NITRD

Networking and Information Technology Research and Development

FY 2004

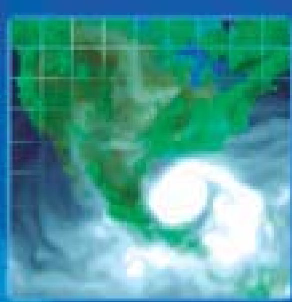
EXECUTIVE OFFICE OF THE PRESIDENT OF THE UNITED STATES

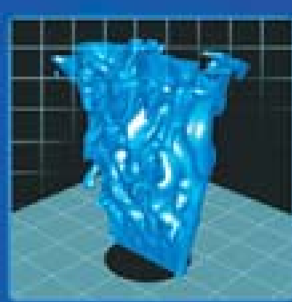
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

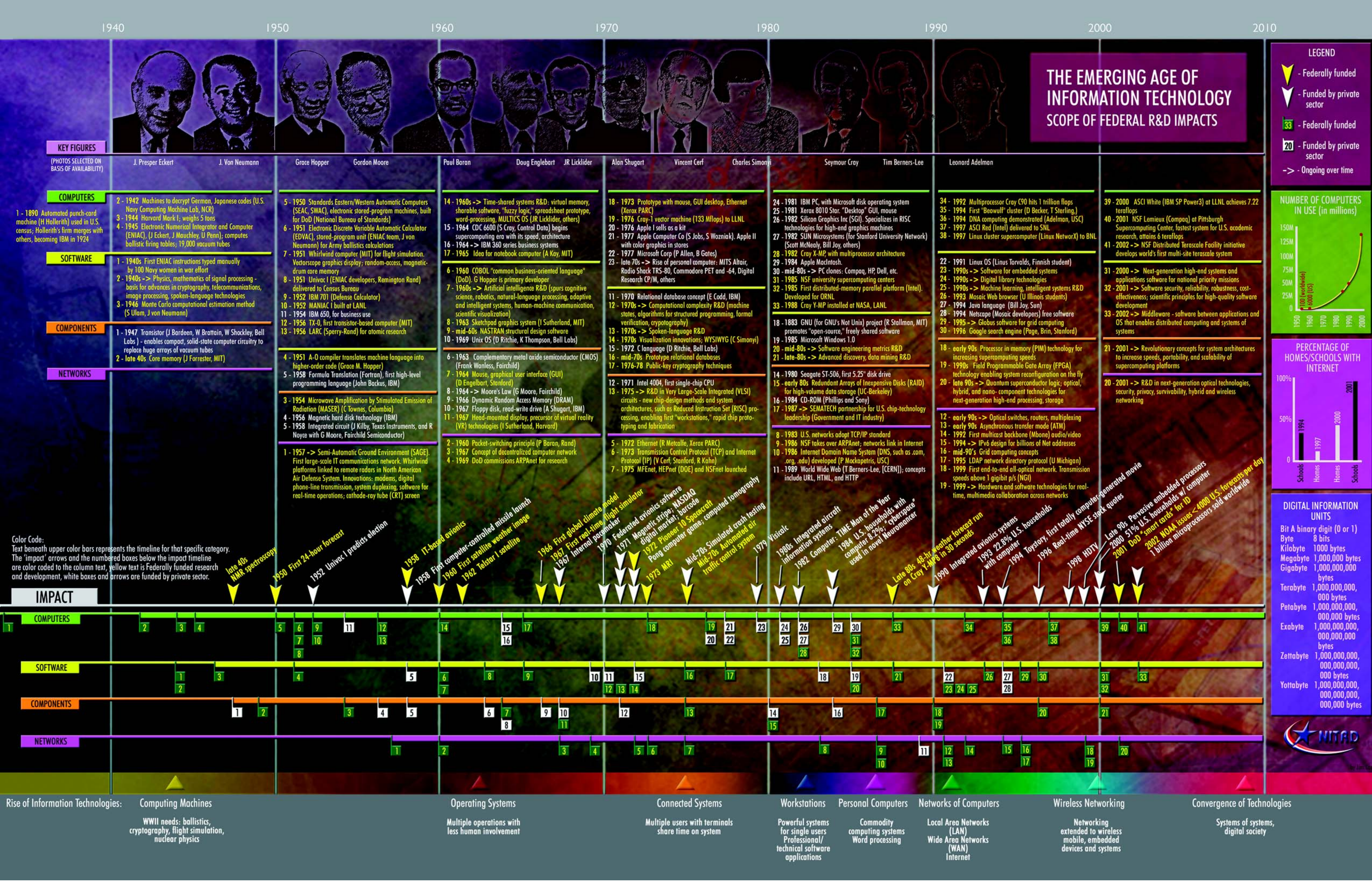
Networking and Information Technology Research and Development

