Assessing the Impact of Changes in the Information Technology Research and Development Ecosystem

Perspectives on the IT R&D Ecosystem

National Academy of Sciences
November 2, 2006

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National Center for Research Resources
National Institutes of Health

What are your agency's investment philosophy, strategy, and interests for IT research?

NIH invests $500M/yr in Bioinformatics and Computational Biology

- High end computing infrastructure and applications (40%)
- Human-computer interaction and information management (35%)
- Large scale networking (15%)

Infrastructure for biomedical computation

THEORETICAL *and* COMPUTATIONAL BIOPHYSICS GROUP

NIH RESOURCE FOR MACROMOLECULAR MODELING AND BIOINFORMATICS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

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Highlights of our Work

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Most forms of life need to detect and respond to changes in their environment for survival and optimal growth. For this purpose organisms rely on receptors that are based on sensory proteins. In plants, several sensory proteins detect the ambient light for optimal exposure of their photosynthetic apparatus. One class of plant light sensors, the phototropins, influence photosynthesis and induce the transition between root and stem growth when seedlings emerge out of the ground. Induction is activated through several protein domains, two of which actually absorb light and for their sensitivity to light, oxygen, and voltage, are called LOV1 and LOV2 domains. Understanding the LOV domains' involvement in activation is important for studying the activation mechanisms of other types of sensory proteins. Strangely, light absorbed by LOV domains is observed to lead to a distinct, but only very minute, structural change that does not explain how activation might come about. **NAMD**-based molecular dynamics simulations of the LOV domain have now revealed, as reported in a **recent publication**, that photoactivated LOV domains exhibit altered patterns of motion that can induce a signal for plant cells. More information may be found on our **biological photoreceptors** website.

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Recent Publications

Stability and dynamics of virus capsids described by coarse-grained modeling. *Structure*, 2006. In press.

Ion conduction through MscS as determined by electrophysiology and simulation. *Biophysical Journal*, 2006. In press.

All Publications

Software

VMD - Molecular Graphics Viewer
NAMD - Molecular Dynamics Simulator
BioCoRE - Collaboratory Environment
MD Service Suite
Structural Biology Software Database

Announcements

13 Oct 2006 - Upcoming Cluster Workshop - Nov 2006
21 Sep 2006 - One Protein, Two Channels
18 Sep 2006 - VMD Adds Evolutionary View
12 Sep 2006 - Aksimentiev in Synergy magazine
11 Sep 2006 - Postdoctoral Position
31 Aug 2006 - NAMD 2.6 released
25 Aug 2006 - VMD 1.8.5 released
25 Aug 2006 - VMD MultiSeq in BMC Bioinformatics

In the News - Archive

Research

Membrane Biophysics
Mechanobiology
Nanoengineering
Bioenergetics
Steered/Interactive Molecular Dynamics
Quantum Biology
Neurobiology
Other Topics
Collaborations

Outreach

TCB Group Overview
Group Members - Recent Photos
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Tutorials
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Training and Workshops
Picture, Movie, and Poster Galleries
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Upcoming Seminars

