National Strategic Computing Initiative: NIH Participation

Susan K. Gregurick, Ph.D. Division Director
Biomedical Technology, Bioinformatics and Computational Biology
To seek fundamental knowledge about the nature and behavior of living systems and the application of that knowledge to enhance health, lengthen life, and reduce illness and disability.

In support of this mission, NIH makes optimal use of computer science and computing technologies to address current challenges in biology and medicine.
The mission of BISTI is to make optimal use of computer science and technology to address problems in biology and medicine by fostering new basic understandings, collaborations, and transdisciplinary initiatives between the computational and biomedical sciences.

In support of this mission, the BISTI coordinates research grants, training opportunities, and scientific symposia associated with biomedical computing across NIH. Regular monthly meetings are conducted to discuss program status, future needs and directions, and topics of interest to the bioinformatics community.

http://www.bisti.nih.gov
# Biocomputing across NIH

<table>
<thead>
<tr>
<th>Networking and Information Technology Research and Development Program (NITRD)</th>
<th>$612 million/year in 2014</th>
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<tbody>
<tr>
<td>High End Computing</td>
<td>$189 million/year</td>
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<tr>
<td>Information management</td>
<td>$251 million/year</td>
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<tr>
<td>High Confidence Software &amp; Systems</td>
<td>$242 million/year</td>
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<td>Software Design &amp; Productivity</td>
<td>$92 million/year</td>
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Assembling and Sustaining the ‘Acid Mantle’ of the Human Skin Barrier
PI: Michael Klein, Temple University
Summary: Study the cohesive forces between the microscopic layers of human skin and thus build models to evaluate the impact of chemicals on one of the body's largest organs
CPU: 75M

Multiscale Simulations of Human Pathologies
PI: George Karniadakis, Brown University
Summary: This research project aims to simulate blood flow and thrombus biomechanics in thoracic aortic aneurysms and dissections (TAADs).
CPU: 45M

Studies of Large Conformational Changes in Biomolecular Machines
PI: Benoît Roux, University of Chicago
Summary: Calculating all conformational states of two membrane proteins to provide mechanistic perspective of membrane protein function, linking structure to dynamics, by characterizing the free energy landscape that governs functional motions
CPU: 55M

Petascale Computing of Biomolecular Systems
PI: Klaus Schulten, University of Illinois at Urbana-Champaign
Summary: Petascale resources to investigate three biomolecular systems: the assembly of the HIV capsid, the process of peptide bond formation in ribosomes, and the basic process of photosynthesis.
CPU: 150M
Strategic Objectives of NSCI Initiative

1. **Accelerating delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 100 times the performance of current 10 petaflop systems across a range of applications representing government needs.**

2. **Increasing coherence between the technology base used for modeling and simulation and that used for data analytic computing.**

3. **Establishing, over the next 15 years, a viable path forward for future HPC systems even after the limits of current semiconductor technology are reached (the "post-Moore's Law era").**

4. **Increasing the capacity and capability of an enduring national HPC ecosystem by employing a holistic approach that addresses relevant factors such as networking technology, workflow, downward scaling, foundational algorithms and software, accessibility, and workforce development.**

5. **Developing an enduring public-private collaboration to ensure that the benefits of the research and development advances are, to the greatest extent, shared between the United States Government and industrial and academic sectors.**
NIH Role and Responsibility

• **DOE and NSA**: Lead agencies, charged with primary delivery of the next generation of integrated computing capability
  - **DOE** focus on scientific computing through a CMOS-based, *capable exascale* program
    - seek major improvements in memory bandwidth, interconnect performance, energy efficiency, & resiliency
    - commensurate improvements in system software, algorithms, application code efficiency, uncertainty quantification etc.
    - *increase emphasis on “Big Data” analytic computing for DOE missions in large science and national security*
  - **NSA** focus on next generation cryptanalytic and data analytic computing
  - **Joint**: Engage in synergistic, mutually supportive technology develop.

• **NSF, DOD, DNI and NIST**: foundational R&D (hardware and software).

• **NSF**: central role in education (*all agencies will participate in workforce development as appropriate*).

• **DOD, NASA, NIST, NIH and NOAA**: engage in and track early stages of design and on effective mission deployment in their contexts.
NIH Role and Responsibility

• Consistent with Strategic Objective 2, provide research leadership in developing the necessary computational methods, algorithms, and sustainable software applications that will exploit NSCI technology advances and that are in support of the biomedical research community.

• Participate in activities of the cross-agency steering group to optimize a national HPC infrastructure.

• Recognize and plan for emerging uses of HPC (Strategic Objectives 2, 4, and 5).

Activities in FY 2016 and 2017

• Participate with NSF and DOE in the NSCI Exascale Request for Information (RFI) in FY 2016.

• By FY 2017, identify and report on the research requirements for HPC and capable exascale computing that are unique to the biomedical research community.
NSCI Exascale Request for Information (RFI, NOT-GM-15-122)

- The specific scientific and research challenges that would need the projected 100-fold increase in performance
- The potential impact of the research to the scientific community, national economy, and society.
- The specific limitations/barriers of existing HPC systems must overcome
- Any related research areas you foresee that would benefit from this level of augmented computational capability.
- Important computational and technical parameters of the problem as you expect them to be in 10 years (2025)
- Alternative models of deployment and resource accessibility arising out of exascale computing
- Capabilities needed by the end-to-end system, including data requirements such as data analytics and visualization tools, shared data capabilities, and data services which includes databases, portals and data transfer tools/nodes.
- Foundational issues that need to be addressed such as training, workforce development or collaborative environments.
- Other areas of relevance for the Agencies to consider.

NIGMS_exascale@nigms.nih.gov by November 13, 2015
Specific areas where Exascale Computing enhances NIH research

The BRAIN Initiative:

*Brain Research through Advancing Innovative Neurotechnologies*

- Launched by the President in April 2013 as a bold new effort to revolutionize our understanding of the human brain

- **Goal**: Produce a clearer, dynamic picture of the brain that can show, for the first time, how individual cells and complex neural circuits interact in both time and space

- Leverages high-performance computing resources to simulate the complexities of neural circuitry

- Multi-agency initiative: NIH, DARPA, NSF, FDA, and IARPA
Specific areas where Exascale Computing enhances NIH research

Advanced Cellular Imaging

- Imaging technologies can pinpoint the inner workings of living tissues at extraordinary detail, making three-dimensional molecular movies and capturing nanoscale chemical reactions in real time
  - X-ray free-electron lasers
  - Electron cryomicroscopy
  - Light microscopy

- Novel approaches need to be developed to analyze the deluge of data produced by advanced cellular imaging tools
Specific areas where Exascale Computing enhances NIH research

Precision Medicine

• Tailor treatments to individual patient’s characteristics

• Proposal: National cohort of >1 million individuals who volunteer to share their genetic information in the context of other health data over time
  – Link data to electronic health records
  – Foundation for research studies leading to prevention strategies, novel therapeutics, and medical devices
  – Improve how drugs are prescribed (choice, dosage)
Specific areas where Exascale Computing enhances NIH research

Big Data to Knowledge (BD2K)

• Coordinate access to and analysis of the many types of biological and behavioral ‘big data’ being generated by biomedical scientists

• Develop innovative and transformative computational approaches, tools, and infrastructures to make ‘big data’ and data science a prominent component of biomedical research

• Enable data sharing and utilization through the development of a new shared, interoperable cloud computing environment: the ‘Commons’
Thank You!