Advanced Foundations for American Innovation

Supplement to the President's Budget







1940
1950
1960
1970
1980
1990
2000
2010
THE EMERGING AGE OF INFORMATION TECHNOLOGY
SCOPE OF FEDERAL R&D IMPACTS
LEGEND
- Federally funded
- Funded by private sector
33 - Federally funded
20 - Funded by private sector
-> - Ongoing over time
KEY FIGURES
(PHOTOS SELECTED ON BASIS OF AVAILABILITY)
J. Presper Eckert
J. Von Neumann
Grace Hopper
Gordon Moore
Paul Baran
Doug Englebart
JR Licklider
Alan Shugart
Vincent Cerf
Charles Simonyi
Seymour Cray
Tim Berners-Lee
Leonard Adelman
COMPUTERS
1 - 1890 Automated punch-card machine (H Hollerith) used in U.S. census; Hollerith's firm merges with others, becoming IBM in 1924
2 - 1942 Machines to decrypt German, Japanese codes (U.S. Navy Computing Machine Lab, NCR)
3 - 1944 Harvard Mark I; weighs 5 tons
4 - 1945 Electronic Numerical Integrator and Computer (ENIAC), (J Eckert, J Mauchley, U Penn); computes ballistic firing tables; 19,000 vacuum tubes
5 - 1950 Standards Eastern/Western Automatic Computers (SEAC, SWAC), electronic stored-program machines, built for DoD (National Bureau of Standards)
6 - 1951 Electronic Discrete Variable Automatic Calculator (EDVAC), stored-program unit (ENIAC team, J von Neumann) for Army ballistics calculations
7 - 1951 Whirlwind computer (MIT) for flight simulation. Vectorscope graphics display; random-access, magnetic-drum core memory
8 - 1951 Univac I (ENIAC developers, Remington Rand) delivered to Census Bureau
9 - 1952 IBM 701 (Defense Calculator)
10 - 1952 MANIAC I built at LANL
11 - 1954 IBM 650, for business use
12 - 1956 TX-0, first transistor-based computer (MIT)
13 - 1956 LARC (Sperry-Rand) for atomic research
14 - 1960s -> Time-shared systems R&D: virtual memory, sharable software, "fuzzy logic," spreadsheet prototype, word-processing, MULTICS OS (JR Licklider, others)
15 - 1964 CDC 6600 (S Cray, Control Data) begins supercomputing era with its speed, architecture
16 - 1964 -> IBM 360 series business systems
17 - 1965 Idea for notebook computer (A Kay, MIT)
18 - 1973 Prototype with mouse, GUI desktop, Ethernet (Xerox PARC)
19 - 1976 Cray-1 vector machine (133 Mflops) to LLNL
20 - 1976 Apple I sells as a kit
21 - 1977 Apple Computer Co (S Jobs, S Wozniak). Apple II with color graphics in stores
22 - 1977 Microsoft Corp (P Allen, B Gates)
23 - late 70s -> Rise of personal computer: MITS Altair, Radio Shack TRS-80, Commodore PET and -64, Digital Research CP/M, others
24 - 1981 IBM PC, with Microsoft disk operating system
25 - 1981 Xerox 8010 Star. "Desktop" GUI, mouse
26 - 1982 Silicon Graphics Inc (SGI). Specializes in RISC technologies for high-end graphics machines
27 - 1982 SUN Microsystems (for Stanford University Network) (Scott McNealy, Bill Joy, others)
28 - 1982 Cray X-MP, with multiprocessor architecture
29 - 1984 Apple MacIntosh.
30 - mid-80s -> PC clones: Compaq, HP, Dell, etc.
31 - 1985 NSF university supercomputing centers
32 - 1985 First distributed-memory parallel platform (Intel). Developed for ORNL
33 - 1988 Cray Y-MP installed at NASA, LANL
34 - 1992 Multiprocessor Cray C90 hits 1 trillion flops
35 - 1994 First "Beowulf" cluster (D Becker, T Sterling,)
36 - 1994 DNA computing demonstrated (Adelman, USC)
37 - 1997 ASCI Red (Intel) delivered to SNL
38 - 1997 Linux cluster supercomputer (Linux NetworX) to BNL
39 - 2000 ASCI White (IBM SP Power3) at LLNL achieves 7.22 teraflops
40 - 2001 NSF Lemieux (Compaq) at Pittsburgh Supercomputing Center, fastest system for U.S. academic research, attains 6 teraflops
41 - 2002 -> NSF Distributed Terascale Facility initiative develops world's first multi-site terascale system
SOFTWARE
1 - 1940s First ENIAC instructions typed manually by 100 Navy women in war effort
2 - 1940s -> Physics, mathematics of signal processing - basis for advances in cryptography, telecommunications, image processing, spoken-language technologies
3 - 1946 Monte Carlo computational estimation method (S Ulam, J von Neumann)
4 - 1951 A-0 compiler translates machine language into higher-order code (Grace M. Hopper)
5 - 1958 Formula Translation (Fortran), first high-level programming language (John Backus, IBM)
6 - 1960 COBOL "common business-oriented language" (DoD). G Hopper is primary developer
7 - 1960s -> Artificial intelligence R&D (spurs cognitive science, robotics, natural-language processing, adaptive and intelligent systems, human-machine communication, scientific visualization)
8 - 1963 Sketchpad graphics system (I Sutherland, MIT)
9 - mid-60s NASTRAN structural design software
10 - 1969 Unix OS (D Ritchie, K Thompson, Bell Labs)
11 - 1970 Relational database concept (E Codd, IBM)
12 - 1970s -> Computational complexity R&D (machine states, algorithms for structured programming, formal verification, crypotography)
13 - 1970s -> Spoken-language R&D
14 - 1970s Visualization innovations; WYSIWYG (C Simonyi)
15 - 1972 C language (D Ritchie, Bell Labs)
16 - mid-70s Prototype relational databases
17 - 1976-78 Public-key cryptography techniques
18 - 1883 GNU (for GNU's Not Unix) project (R Stallman, MIT) promotes "open-source," freely shared software
19 - 1985 Microsoft Windows 1.0
20 - mid-80s -> Software engineering metrics R&D
21 - late-80s -> Advanced discovery, data mining R&D
22 - 1991 Linux OS (Linus Torvalds, Finnish student)
23 - 1990s -> Software for embedded systems
24 - 1990s -> Digital library technologies
25 - 1990s -> Machine learning, intelligent systems R&D
26 - 1993 Mosaic Web browser (U Illinois students)
27 - 1994 Java language (Bill Joy, Sun)
28 - 1994 Netscape (Mosaic developers) free software
29 - 1995 -> Globus software for grid computing
30 - 1996 Google search engine (Page, Brin, Stanford)
31 - 2000 -> Next-generation high-end systems and applications software for national priority missions
32 - 2001 -> Software security, reliability, robustness, cost-effectiveness; scientific principles for high-quality software development
33 - 2002 -> Middleware - software between applications and OS that enables distributed computing and systems of systems
COMPONENTS
1 - 1947 Transistor (J Bardeen, W Brattain, W Shockley, Bell Labs) - enables compact, solid-state computer circuitry to replace huge arrays of vacuum tubes
2 - late 40s Core memory (J Forrester, MIT)
3 - 1954 Microwave Amplification by Stimulated Emission of Radiation (MASER) (C Townes, Columbia)
4 - 1956 Magnetic hard disk technology (IBM)
5 - 1958 Integrated circuit (J Kilby, Texas Instruments, and R Noyce with G Moore, Fairchild Semiconductor)
6 - 1963 Complementary metal oxide semiconductor (CMOS) (Frank Wanless, Fairchild)
7 - 1964 Mouse, graphical user interface (GUI) (D Engelbart, Stanford)
8 - 1964 -> Moore's Law (G Moore, Fairchild)
9 - 1966 Dynamic Random Access Memory (DRAM)
10 - 1967 Floppy disk, read-write drive (A Shugart, IBM)
11 - 1967 Head-mounted display, precursor of virtual reality (VR) technologies (I Sutherland, Harvard)
12 - 1971 Intel 4004, first single-chip CPU
13 - 1975 -> R&D in Very Large-Scale Integrated (VLSI) circuits - new chip-design methods and system architectures, such as Reduced Instruction Set (RISC) processing, enabling first "workstations," rapid chip prototyping and fabrication
14 - 1980 Seagate ST-506, first 5.25" disk drive
15 - early 80s Redundant Arrays of Inexpensive Disks (RAID) for high-volume data storage (UC-Berkeley)
16 - 1984 CD-ROM (Phillips and Sony)
17 - 1987 -> SEMATECH partnership for U.S. chip-technology leadership (Government and IT industry)
18 - early 90s Processor in memory (PIM) technology for increasing supercomputing speeds
19 - 1990s Field Programmable Gate Array (FPGA) technology enabling system reconfiguration on the fly
20 - late 90s -> Quantum superconductor logic; optical, hybrid, and nano- component technologies for next-generation high-end processing, storage
21 - 2001 -> Revolutionary concepts for system architectures to increase speeds, portability, and scalability of supercomputing platforms
NETWORKS
1 - 1957 -> Semi-Automatic Ground Environment (SAGE). First large-scale IT communications network. Whirlwind platforms linked to remote radars in North American Air Defense System. Innovations: modems, digital phone-line transmission, system duplexing, software for real-time operations; cathode-ray tube (CRT) screen
2 - 1960 Packet-switching principle (P Baran, Rand)
3 - 1967 Concept of decentralized computer network
4 - 1969 DoD commissions ARPAnet for research
5 - 1972 Ethernet (R Metcalfe, Xerox PARC)
6 - 1973 Transmission Control Protocol (TCP) and Internet Protocol (IP) (V Cerf, Stanford, R Kahn)
7 - 1975 MFEnet, HEPnet (DOE) and NSFnet launched
8 - 1983 U.S. networks adopt TCP/IP standard
9 - 1986 NSF takes over ARPAnet; networks link in Internet
10 - 1986 Internet Domain Name System (DNS, such as .com, .org, .edu) developed (P Mockapetris, USC)
11 - 1989 World Wide Web (T Berners-Lee, [CERN]); concepts include URL, HTML, and HTTP
12 - early 90s -> Optical switches, routers, multiplexing
13 - early 90s Asynchronous transfer mode (ATM)
14 - 1992 First multicast backbone (Mbone) audio/video
15 - 1994 -> IPv6 design for billions of Net addresses
16 - mid-90's Grid computing concepts
17 - 1995 LDAP network directory protocol (U Michigan)
18 - 1999 First end-to-end all-optical network. Transmission speeds above 1 gigibit p/s (NGI)
19 - 1999 -> Hardware and software technologies for real-time, multimedia collaboration across networks
20 - 2001 -> R&D in next-generation optical technologies, security, privacy, survivability, hybrid and wireless networking
Color Code:
Text beneath upper color bars represents the timeline for that specific category. The 'impact' arrows and the numbered boxes below the impact timeline are color coded to the column text, yellow text is Federally funded research and development, white boxes and arrows are funded by private sector.
IMPACT
late 40s NMR spectroscopy
1950 First 24-hour forecast
1952 Univac I predicts election
1958 IT-based avionics
1958 First computer-controlled missile launch
1960 First satellite weather image
1962 Telstar I satellite
1966 First global climate model
1967 First real-time flight simulator
1967 Internal pacemaker
1970 Federated avionics software
1971 Magnetic stripe; NASDAQ digital market; barcode
1972 Pioneer 10 Spacecraft
Pong computer game; computed tomography
1973 MRI
Mid-70s Simulated crash testing
Mid-70s Automated air traffic control system
1979 Visicalc
1980s Integrated aircraft information systems
1982 Computer: TIME Man of the Year
1984 U.S. households with computer 8.2%; "cyberspace" used in novel Neuromancer
Late 80s 48-hr weather forecast run on Cray Y-MP8 in 30 seconds
1990 Integrated avionics systems
1993 22.8% U.S. households with computer
1994 Toystory, first totally computer-generated movie
1996 Real-time NYSE stock quotes
1998 HDTV
Late 90s Pervasive embedded processors
2000 51% U.S. households w/ computer
2001 DoD "smart cards" for ID
2002 NOAA issues <4000 U.S. forecasts per day
1 billion microprocessors sold worldwide
COMPUTERS
SOFTWARE
COMPONENTS
NETWORKS
NUMBER OF COMPUTERS IN USE (in millions)
150M
125M
100M
75M
50M
25M
0
100 (worldwide)
6000 (US)
1950
1960
1970
1980
1990
2000
PERCENTAGE OF HOMES/SCHOOLS WITH INTERNET
100%
50%
0
1994
1997
2000
2001
Schools
Homes
Homes
Schools
DIGITAL INFORMATION UNITS
Bit A binary digit (0 or 1)
Byte 8 bits
Kilobyte 1000 bytes
Megabyte 1,000,000 bytes
Gigabyte 1,000,000,000 bytes
Terabyte 1,000,000,000,000 bytes
Petabyte 1,000,000,000,000,000 bytes
Exabyte 1,000,000,000,000,000,000 bytes
Zettabyte 1,000,000,000,000,000,000,000 bytes
Yottabyte 1,000,000,000,000,000,000,000,000 bytes
NITRD
Rise of Information Technologies:
Computing Machines
WWII needs: ballistics, cryptography, flight simulation, nuclear physics
Operating Systems
Multiple operations with less human involvement
Connected Systems
Multiple users with terminals share time on system
Workstations
Powerful systems for single users Professional/ technical software applications
Personal Computers
Commodity computing systems Word processing
Networks of Computers
Local Area Networks (LAN)
Wide Area Networks (WAN)
Internet
Wireless Networking
Networking extended to wireless mobile, embedded devices and systems
Convergence of Technologies
Systems of systems, digital society

THE EMERGING AGE OF INFORMATION TECHNOLOGY: SCOPE OF FEDERAL R&D IMPACTS

The graphic timeline at left (please fold out front cover) provides an overview of the role of Federally funded research in the history of information technologies in the United States. The timeline's aim is to show the developing outlines of the digital revolution and some societal indicators of technological transformation. It is not intended to be comprehensive.