09 Nov 2006 - Dr. Lloyd Demetrius - The Origin of Allometric Scaling Laws in Biology

Recent Seminars

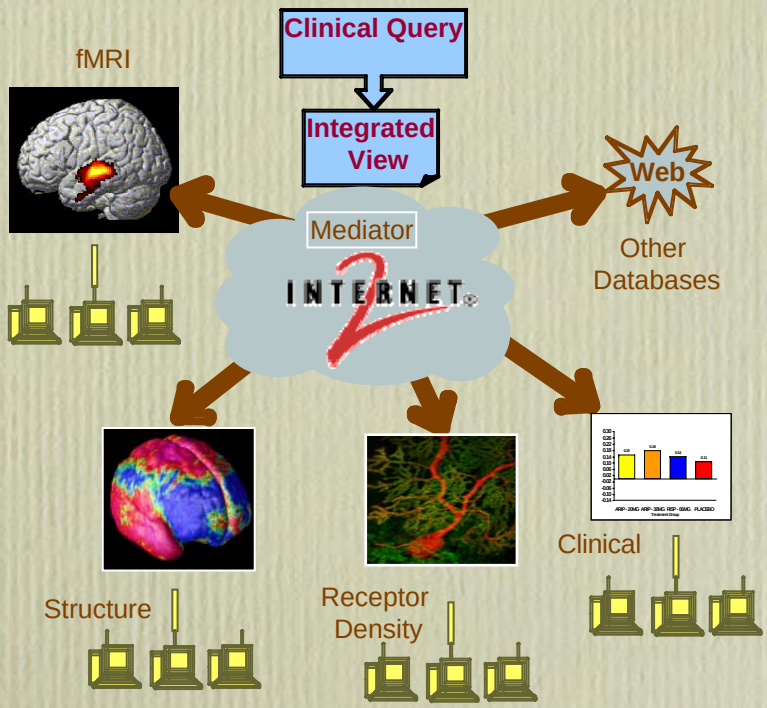
http://www.ks.uiuc.edu

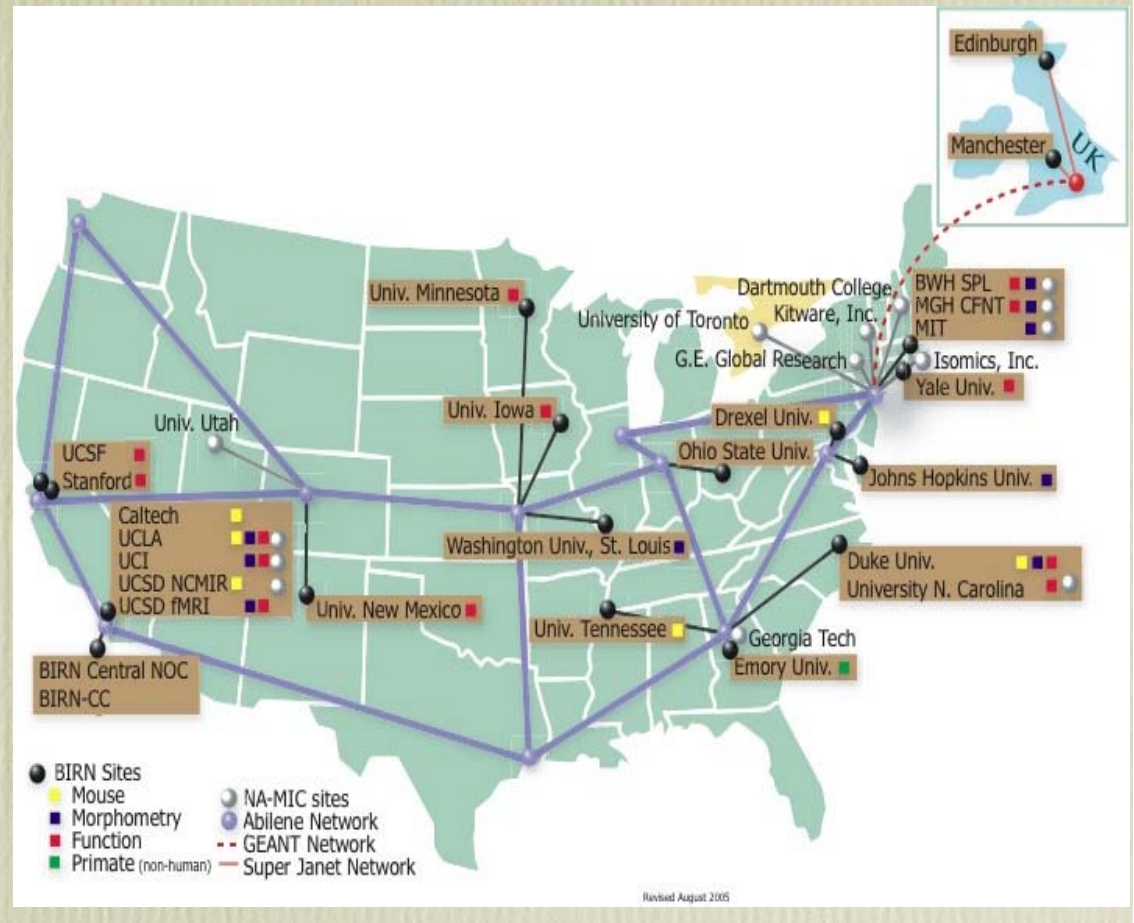
National Centers for Biomedical Computing

