NSF Ideas for Future Investment

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Harnessing Data for 21st Century Science and Engineering

The increasing volume, variety, and velocity of data are giving rise to a profound transformation of research in all fields of science and engineering. New types of questions are being asked, and new challenges addressed; indeed, the very nature of scientific inquiry is changing. Building on NSF’s past investments, we propose a bold initiative to engage NSF’s research community in the pursuit of fundamental research in data science and engineering, the development of a cohesive, federated, national-scale approach to research data infrastructure, and the development of a 21st-century data-capable workforce. Advances will be required across the breadth of NSF’s research community, from

- **fundamental research in mathematics, statistics and computational science** that will enable data-driven discovery and decision-making through visualization, modeling and analysis of complex data; to

- **fundamental research on data topics** such as data discovery and integration, predictive analytics, data mining, machine learning; data semantics, open data-centric architectures and systems, reproducibility, privacy and protection, and the human-data interface; to

- **the engagement of the research domains** supported across NSF in using the advances in data science and the cyberinfrastructure to further their research; to

- **the embodiment of these innovations in a robust, comprehensive, open, science-driven, cyberinfrastructure (CI) ecosystem** capable of accelerating a broad spectrum of data-intensive research, including that in large-scale and MREFC facilities; to

- **the development and evaluation of innovative learning opportunities and educational pathways**, grounded in an education-research-based understanding of the knowledge and skill demands needed by a 21st-century data-capable workforce.

This initiative will enable and accelerate future discovery by providing the fundamental techniques, tools, research cyberinfrastructure, and educational foundations to harness the data revolution. The initiative itself could include (i) the creation of a network of national center-scale activities, each with a specific focus but linked with each other and with industry, government and international partners to maximize collective impact; (ii) increased directorate and cross-directorate activities and investments; (iii) the development, deployment, operation and evolution of national-scale, open, data-centric CI, that is integrated with NSF’s existing CI capabilities and evolved through mid-scale pilot activities. As the only federal agency broadly funding fundamental research, NSF can uniquely lead a bold initiative to create a data-enabled future for the Nation’s science, engineering and educational enterprises, and for the country more broadly.
Shaping the New Human---Technology Frontier

We envision a world in which technologies – sensors, communication, computation, and intelligence – are embedded around, on, and in us. We propose a bold initiative to catalyze the interdisciplinary science and engineering needed to shape that future and the human centered engineered and social systems that those technologies will enable.

The research challenges range broadly from:

- developing new machine learning algorithms, computing system structures, and underlying neuromorphic architectures for machine intelligence and “brain like” computations; to
- dramatically increasing the energy efficiency of sensing, communications, and computing; to
- designing, building and deploying the human-centered engineered systems with cognitive and adaptive capacities that are best matched to collaboration with humans, individually and in their smart-and-connected communities; to
- understanding how technologies affect human behavior and social organizations -- from individual psychology to the very nature of work and the work place to skills, jobs, and employment -- and how technologies are and can be shaped through interactions with people and designers; to
- determining how new learning will be possible and will be needed, and how technology can improve and extend learning to support the next generation of science; and designing, implementing, and testing new learning environments inside and outside of schools that incorporate that knowledge; and, to
- addressing the technical and social research challenges in privacy and security

NSF will fund networked center activities, living labs and community-scale testbeds as well as coordinated directorate-level investments. This integrated interdisciplinary initiative will enable the creation of the human-centered technologies and the technology-rich environments that will serve the pursuit of more satisfying, happier and productive lives.
Understanding the Rules of Life:  
Predicting Phenotype

The universally recognized biggest gap in our biological knowledge is our inability to predict the phenotype of a cell or organism from what we know about the genome and environment. The traits of an organism are emergent properties of multiple types of information processed across multiple scales, e.g., biophysical, genomic, evolutionary, ecological, environmental, time. It is an enormous challenge to unravel because of the complexity of information and nonlinear processes involved; we simply do not understand the rules that govern phenotypic emergence at this scale. Unpacking phenotypic complexity will require convergence of research across biology, computer science, mathematics, the physical sciences, behavioral sciences and engineering.

Key Questions

1) How can computational modeling and informatics methods enable data integration for the purpose of analysis and prediction of complex living systems?

2) Variation in traits expressed by organisms is a feature of all life; what are the genetic, epigenetic and environmental factors that explain its magnitude and occurrence?

3) How to predict the behavior of living systems, from single molecules to whole cells, whole organisms, and whole ecosystems? To what degree do group interactions and behavior affect phenotypic expression?

4) To what degree is an organism’s phenome a result of the microorganisms that live in symbiosis with it? To what degree is the production of a phenotype a ‘joint effort’ among genomes of different organisms?

5) Can we synthesize cells and organisms based on knowledge of genome sequence and physical features of other basic molecules?