Reading the timeline

Four information technology areas are highlighted by color (computers, software, components, and networks). Numbered descriptions of developments in each IT area, by decade, run across the top, with Federally funded activities in yellow. Below, corresponding timelines for each area show the sequence of these developments. Arrows indicate impact milestones.

Selected sources: Federal agencies and laboratories; IT industry Web sites; *Funding a Revolution,* National Research Council, National Academy Press, Washington, D.C., 1999; Computer History Museum; Greatest Engineering Feats of the 20th Century, National Academy of Engineering; History of Computing Project; IEEE History Center; History of Computing, J.A.N. Lee, former editor, IEEE Annals of the History of Computing; History in the Computing Curriculum, Association for Computing Machinery (ACM); Chronology of Personal Computers, Ken Polsson; Common Gateway Interface (CGI) Historical Timeline, Wayne E. Carlson.

Disclaimer: Dates given for key developments often vary among IT histories. The variations typically do not change the broad direction of advances. Nonetheless, the editors regret any inadvertent errors in this timeline.

Networking and Information Technology Research and Development

Advanced Foundations for American Innovation

Supplement to the President's FY 2004 Budget

A Report by the Interagency Working Group on Information Technology Research and Development

Committee on Technology
National Science and Technology Council

September 2003

About the National Science and Technology Council

The National Science and Technology Council (NSTC) was established by Executive Order on November 23, 1993. This Cabinet-level council is the principal means for the President to coordinate science, space, and technology policies across the Federal government. NSTC acts as a "virtual agency" for science and technology to coordinate the diverse parts of the Federal research and development enterprise. The NSTC is chaired by the President. Membership consists of the Vice President, Assistant to the President for Science and Technology, Cabinet Secretaries, agency heads with significant science and technology responsibilities, and other White House officials.

The NSTC Web site is: www.nstc.gov. To obtain additional information regarding the NSTC, please contact the NSTC Executive Secretariat at (202) 456-6100.

About the Office of Science and Technology Policy

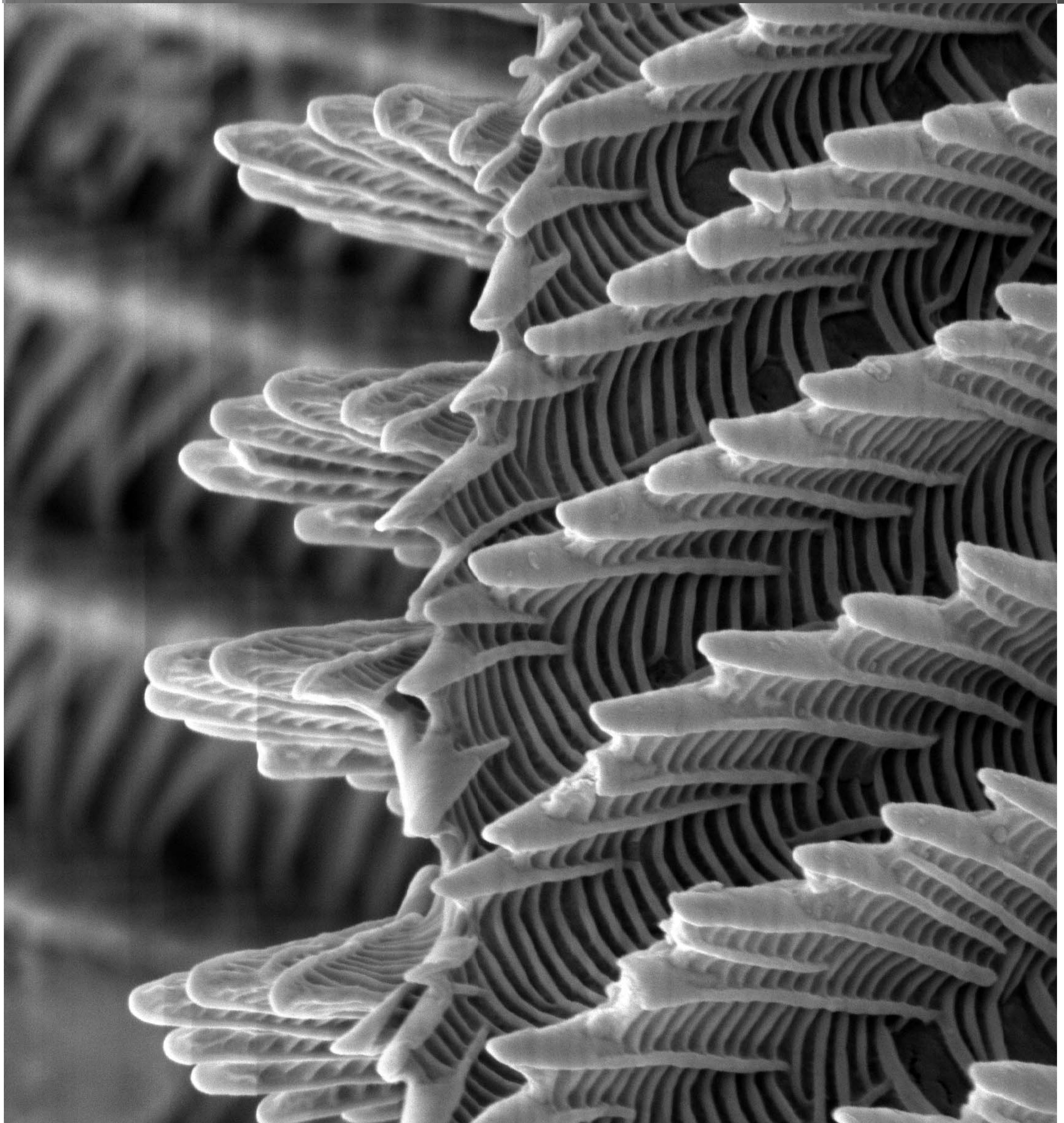
The Office of Science and Technology Policy (OSTP) was established by the National Science and Technology Policy, Organization, and Priorities Act of 1976. OSTP's responsibilities include advising the President in policy formulation and budget development on all questions in which science and technology are important elements; articulating the President's science and technology policies and programs; and fostering strong partnerships among Federal, state, and local governments, and the scientific communities in industry and academe. The Assistant to the President for Science and Technology serves as the Director of the OSTP and directs the NSTC on behalf of the President.

The OSTP Web site is: www.ostp.gov. For additional information about OSTP, please call (202) 456-7116.

Cover and Book Design

The cover, book design, historical timeline, and selected illustrations for this report are the work of James J. Caras of NSF's Design and Publishing Division. The cover illustration suggests the 21st century digital world and its metaphoric and scientific connections with the fundamental elements of earth, wind, fire and water.

Copyright Information



INVISIBLE WORLDS: In NSF's Bugscope Project (http://bugscope.beckman.uiuc.edu), state-of-the-art scanning electron microscopy enables grade-school students to examine nature's extraordinary complexity. This high-definition digital image made for the program by scientist Scott J. Robinson reveals the intricacy in a tiny part of one elegant winged creature. *For details, see page 50.*