www.bisti.nih.gov/ncbc

Infrastructure for data & tool sharing

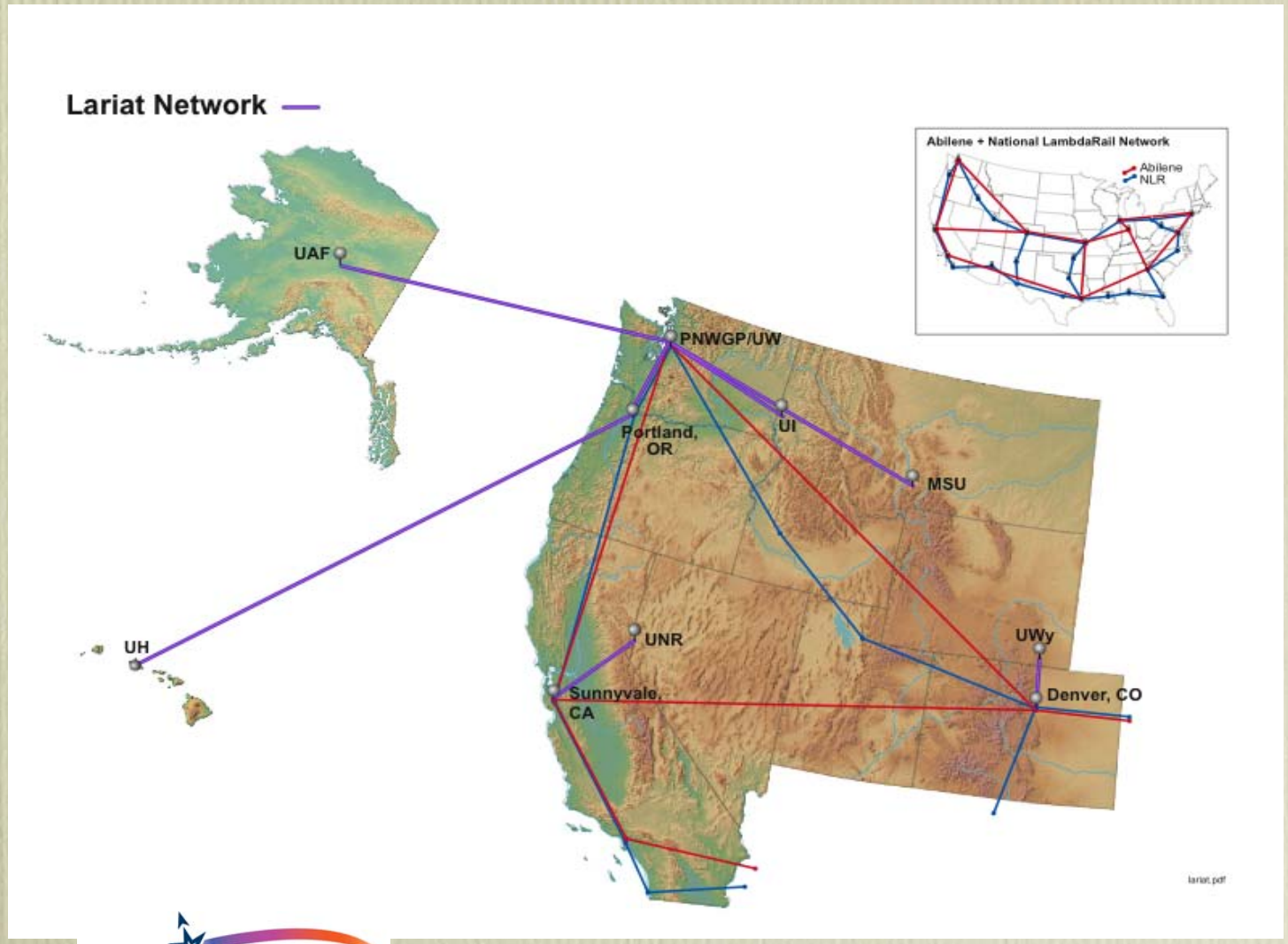
Biomedical Informatics Research Network (BIRN)





http://www.nbirn.net/

Collaborative infrastructure



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www.lariat-west.org

Large-scale Modeling

Models of Infectious Disease Agent Study (MIDAS)