The Quantum Leap: Leading the Next Quantum Revolution

The world is on the threshold of the next quantum revolution, and the NSF has a leading role to play. The Quantum Leap is a cross-NSF approach to identifying and supporting research that answers deep questions about quantum behavior and develops the means of accessing and manipulating quantum systems. The goal is to couple together experiment, computation, and theory to attack fundamental questions, with an eye toward enabling more efficient computation, communication and simulation. NSF can drive this compelling basic research and its potentially significant applications across a broad swath of science and engineering.

Quantum mechanics is a powerful concept that has led to many of the transformative technologies of today. The next quantum revolution will exploit quantum phenomena, such as superposition, entanglement, and squeezing, to capitalize on the rich behavior of many-body systems. Superposition allows simultaneous determination of all possible outcomes, entanglement produces correlation of even widely separated particles, and squeezing manipulates inherent uncertainty to increase vastly the precision of measurements. Applying these phenomena to collections of particles leads to revolutionary developments such as

- quantum sensors,
- quantum computation,
- quantum communications, and
- quantum simulators.

Intellectual opportunity, broad national interest, and international competition make The Quantum Leap a compelling topic that draws physical science, mathematics, computer science, and engineering together in a transformative (high risk – high reward) enterprise to answer fundamental questions, such as,

- How do we prepare and manipulate complex or dynamic quantum states?
- How do we control material-light interactions to create new quantum phenomena?
- What are the mathematics that describe emergent quantum behavior?
- How do we design and engineer systems that use quantum effects extensively?

Competition is fierce and the US needs to stay at the forefront to ensure our security, economic growth, and global competitiveness. Research in quantum materials will also prepare the broadly educated individuals to make and implement the discoveries of the next quantum revolution. There will be strong connections to industry, federal agencies, and international partners.
Navigating the New Arctic

Vision

The Arctic is warming at twice the rate of the rest of the Earth, with far-reaching consequences for Arctic residents, particularly indigenous peoples. Arctic change will fundamentally alter climate, weather, and ecosystems globally in ways that we do not yet understand, but which will have profound impacts on the world’s economy and security. Rapid loss of Arctic sea ice and other changes will also bring new access to this frontier and its natural resources like fossil fuels, minerals, and new fisheries which are already attracting international attention from industry and nations seeking new resources.

NSF proposes to establish an observing network of mobile and fixed platforms and tools across the Arctic to document these rapid biological, physical, chemical and social changes, leveraging participation by other federal agencies. Current Arctic observations are sparse and inadequate to enable discovery or simulations of the processes underlying Arctic System change on a wide range of spatial and temporal scales, and to assess their environmental and economic impacts on the broader Earth System.

Summertime heating at 71°N on the central Baffin Island plateau in 2009 produced deep convection with accompanying thunder and lightning… nearly unheard of in earlier decades (NAS 2014). Other major environmental changes in the Arctic include a rapidly diminishing sea ice cover, altered freshwater cycling, greening of the tundra, thawing permafrost, coastal erosion, and widespread fires.

NSF Uniqueness and Readiness

Among the Federal Agencies, NSF is unique in its ability to fund bottom-up research driven by the U.S. academic research community across the physical, biological, social, engineering and computational sciences. Growing human capacity via education and training of the next generation of Arctic researchers can be undertaken. Arctic system science and creating an Arctic observing network are efforts that NSF has led. NSF also supports the most capable Arctic logistics infrastructure of any agency.

Some Key Questions

How will the dramatic changes in sea ice alter marine ecosystem structure and primary productivity? How will the new Arctic Ocean ecosystem function?

What new indicators and theory are needed to understand adaptive capacity of Arctic individuals and communities experiencing the unprecedented rate of Arctic environmental and social change?

How will permafrost thaw and the changing Arctic water cycle alter Arctic terrestrial ecosystems and greenhouse gas emissions?

What is are the linkages between Arctic warming and changing mid-latitude weather patterns?
Windows on the Universe: The Era of Multi-messenger Astrophysics

Observing the cosmos through three different windows - opened by detecting electromagnetic waves, particles, and gravitational waves - can answer some of the most profound questions before humankind.

- How did the universe begin?
- Why is the universe accelerating?
- What is the unseen matter that constitutes much of the universe?
- How does gravity work under the most extreme conditions?
- What are the properties of the most exotic objects in the universe?

We have come to a special moment in understanding the universe. We have been observing across the electromagnetic spectrum from radio waves to gamma rays, and now we are able for the first time to look in fundamentally different ways using a powerful and synthetic collection of approaches. Just as electromagnetic radiation gives us one view, particles such as neutrinos and cosmic rays provide a different view, and gravitational waves give yet another. Together they will provide unique insights into the nature and behavior of matter and energy.