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF SCIENCE AND TECHNOLOGY POLICY
WASHINGTON, D.C. 20502

August 29, 2003

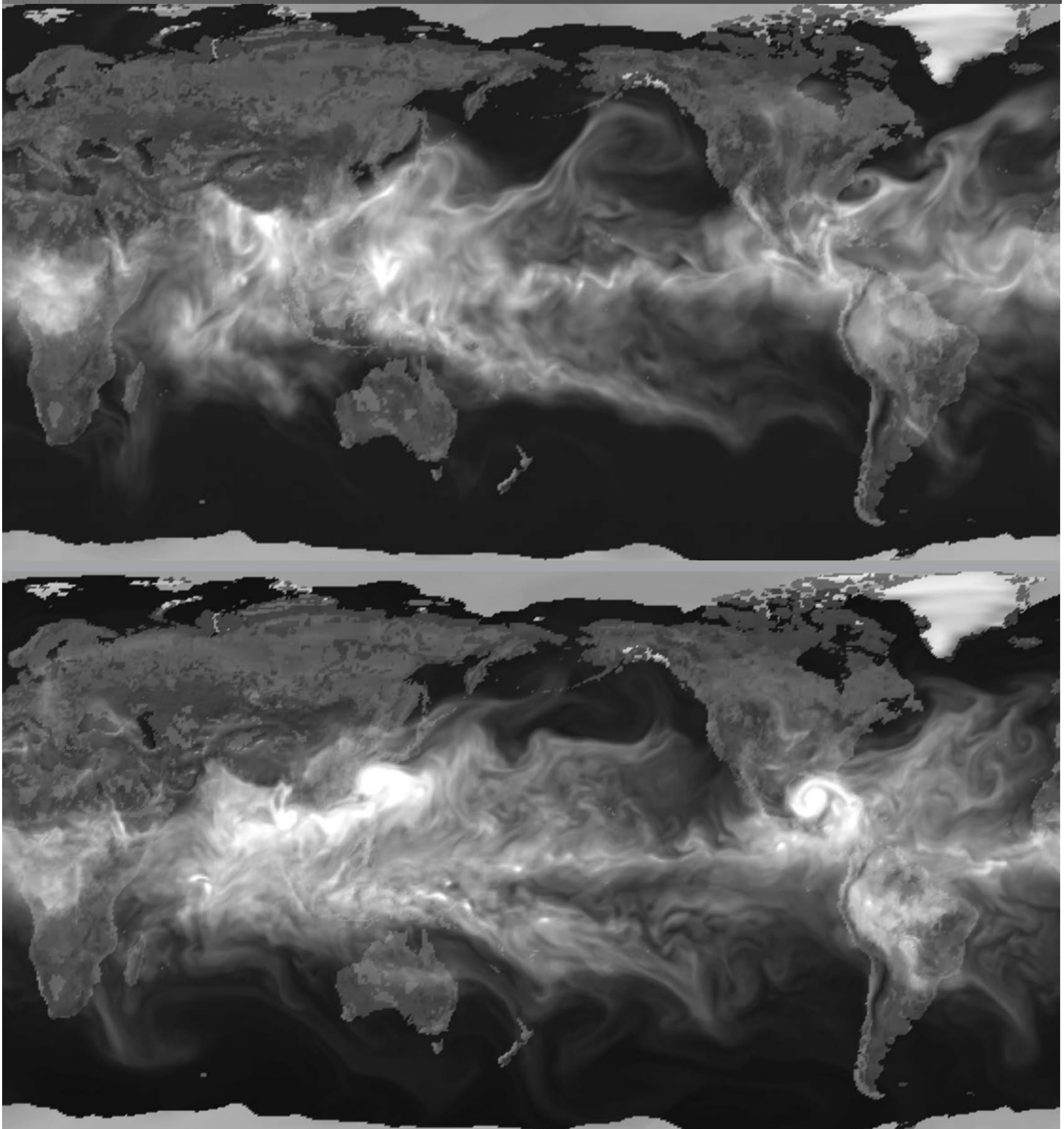
MEMBERS OF CONGRESS:

I am pleased to forward with this letter the annual report on the multiagency Networking and Information Technology Research and Development (NITRD) Program. This Supplement to the President's Budget for Fiscal Year 2004 describes advanced networking and information technologies developed through Federal NITRD investments. These investments continue to foster an unrivalled U.S. capacity for innovation–the Nation's most vital resource for national security, economic development, and continuous improvements in living standards for all Americans.

The broad-based impacts of the NITRD Program cited in this document represent achievements not only of the NITRD research community, but also of other Federal programs, public-private partnerships, and the private sector. The FY 2004 Supplement focuses on the outcomes of Federal NITRD research, organized around the Program's contributions to foundations for national security, scientific leadership, research, learning, and the 21st century society. The report places Federal NITRD research in its context as a strategic national resource that provides the essential technological underpinnings for far-reaching innovations that will influence the Nation's development in the years to come.

Sincerely,

John H. Marburger, III
Director



HUMIDITY, NOT CLOUDS: Visualizations of computed specific humidity from a high-resolution run of the general circulation model (GCM), which simulates global atmospheric dynamics. The GCM is a joint effort of NASA and the NSF-supported National Center for Atmospheric Research. GCM data play a central role in climate research and weather prediction. Technical details on page 50.

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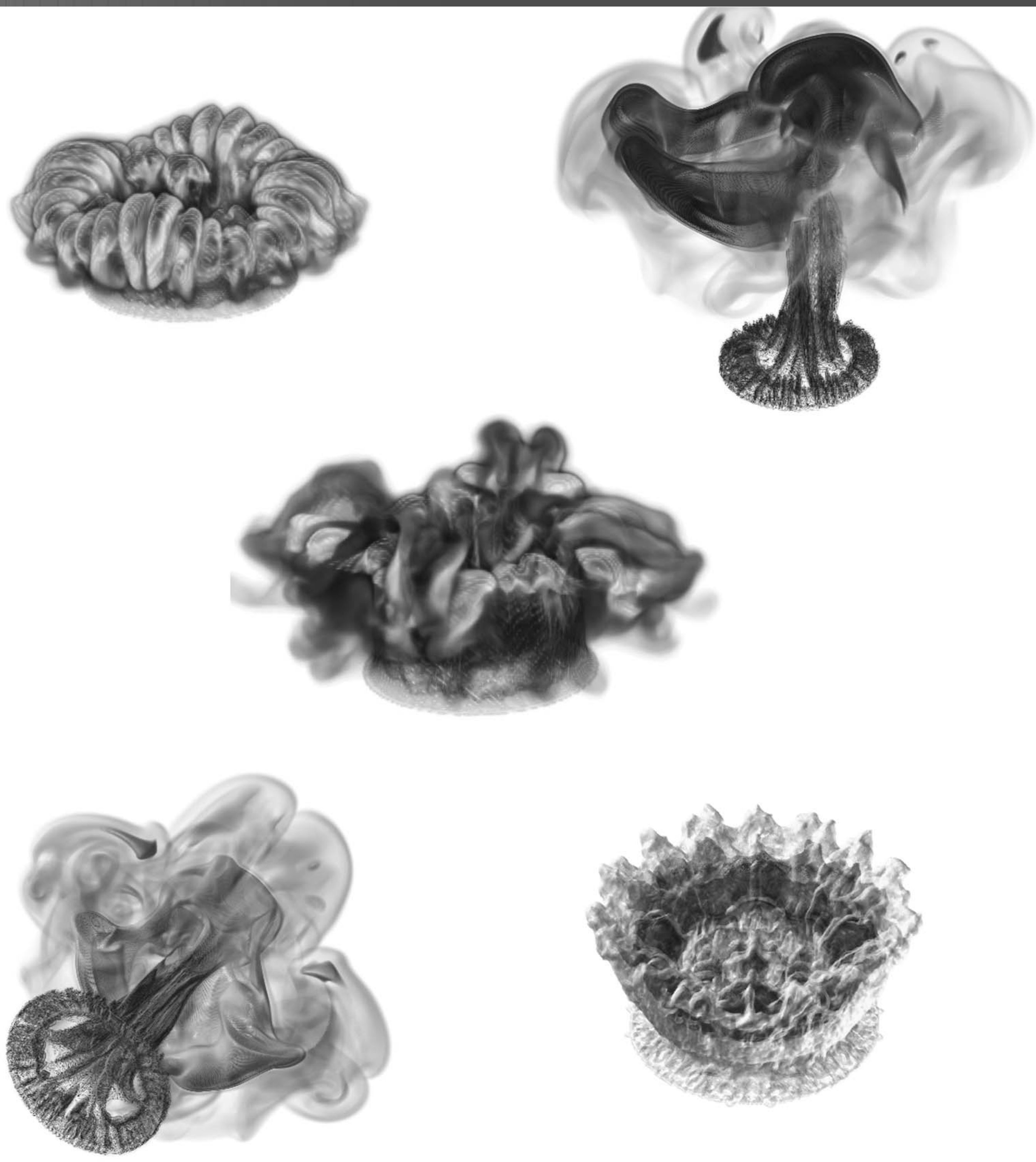


THE SHAPES OF FIRE: Images from simulations of a spreading heptane-pool fire show 3-D dynamics of fire temperatures (darker areas hottest). Generated from data by the Center for the Simulation of Accidental Fires and Explosions (C-SAFE), part of DOE/NNSA's Advanced Simulation and Computing (ASCI) program. C-SAFE's aim is to use high-end modeling techniques to improve understanding of fire and explosive processes to aid emergency planning and response activities. Details on page 50.

INTRODUCTION

"The role of government is not to create wealth. The role of our government is to create an environment in which the entrepreneur can flourish, in which minds can expand, in which technologies can reach new frontiers."

– President George W. Bush

The American imagination, challenged to invent new technologies to meet vital national needs, launched and powered a digital revolution that ultimately swept around the globe. Today U.S. ingenuity is extending advances in computing, networking, software, and information management technologies to a vast array of new applications and devices that are shaping national defense and national security capabilities, driving rising economic productivity, supporting leading-edge scientific and medical research, and adding powerful new dimensions to the ways citizens work, learn, communicate, and interact with government.