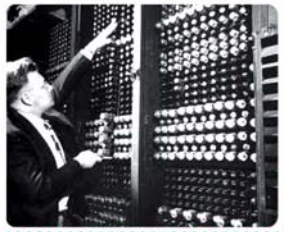
MIDAS is a collaboration of research and informatics groups to develop computational models of the interactions between infectious agents and their hosts, disease spread, prediction systems, and response strategies. The models will be useful to policymakers, public health workers, and other researchers who want to better understand and respond to emerging infectious diseases. If a disease outbreak occurs, the MIDAS network may be called upon to develop specific models to aid public officials in their decision-making processes.

http://www.nigms.nih.gov/Initiatives/MIDAS/

MILESTONES IN SCIENTIFIC COMPUTING

PRE 1960s>>

1946 ENIAC, widely thought of as the first electronic digital computer, is formally unveiled. Designed to compute ballistics during the Second World War, it performs calculations in a variety of scientific fields including random-number studies, wind-tunnel design and weather prediction. Its first 24-hour forecast takes about 24 hours to do.



1951 Marvin Minsky, later of the Massachusetts Institute of Technology (MIT), builds SNARC, the first machine to mimic a network of neurons.

1954 John Backus and his team at IBM begin developing the scientific programming language Fortran.

1956 Building on earlier experiments at the University of Manchester, UK, and elsewhere, MANIAC at the Los Alamos National Laboratory in New Mexico becomes the first computer to play a full game of chess. In 1996, IBM's Deep Blue computer will defeat world chess champion Garry Kasparov.

1959 John Kendrew of the University of Cambridge, UK, uses computers to build an atomic model of myoglobin using crystallography data.

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1960s>>

1962 Charles Molnar and Wesley Clark at MIT's Lincoln Laboratory design the Laboratory Instrument Computer (LINC) for researchers at the National Institutes of Health. It is the first lab-based computer to process data in real time.

1963 In California, the Rancho Arm becomes the first artificial robot arm to be controlled by a computer.

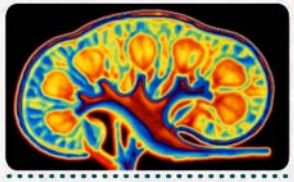
1966 Cyrus Levinthal at MIT designs the first program to represent and interpret protein structures.

1967 ARPANET — the predecessor of the Internet — is proposed by the US Department of Defense for research networking.

1969 Results of the first coupled ocean–atmosphere general circulation model are published by Syukuro Manabe and Kirk Bryan, paving the way for later climate simulations that become a powerful tool in research on global warming.

1970s>>

1971 Computing power shows its potential in medical imagery with a prototype of the first computerized tomography (CT) scanner.



1971 The Protein Data Bank is established at Brookhaven National Laboratory in Upton, New York.

1972 Hewlett Packard releases the HP-35, the first hand-held scientific calculator, rendering the engineer's slide rule obsolete.

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>> MAINFRAMES... >> WORKSTATIONS...

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1976 At Los Alamos, Seymour Cray installs the first Cray supercomputer, which can process large amounts of data at fast speeds.

DALE BOYER / SCIENCE PHOTO LIBRARY

1980s>>

1983 Danny Hillis develops the Connection Machine, the first supercomputer to feature parallel processing. It is used for artificial intelligence and fluid-flow simulations.

1985 After receiving reports of a lack of high-end computing resources for academics, the US National Science Foundation establishes five national supercomputing centres.

1989 Tim Berners-Lee of the particle-physics laboratory CERN in Geneva develops the World Wide Web — to help physicists around the globe to collaborate on research.

MICHAEL QUAN/ZUMA PRESS

1990s>>

1990 The widely used bioinformatics program Basic Local Alignment Search Tool (BLAST) is developed, enabling quick database searches for specific sequences of amino acids or base pairs.

1996 George Woltman combines disparate databases and launches the Great Internet Mersenne Prime Search. It has found nine of the largest known Mersenne prime numbers (of the form 2^n-1), including one that is 9,152,052 digits long.

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>> PERSONAL COMPUTERS... >> INTERNET...

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1996 Craig Venter develops the shotgun technique, which uses computers to piece together large fragments of DNA code and hastens the sequencing of the entire human genome.

1998 The first working quantum computers based on nuclear magnetic resonance are developed.

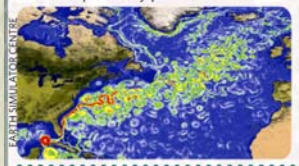
21st CENTURY>>

2001 The National Virtual Observatory project gets under way in the United States, developing methods for mining huge astronomical data sets.

