform?

Is there strong set of expected deliverables to the Cyber Platform?

Is there an effective strategic plan to achieve the deliverables and strong milestone chart showing the timing of the deliverables?

Are there a comprehensive analysis of the state of the art and description of existing user-tested tools for baseline quality and

identification of needs grounded in theory?

Given that analysis, are there effective plans to develop needed new computation and simulation tools that enable analyses of scaling up from the nanoscale to devices and systems, including design and manufacturing constraints?

Are there plans to link theory to experimentation to improve these tools, including appropriate lings to already funded groups/centers of experimentalists?

Is there a workable methodology for user-testing deliverables for the Cyber Platform?

Are educational materials developed to link nanoscience to nanotechnology applications of value to high school, community college, and university students as well as industry and regulatory professionals?

Are there plans for ongoing collaboration with and delivery to the NCN Cyber Platform?

Are there plans for extracting relevant findings and lessons that might be shared across the other new Nodes?

# B. Review and Selection Process

Proposals submitted in response to this program solicitation will be reviewed by

Ad hoc Review and/or Panel Review, or Reverse Site Review.

The three sets of Node proposals will be reviewed by a panel or panel(s) that will make recommendations for an award.

Reviewers will be asked to evaluate proposals using two National Science Board approved merit review criteria and, if applicable, additional program specific criteria. A summary rating and accompanying narrative will generally be completed and submitted by each reviewer and/or panel. 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 strives to be able to tell applicants whether their proposals have been declined or recommended for funding within six months. Large or particularly complex proposals or proposals from new awardees may require additional review and processing time. The time interval begins on the deadline or target date, or receipt date, whichever is later. The interval ends when the Division Director acts upon the Program Officer's recommendation.

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. After an administrative review has occurred, Grants and Agreements Officers perform 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.

Once an award or declination decision has been made, Principal Investigators are provided feedback about their proposals. In all cases, reviews are treated as confidential documents. Verbatim copies of reviews, excluding the names of the reviewers or any reviewer-identifying information, 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.

# 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 notice, 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 notice; (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 notice. Cooperative agreements also are 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 <a href="http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=aag">http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=aag</a>.

# **Special Award Conditions:**

Post-award oversight through annual site visits and PI meetings: In addition to the annual report, each NCN Node will be reviewed by an advisory site visit team (SVT), comprising external reviewers, that will evaluate the annual performance on site at the lead institution or one of the domestic partner campuses. At the conclusion of the visit, the SVT generates a consensus site visit report that includes analyses of the strengths and weaknesses of each of the key features of the Node. The SVT recommends whether or not support should continue and provides a budget recommendation. This recommendation will be advisory to the NSF to make decisions of the terms of renewal of the corresponding NCN node. In addition, the NCN Program will host annual meetings for NCN Node Leadership Teams and NSF staff. The purpose of the meeting is to bring members of the NCN Nodes' leadership teams together to share best practices, provide input to NSF on program management issues, and receive program updates from NSF.

# 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 no later than 90 days prior to the end of the current budget period. (Some programs or awards require submission of more frequent project reports). No later than 120 days following 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 all identified PIs and co-PIs on a given award. PIs should examine the formats of the required reports in advance to assure availability of required data.

Pls are required to use NSF's electronic project-reporting system, available through Research.gov, for preparation and submission of annual and final project reports. Such reports provide information on accomplishments, project participants (individual and organizational), publications, and other specific products and impacts of the project. Submission of the report via Research.gov constitutes certification by the PI that the contents of the report are accurate and complete. The project outcomes report also 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 <a href="http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=aag">http://www.nsf.gov/publications/pub\_summ.jsp?ods\_key=aag</a>.

# **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:

- Eduardo A. Misawa, ENG/EEC, telephone: (703) 292-5353, email: emisawa@nsf.gov
- Khershed Cooper, ENG/CMMI, telephone: (703) 292-7017, email: khcooper@nsf.gov
- William Olbricht, ENG/CBET, telephone: (703) 292-2563, email: wolbrich@nsf.gov
- Dimitri Pavlidis, ENG/ECCS, telephone: (703) 292-2216, email: dpavlidi@nsf.gov
- Rajiv Ramnath, CISE/ACI, telephone: (703) 292-4776, email: rramnath@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, "NSF Update" is an information-delivery system 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 Grants Conferences. Subscribers are informed through e-mail or the user's Web browser each time new publications are issued that match their identified interests. "NSF Update" also is available on NSF's website.

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

# 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.

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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 (703) 292-5111

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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 Office of the General Counsel National Science Foundation Arlington, VA 22230



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