The Federal agencies whose fundamental information technology (IT) research is described in this document sponsored many of the scientific breakthroughs that set the foundations for the information age (see timeline on front-cover foldout). Working collaboratively in the multiagency Federal Networking and Information Technology Research and Development (NITRD) Program, these agencies continue to foster an unrivalled U.S. capacity for innovation – the Nation's most vital resource for national security, economic development, and continuous improvements in living standards for all Americans.

This Supplement to the President's Budget for Fiscal Year (FY) 2004 summarizes the NITRD agencies' coordinated research activities and FY 2004 plans, as required by the High-Performance Computing Act of 1991. The FY 2004 Supplement, also known as the Blue Book, focuses in particular on the critical role of fundamental IT research in providing advanced foundations for innovation in every dimension of the national interest.

Networking and computing technologies are often called "enabling" technologies because their utility – and broader significance – are realized in the human advances and capabilities they make possible. It is these advances that are the focus of the report's main sections – Foundations for National Security, Foundations for Scientific Leadership, Foundations for Research and Learning, and Foundations for 21st Century Society. The broad-based impacts of the NITRD Program cited in this document represent achievements not only of the NITRD research community, but also of other Federal programs, public-private partnerships, and the private sector. The FY 2004 Blue Book places Federal NITRD research in its context as a strategic national resource, which provides the essential technological underpinning for far-reaching innovations that will influence the Nation's development over the course of the 21st century.

For an overview of the NITRD Program, please see pages 2 and 3. Additional details about the NITRD agencies' specific research interests, proposed research activities for FY 2004, and NITRD Program budgets are presented on pages 35-41.

The NITRD Agencies

Agency for Healthcare Research and Quality
(AHRQ)

Defense Advanced Research Projects Agency
(DARPA)

Defense Information Systems Agency
(DISA)

Department of Defense, Office of the Director,
Defense Research & Engineering
(ODDR&E)

Department of Energy
National Nuclear Security Administration
(DOE/NNSA)

Department of Energy
Office of Science
(DOE/SC)

Environmental Protection Agency
(EPA)

National Aeronautics and
Space Administration
(NASA)

National Institutes of Health
(NIH)

National Institute of
Standards and Technology
(NIST)

National Oceanic and
Atmospheric Administration
(NOAA)

National Security Agency
(NSA)

National Science Foundation
(NSF)

THE NITRD PROGRAM: E PLURIBUS UNUM

Chartered by Congress under the High-Performance Computing Act of 1991 (P.L. 102-194) and the Next Generation Internet Act of 1998 (P.L. 105-305), the NITRD Program is the collaborative framework of Federal agencies that conduct fundamental R&D in advanced networks, computing systems, software, and information-management technologies, as well as in the socioeconomic and workforce implications of these new technologies. One of the few formal interagency enterprises in the Federal government, the successful NITRD effort enables the major IT research agencies to coordinate their plans and activities to leverage strengths, avoid duplication, and increase the interoperability of research accomplishments to maximize the utility of Federal R&D investments.

The NITRD agencies' balanced, diversified portfolio of R&D efforts across Federal laboratories, universities, research institutions, and partnerships with industry helps meet critical Federal requirements for leading-edge IT capabilities, which are rarely available in the commercial marketplace. The multiagency push toward highest-performance and next-generation technologies yields not only advances for national defense, national security, and scientific research but broader applications that directly contribute to overall U.S. preeminence in the sciences, in engineering, and in advanced industrial technologies.

Flow of results to private sector

The Federal emphasis on long-range IT progress complements the private sector's necessary competitive focus on short-term research and rapid product development. IT industry leaders point out that NITRD activities serve the essential purpose of filling the American research pipeline with revolutionary ideas and technological concepts that can be turned downstream into new generations of commercial innovations. Moreover, NITRD research dollars constitute the principal source of support for the advanced education and training of the Nation's leading IT researchers, entrepreneurs, inventors, and technical professionals.

The flow of ideas from Federal R&D into the larger economy is cited by the President's Council of Advisors on Science and Technology (PCAST) in a 2002 study assessing the role of Federally funded research. The PCAST notes that "activities emanating from R&D investments that produced new economic growth have never been higher, including increasing numbers of patents and discovery disclosures." Fully 40 percent of all patents, the PCAST reports, cite Federal research as their source even though Federal R&D constitutes only 30 percent of total U.S. R&D investment.

FY 2004 Administration R&D priority

The President's Budget for FY 2004 highlights the strategic national significance of Federal R&D, proposing a record $123 billion for R&D activities over all, up 7 percent from FY 2003. The NITRD Program is a top Administration R&D priority that is critical to achieving the President's goals of winning the war on terrorism, protecting the homeland, and strengthening the U.S. economy. The FY 2004 plan provides $2,147 million for the NITRD Program, a $171 million increase over the FY 2003 appropriations of $1,976 million. For more information on the NITRD agencies' research plans for FY 2004, please see pages 36-39. Details of the NITRD budget appear on page 39.

Coordinated management

NITRD activities are coordinated by an Interagency Working Group (IWG) of the Committee on Technology, National Science and Technology Council (NSTC). The IWG members include representatives from each of the participating agencies and from OSTP, NSTC, the Office of Management and Budget (OMB), and the National Coordination Office (NCO) for IT R&D. The IWG is co-chaired by one agency representative (currently NSF's Assistant Director for the Computer and Information Science and Engineering Directorate) and the Director of the NCO. Participating agencies, working with OMB and the Congress, fund their NITRD research through standard agency budgeting processes and appropriations measures that are signed into law by the President.

The NCO provides overall support for the NITRD Program, including extensive technical and administrative activities on behalf of the IWG and planning, budget, and assessment activities for the Program. The NCO also supports the President's Information Technology Advisory Committee (PITAC), a private-sector panel appointed by the President to provide independent reviews and guidance on IT research and development questions.

Copies of NCO publications, including this report, information about NITRD activities, and links to participating agency and related Web sites can be found at: http://www.nitrd.gov/

PCA R&D Structure

The collaborative research agenda of the NITRD agencies is carried out in Program Component Areas (PCAs), which focus on particular aspects of fundamental, long-term research in computing and networking technologies. In each PCA, a Coordinating Group made up of agency program managers in the relevant research fields meets monthly to exchange information and support multiagency activities in their areas.

The PCAs and their major research interests are:

- High End Computing (HEC) has two PCAs – Infrastructure & Applications (I&A) and R&D – which together include advances in hardware, software, architecture, and application systems; advanced concepts in quantum, biological, and optical computing; algorithms for modeling and simulation of complex physical, chemical, and biological systems and processes; and information-intensive science and engineering applications.
- Human Computer Interaction & Information Management (HCI & IM) – R&D in advanced technologies that expand modes and methods of human-computer interaction, improve human ability to manage and make use of information resources, and enable preservation and utility of electronic information archives
- Large Scale Networking (LSN) – R&D in wireless, optical, and mobile communications; networking software for distributed applications and for information dissemination; measuring, modeling, and scaling the Internet; improving end-to-end performance; and testbeds and R&D infrastructure. LSN also fields three special teams: Joint Engineering Team (JET), Middleware and Grid Infrastructure Coordination (MAGIC), and Networking Research Team (NRT).
- Software Design and Productivity (SDP) – R&D to improve software development and software quality, including understanding the trade-offs between cost and quality; software engineering of complex systems; end-user programming (such as domain-specific languages and programming by example); component-based software development; embedded and autonomous software; middleware for distributed systems
- High Confidence Software and Systems (HCSS) – R&D in critical technologies needed to enable computer systems to achieve high levels of availability, reliability, safety, security, survivability, protection and restorability of information services
- Social, Economic, and Workforce Implications of IT and IT Workforce Development (SEW) – Multidisciplinary R&D in complex interactions of information technologies with people and society, such as IT impacts on organizations, economic markets, and communications processes; privacy and intellectual property rights; and participation in digital society

Foundations for NATIONAL SECURITY

TECHNOLOGIES AT WORK ON THE FRONT LINE

The NITRD Program is the principal source of fundamental advances in the digital technologies powering vital national defense, national security, and homeland security capabilities – from precision command-and-control, communications, and weapons systems, to advanced systems for intelligence gathering and analysis, to technologies and tools for detecting and preventing terrorist attacks on U.S. soil and increasing security for all Americans. The NITRD agencies' expertise is also aiding Administration efforts to coordinate and mobilize Federal technological resources in support of Department of Homeland Security (DHS) applications.

High-priority NITRD research plans for FY 2004 continue to focus on strengthening the overall security, reliability, and robustness of critical U.S. networks, high-end computing systems, and digital infrastructures. This work includes development of "trust" technologies for broadband, optical, wireless, and other ad hoc networks; cost-effective methods for designing highly reliable software; and new science and engineering approaches to achieve unprecedented dependability and security – called "high confidence" – in complex systems and software. Other efforts focus on advanced computational capabilities, such as data mining and language translation, for national security applications. Working with NSTC, the NITRD agencies are also developing a comprehensive plan to guide federal investments in high-end computing to meet critical mission needs ranging from national security and defense to basic science.