SDSS

2001 The US National Institutes of Health launches the Biomedical Informatics Research Network (BIRN), a grid of supercomputers designed to let multiple institutions share data.

2002 The Earth Simulator supercomputer comes online in Japan, performing more than 35 trillion calculations each second in its quest to model planetary processes.



EARTH SIMULATOR CENTRE

2005 The IBM Blue Gene family of computers is expanded to include Blue Brain, an effort to model neural behaviour in the neocortex — the most complex part of the brain.

2007 CERN's Large Hadron Collider in Switzerland, the world's largest particle accelerator, is slated to come online. The flood of data it delivers will demand more processing power than ever before.

Jacqueline Ruttimann

>> IMPLICIT COMPUTING...

Nature 440 (23 March 2006)

From your perspective, what is the state of the IT R&D ecosystem? Has this changed or do you see it changing?

- Interdisciplinarity
- Data (tool) sharing

What studies and data, including funding data, do you think the Committee should take into account?

The Biomedical Information Science and Technology Initiative

Prepared by the Working Group on Biomedical Computing
Advisory Committee to the Director, National Institutes of Health
June 3, 1999

http://www.nih.gov/about/director/060399.htm

Supplement to the President's Budget for Fiscal Year 2007

The Networking and Information Technology Research and Development Program

A report by the Subcommittee on Networking and Information Technology Research and Development
Committee on Technology, National Science and Technology Council

http://www.nitrd.gov/pubs/2007supplement/

Agency		High End Computing Infrastructure & Applications (HEC I&A)	High End Computing Research & Development (HEC R&D)	Cyber Security & Information Assurance[1] (CSIA)	Human-Computer Interaction & Information Management (HCI &IM)	Large Scale Networking (LSN)	High Confidence Software & Systems (HCSS)	Social, Economic, & Workforce Implications of IT (SEW)	Software Design & Productivity (SDP)	Total
NSF	2006 Estimate	220.3	62.7	57.6	207.4	82.2	41.3	91.1	47.9	810.3
	2007 Request	**272.4**	**64.1**	**67.6**	**220.9**	**84.0**	**51.3**	**92.9**	**50.7**	**903.7**
OSD and DoD Service research orgs.[2,3]		214.6	9.8	0.6[4]	138.5	141.8	31.2	0.2	6.9	543.7
		186.0	**8.7**	**0.7[4]**	**135.6**	**130.7**	**29.1**	**0.3**	**6.8**	**497.8**
NIH[5]		198.5			188.7	74.9	8.4	12.3	17.9	500.6
		194.7			**183.2**	**74.6**	**8.3**	**12.2**	**17.7**	**490.7**
DARPA[3]			94.1	78.7	174.2	21.3				368.3
			117.7	**81.6**	**233.2**	**33.2**				**465.7**
DOE/SC[6]		104.4	109.1			38.9		3.5		255.8
		135.3	**160.4**			**45.0**		**4.0**		**344.7**
NSA[3]			89.2	14.1		1.0	36.2			140.5
			62.4	**13.3**		**2.3**	**39.9**			**117.9**
NASA		60.3		1.3	2.0	5.7	7.0		1.8	78.1
		63.9		**1.3**	**2.0**	**6.0**	**7.0**		**1.8**	**82.0**
AHRQ[5]					40.1	21.6				61.7
					37.3	**20.0**				**57.3**
NIST[7]		2.3	1.2	9.1	7.8	4.3	9.6		4.6	38.9
		2.3	**1.2**	**11.1**	**9.8**	**4.3**	**9.6**		**4.6**	**42.9**
DOE/NNSA[6]		10.0	15.9			1.6		4.6	3.3	35.4
		9.5	**23.4**			**1.6**		**4.6**	**2.8**	**41.9**
NOAA[7]		11.4	1.9		0.2	0.7			1.6	15.8
		16.4	**1.9**		**0.5**	**2.9**			**1.6**	**23.3**
EPA		3.3			3.0					6.3
		3.3			**3.0**					**6.3**
TOTAL (2006 Estimate)		825.0	383.9	161.3	761.9	393.9	133.6	111.6	84.0	2,855
TOTAL (2007 Request)		**883.8**	**439.9**	**175.5**	**825.4**	**404.5**	**145.2**	**114.0**	**85.9**	**3,074**

http://www.nitrd.gov/pubs/2007supplement/