These research goals and topics are clearly at the heart of the fundamental mission of the NSF to promote the progress of science. The history of the Foundation in ground-based astronomy, particle astrophysics, and gravitational physics puts it clearly in the center of the action for all of these messengers. As the one agency engaged in all three types of multi-messenger astrophysics, NSF is uniquely positioned to promote interagency and international collaborations.
Growing Convergent Research at NSF

Context: The NAS report depicted here states: “The key message of convergence, however, is that merging ideas, approaches, and technologies from widely diverse fields of knowledge at a high level of integration is one crucial strategy for solving complex problems and addressing complex intellectual questions underlying emerging disciplines.” The convergence paradigm augments a more traditional transdisciplinary approach to research by framing challenging research questions at inception, and fostering the collaborations needed for successful inquiry. An effective approach to convergence would address the key technical, organizational and logistical challenges that hinder truly transdisciplinary research. Today’s grand challenges invite a convergence approach, and NSF is well positioned to foster convergence because of its deep connections to all fields of science and engineering.

Goal: NSF would strategically support research projects and programs which are motivated by intellectual opportunities and/or important societal problems, and which would benefit from the convergence of (subsets) of physical sciences, biological sciences, computing, engineering, and the social and behavioral sciences.

Key Questions:

How can we structure the criteria and metrics for assessing potential research challenges to match the promise of the convergence research paradigm?

How might we adapt our merit review processes to represent the broad spectrum of disciplinary expertise needed to most effectively ensure that excellent convergent research projects are funded?

What are the grand challenges or emerging areas of research that might benefit from a convergence approach?

How do we further increase interagency and private partnerships to augment the best convergence research?
Mid-scale Research Infrastructure

Rapidly changing patterns of research require a new approach to research infrastructure for NSF’s science and engineering activities because today they

- rely increasingly on cyberinfrastructure, broadly defined,
- use infrastructure that is diverse in space, cost, and implementation time, and
- require dynamic and nimble responses to new challenges.

We face a gap in the funding structure available at NSF to respond to this new reality. NSF funds relatively small research infrastructure projects through individual Directorates (up to about $20M) or through the Major Research Instrumentation (MRI) program (up to $4M). There are many important experiments and facilities that fall in the gap between these amounts and the roughly $100M threshold for Major Research Equipment and Facilities Construction (MREFC) funding. Missing that opportunity leaves essential science undone. The long-term consequences of that neglect will be profound for science as well as for our Nation’s economy, security, and competitiveness.

One example is collaborative cyberinfrastructure that is critical across all of science and engineering, an area that requires a more agile approach than currently provided by the MREFC process. Other examples are cosmic microwave background measurements, sensor networks, dark matter experiments, and nuclear astrophysics measurements. This range of “large mid-scale” funding is also potentially critical for existing major experiments and facilities such as the Laser Interferometer Gravitational-Wave Observatory (LIGO) or the National High Magnetic Field Laboratory. Funding projects that fall in the “gap” can propel a facility into an entirely new realm of capability. Importantly, mid-scale infrastructure potentially creates opportunities for parts of NSF beyond the traditionally “facilities-intensive” Directorates.

*NSF must find a way to seize these important opportunities.* One relatively simple approach is to lower the threshold for MREFC expenditures and develop a nimble, but carefully monitored, process for funding experimental research capabilities in the mid-scale range.
Context: The NSF 2050: Integrative Foundational Fund (IFF) will be dedicated to identifying bold, long-term foundational research questions to set the stage for breakthrough science and engineering all the way to NSF’s Centennial in 2050. Visioning exercises will develop research agendas for possible implementation in a set of highly visible, transformational programs to be known as NSF 2050. Similar to NIH’s Common Fund, NSF 2050 will allow for systemic, community input into long-term program development and capture the imagination of critical stakeholders in terms of what might be.

Vision: While long-term program development occurs throughout the Foundation already, it usually occurs in individual directorates or divisions. And cross-cutting programs are usually developed on yearly budget cycles, which may limit vision and scope. NSF 2050 intends to transcend established scientific structures and standard operating procedures to ensure continuous exploration at the frontiers and risk-taking in areas that might not fit into any particular program “box.” New programs might cross boundaries in innovative ways, fill recognized gaps or take advantage of new opportunities. They should all push the frontiers.

Questions:

- How can NSF most effectively maintain and bolster its global leadership in both foundational and cross-cutting research and education, enabling discovery and innovation of unprecedented scope and impact?
- What are the bold, new, long-term research questions that need to be asked today to allow for a future that aligns with human values and captures our imaginations?
- How can NSF emphasize the impact of its research investments and increase its visibility with critical science and engineering stakeholders?
- How can NSF and its research communities take advantage of the changing nature of science and engineering as it becomes more computational- and data-intensive to quicken the pace of discovery?