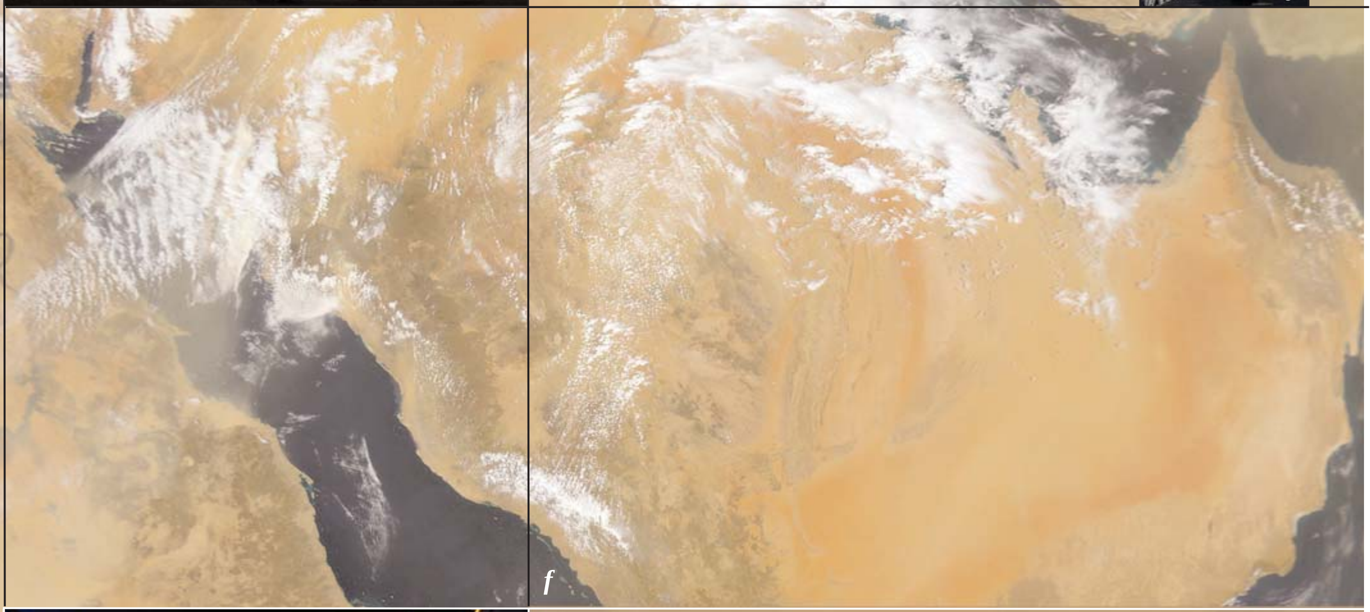
Advanced battlefield capabilities

Applications of NITRD research have been and continue to be deployed on many fronts in the war on terrorism. In Iraq, the unprecedented ensemble of networked high-performance communications, reconnaissance, distributed information management, and precision-guided munitions systems supporting U.S. battlefield operations led *Business Week* to term the conflict the world's first "digital war." Among the new capabilities were DARPA's Phraselator language-translation devices and translingual information detection, extraction, and summarization (TIDES) software for intelligence analysis.

The unmanned aerial vehicle (UAV), one of the "advanced concept" capabilities to play a prominent role in Iraq, has achieved a high level of sophistication that reflects NITRD technological advances in hardware and software components, including remote-sensing, telemetry, and secure wireless networking technologies for remote command and control.

a

a) *U.S. Army Blackhawk helicopter over southern Iraq during Operation Iraqi Freedom. Research on methods and tools for enhancing battlespace visualization for decision making in mobile units and multi-display command-and-control centers is a focus of ODDR&E's Multidisciplinary University Research Initiative.*

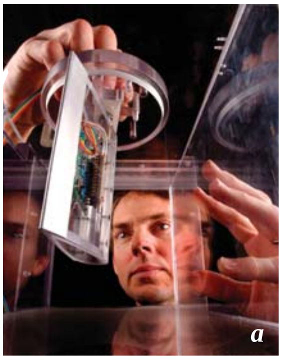


These airborne systems, being deployed by several services in a range of sizes and equipped for varying tasks, provide versatile platforms for wide-area, persistent (many hours at a time), and multimodal (many kinds of sensing and scanning devices) reconnaissance and attack without putting soldiers at risk.

Sensor technologies for hazard detection

The NITRD agencies' research in robotics and in the miniaturization, communications capabilities, and integration of digital components with micro-electromechanical systems (MEMS) such as sensors, actuators, and signal processors enables advanced remote-sensing and networked embedded systems not only for military applications but also for space exploration and scientific research. In the war on terrorism, these technologies are also being applied in small, low-cost

b) *U.S. Air Force Predator unmanned aerial vehicle (UAV) receives ground check before mission.*
c) *Precision-guided Tomahawk cruise missile is fired from U.S.S. Winston Churchill in eastern Mediterranean.*
d) *Air Force officers at coalition operations center in Qatar coordinate multinational mission information.*
e) *Navigator on a B-52 "Superfortress" checks flight details with ground control on wireless computer communications system.*
f) *NASA March 25, 2003, satellite image of Iraq shows severe dust storms (orange streaks). Computer weather models developed by Johns Hopkins University and the University of Colorado also helped coalition forces anticipate dust conditions.*



devices for detecting and identifying biological pathogens, chemical and radiation hazards, and explosive materials.

SnifferSTAR, the result of a DOE/SC-Lockheed Martin Corporation partnership, is a half-ounce unit designed to ride on UAVs to detect nerve gases and blister agents. Operating on half a watt of power, it consists of a butter-pat-sized sensor platform on top of a microprocessor board. The airstream is sampled every 20 seconds by the sensors, which register the mass of airborne particles as electronic frequencies and send the signals to the processor; the digital data are transmitted to the UAV or to a ground link, where they are immediately compared against a library of data patterns for many dangerous gases. Other new sensor technologies include inexpensive microarrays of DNA sensors on a chip that can detect multiple pathogens, such as anthrax and smallpox; acoustic sensors that use sound waves to determine the chemical composition of materials in closed containers; and handheld radiation detectors, now commercially produced and deployed in homeland security activities.

Networks of tiny devices

NITRD advances in software and networking now also make it possible to federate microsensor arrays in ad hoc wireless networks, with potential not only for battlefield reconnaissance but for industrial, health, and environmental monitoring. "Smart dust," a DARPA project in sensor miniaturization, incorporates these new capabilities as a result of work funded by DARPA and NSF at the University of California at Berkeley and a partnership with the Intel Corporation. Researchers re-engineered a sensor prototype to turn it into a modular, component-based computing platform with a processor, sensor, radio, and power distribution system. Because the operating system – TinyOS – and database – TinyDB – are open source software, and Intel is sharing wireless networking technology, developers in many domains are now working on commercial applications.

DOE/SC, NOAA, and corporate partners are linking sensor and mass spectrometry technologies, wireless and wired networking, meteorological instruments, remote telemetry, and computer modeling in a prototype SensorNet, a nationwide system for real-time detection and assessment of chemical, biological, radiological, and nuclear threats. The goal of this effort is to provide immediate, scientifically accurate information to first responders about the nature, severity, and likely dispersion of such agents in the environment. This work complements fundamental investigations by NIH and NSF aimed at developing new methods both to prevent biological and chemical agents from causing harm and to mitigate the severity of contamination incidents.

Assuring technology quality

As the primary measurement and standards laboratory for the United States, NIST conducts research in ultra-precision sensors and works closely with other Federal agencies and industry to develop standards that ensure the accuracy of measurements made by new hazard-detection technologies. A NIST initiative with the Federal Aviation Administration, for example, is using mass spectrometry – a powerful laboratory method supported by IT that identifies a substance's unique chemical fingerprint – to assess the effectiveness of walk-through explosive detectors. Developed with EPA and NIH, NIST's digital library of mass spectral prints for 140,000 chemical compounds is included as the standard reference guide with most mass spectrometers sold today.

Help for first responders

With funding from the National Institute of Justice, NIST is working with the public safety community to standardize techniques and protocols in wireless telecommunications and IT applications for emergency response networks. NIST is also developing Web-based technologies for integrating sensors, real-time video, "smart tags," and embedded microprocessor devices in a next-generation distributed information-gathering and interactive communications system for field deployment by first responders.

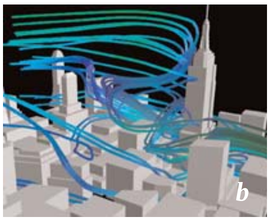
Powerful tools for emergency planning

Today, computational modeling, simulation, and visualization capabilities pioneered in NITRD research are helping emergency planners, first responders, public-health officials, and building engineers better understand

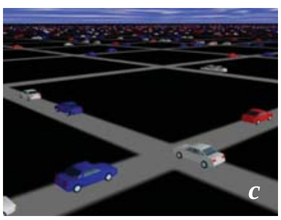
***a)** "Sniffer Star," a butter-pat-size sensor, samples air for toxic agents and relays findings via wireless system to be checked against digital archive of known toxic gases.*

and prepare for the complex impacts of catastrophic events. Some examples:

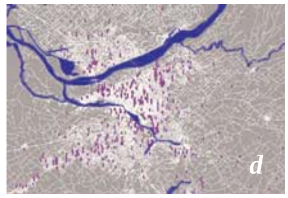
- DOE/SC researchers have developed high-resolution structural dynamics models to simulate the effects of bomb blasts on buildings and other structures. The simulations, which require very high-performance computing capabilities, can be used to evaluate structural vulnerabilities and assist in development of blast-resistant architectural designs and retrofits for existing structures.



- A NIST-developed computational model, the Fire Dynamic Simulator, and related software called SmokeView are enabling investigators of the World Trade Center disaster to study how building geometry, fuel distribution, and wind conditions interacted with the smoke and fires within and outside the towers. In conjunction with its ongoing evaluation of building materials in collaboration with industry, NIST is also preparing a technical assistance package including software tools to help building owners, contractors, designers, and emergency personnel consider how building attributes would factor in a crisis.



- TRANSIMS (Transportation Analysis and Simulation System) – developed for the Department of Transportation by scientists at the National Infrastructure Simulation and Analysis Center (transferred from DOE/SC to DHS) – is a high-end software tool that can integrate tens of millions of interacting variables to represent transportation and traffic flows across an entire urban area over time, from the level of a single pedestrian and traffic light to the aggregate. Designed to provide metropolitan planners with a highly accurate, comprehensive picture of traffic impacts, congestion, and air quality, the tool now is helping emergency planners analyze the effects of disruption on complex urban infrastructures to improve disaster preparedness. IBM Business Consulting Services has licensed TRANSIMS and is working with state and local officials to integrate the tool into their analyses.



- A derivative tool, EpiSIMS (Epidemiological Simulation System), couples models of disease transmission with population-mobility data so that planners can test the efficacy of various public-health response strategies.

NITRD guidance for improving cybersecurity

The NITRD agencies are key contributors to Federal efforts in partnership with the private sector to improve the security of existing networks and computing installations. Work by NIST, NSA, and other DoD agencies underlies the set of "security benchmarks" distributed nationwide in 2002 by the Center for Internet Security, a voluntary consortium of public and private organizations. These instructions and software tools for enhancing security in today's most widely used operating systems and networking technologies are termed "the gold standard" by the IT industry because they reflect public-private consensus on best practices based on thorough evaluation and testing. NIST and NSA jointly support the National Information Assurance Partnership, an international compact among countries that apply validated security standards to assess commercial IT products.

NSF and NIST were authorized by the Cybersecurity R&D Act of 2002 (P.L. 107-305) to take immediate action to address critical national needs in this area. NSF, chartered to take the lead in cybersecurity research and education, has more than doubled its research investment in fundamental security technologies and is supporting training of cybersecurity professionals. NSF plans are underway to expand educational and capacity-building activities in this critical area of workforce development. NIST's responsibilities under the new law include assessing national infrastructure vulnerabilities, fostering public-private partnerships to advance security technologies and standards, establishing postdoctoral cybersecurity fellowships, and coordinating on the IT security research agenda with NSF and other Federal agencies.

NITRD Program representatives participate in NSTC's Critical Information Infrastructure Protection Interagency Working Group, contributing research perspectives and results from long-term NITRD R&D for application in security-related technologies.

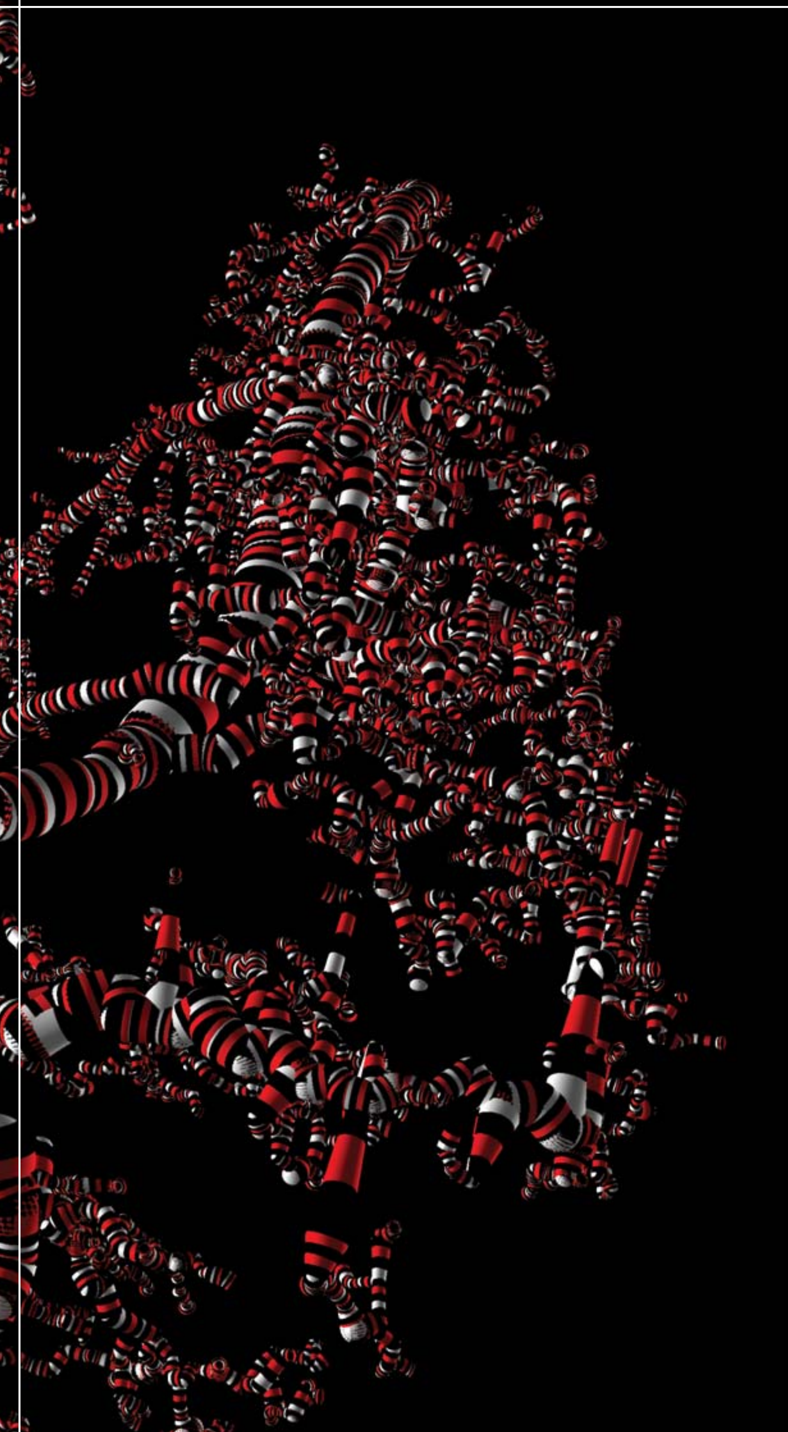
b) *EPA used computational fluid dynamics simulations after 9/11 to help evaluate the spread of materials from the World Trade Center.*
c) *TRANSIMS enables simulations incorporating millions of data points from disaggregated variables, such as pedestrians, vehicles, mass transport, traffic signals, and road characteristics.*

d) *DOE/SC researchers worked with Portland, Oregon officials to simulate the geographic spread (purple shows cases) of a smallpox epidemic in the city, using the EpiSIMS model. Effects of various interventions versus inaction were examined.*

HOW A CRICKET KNOWS

NASA computational scientists are examining the complex neural signaling systems of crickets to learn more about the information-processing capabilities of their nerve cells' three-dimensional branching, tree-like circuitry. In such biological systems for generating and transmitting signals, they hope to find revolutionary new models for tiny computing and other electronic devices.

Visualization by Chris Henze, from data by Gwen Jacobs, of a cricket interneuron, a highly branched nerve cell that "reads" a neural map of input signals transmitted by sensory axons projecting into the insect's abdomen. About 10,000 color bands show precise 3-D geometry of the cell's dendritic branching points and changes in diameter. *Details on page 50.*



In the Nation's science and engineering research laboratories, high-performance computing, networking, software, and information management capabilities enabled by NITRD work are not only accelerating the pace of discovery but transforming the scientific enterprise, from the way individual scientists work to the relationships among the disciplines. Across the physical and biological sciences, at every scale from the vast to the minute, explorations of the structures, properties, and processes of life and of inanimate matter now converge in the high-end virtual laboratory environment made possible by ongoing NITRD advances.

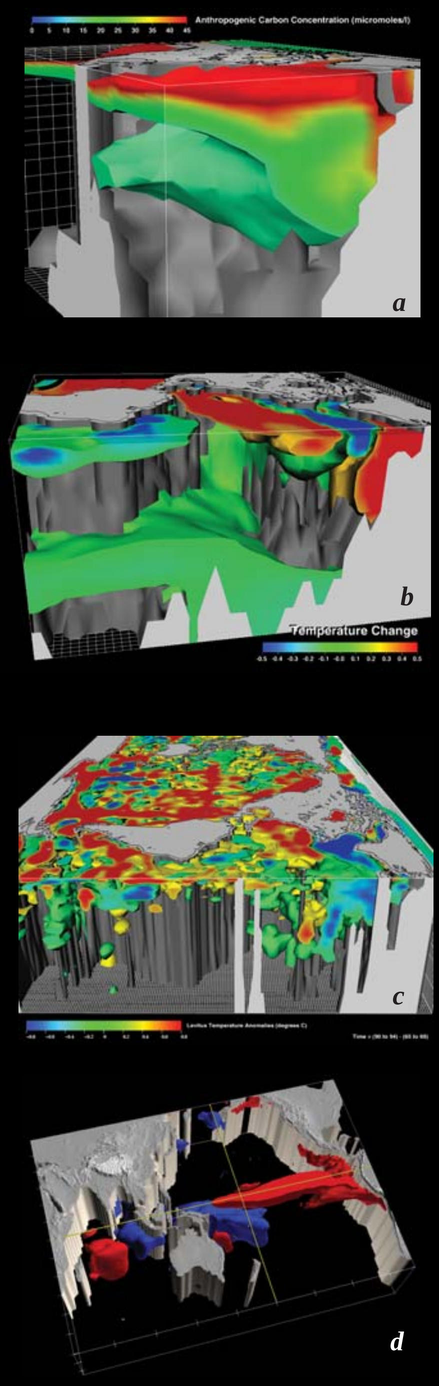
Fundamental breakthroughs in component technologies, system and storage architectures, systems software, and scientific programming environments provide the U.S. scientific community with the world's most extensive and diversified array of high-end computing capabilities for cutting-edge research. NITRD research and engineering in broadband, optical, and wireless networking technologies provides U.S. researchers with access to high-speed research networks. Moreover, NITRD researchers' invention of grid computing and the Globus Toolkit™ of open-source grid software expands the versatility of this high-end connectivity, making possible networked integration and sharing of state-of-the-art instrumentation, data storage, and computing resources.

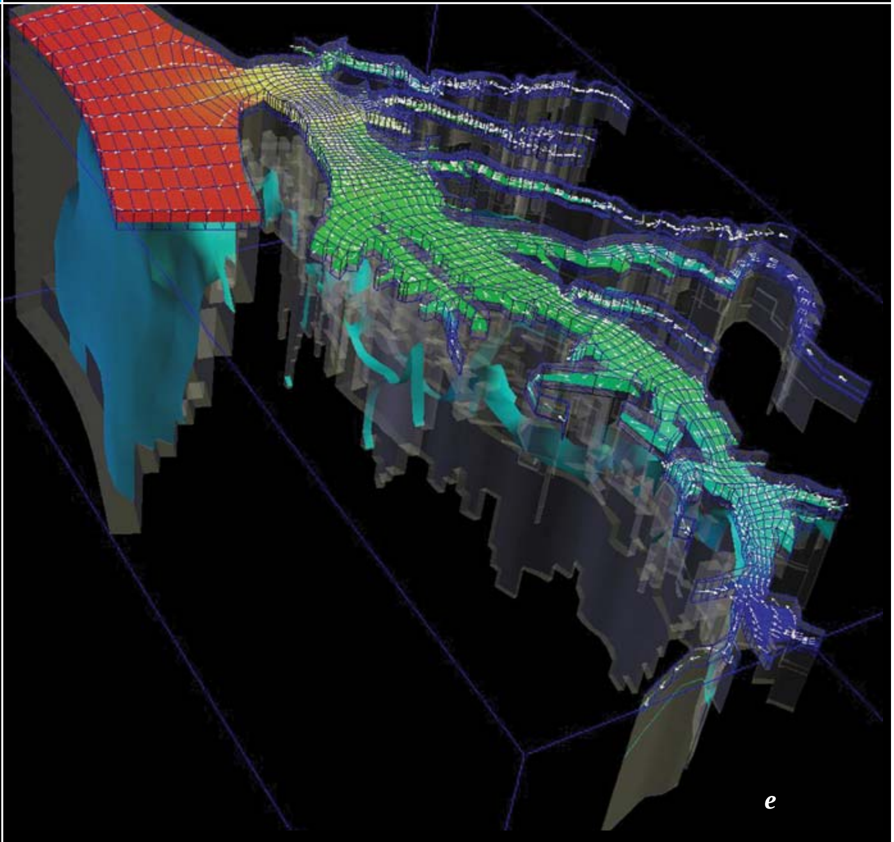
NITRD advances in high-performance hardware and software tools equip scientists with new ways to perform experiments and manage and work with massive data sets. The NITRD focus on digital library technologies, information management, foundational information archives, and new forms of human-computer interaction provide the research and education sectors with unprecedented resources for investigation and learning.

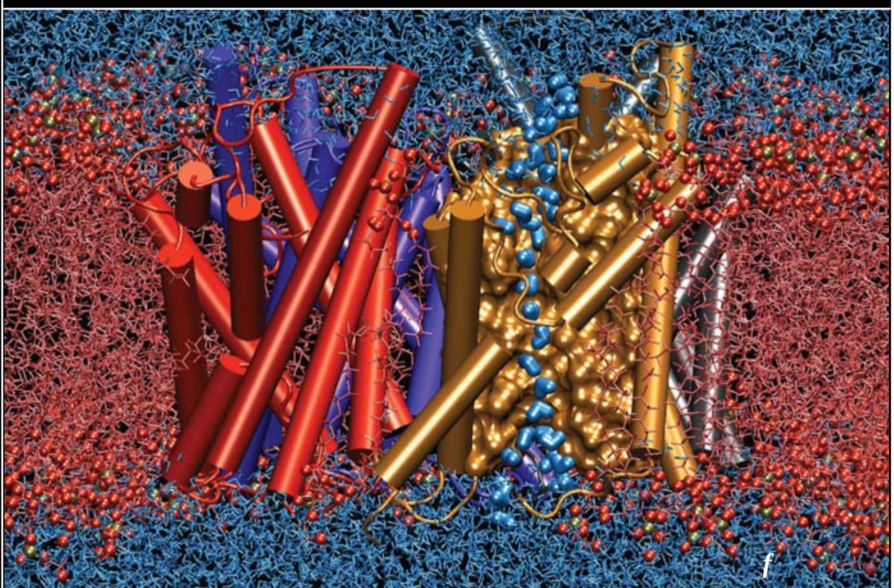
From this growing suite of IT capabilities – almost unimaginable just a decade ago – new modes of 21st century inquiry are rapidly taking shape.

Foundations for SCIENTIFIC LEADERSHIP

NEW WAYS TO 'SEE' AND UNDERSTAND







AIR AND WATER AT EVERY SCALE

*NOAA Geophysical Fluid Dynamics Laboratory models: **a)** Atmospheric carbon (red) concentration. **b)** Atmospheric warming patterns. **c)** Temperature anomalies. **d)** El Niño/La Niña effects on water temperature.*

***e)** Chesapeake Bay looking south, with major tributaries at right. Image shows computed salinity, (high levels red, freshwater dark blue). Rendered from a coupled hydrodynamic/water quality model developed by Army Corps of Engineers and EPA. The first fully 3-D, time-varying model of an estuarine environment, the model has enabled new understanding of multiple eutrophication factors, such as nitrogen from air pollution.*

Beyond the technologies that make high-performance computing and networking possible, no NITRD advances are more profoundly influencing scientific research and industrial innovation than computational modeling, simulation, and visualization. Modeling and simulation enable investigators to examine and experiment with very complex phenomena – such as the chemistry and kinetics of fire, or the mechanisms of viral infection – that exist far outside the boundaries of human vision. These phenomena can be infinitesimal (interactions of atomic particles), hazardous (biotoxins, radiation), multidimensional (combustion, neural signaling systems, air-traffic control), vast (the structures of galaxies), or a combination of factors at many scales (influences on global climate, stress factors in ship design).

Hard to perceive, such aspects of the physical world are even more difficult to explain because they typically represent the interplay of large numbers of disparate processes. Even if we understand individual processes, we cannot easily predict the results of their interactions. With high-performance modeling and simulation techniques, researchers can for the first time create “likenesses,” or simulations, of enormously complicated and dynamic realities – such as the development of tornadoes – and make them visible in imagery.

Trillions of calculations per second

Computational models break a phenomenon under study into very small pieces, each described by mathematics. The model is the scientist’s approximation of how the physical process works as a whole. Very powerful computing platforms then perform the calculations – often many trillions of operations – specified in the model. The resulting simulation also is an approximation, but by comparing the results to observational data, researchers can evaluate how closely the model matches reality. If the data validate the model, it can then be used to predict behavior for which no data exist. Visualization software plays a key role, turning simulation data into three- or four-dimensional renderings of the results. In the case of tornadoes, for example, full-color imagery can highlight such invisible factors as air pressure and wind velocity, revealing relationships that would not be apparent in raw data or photographs.

Because they make complex systems visible and testable, modeling and simulation have become the tools of choice for designing, evaluating, and managing elaborate structures and systems, such as aircraft and avionics, automobiles, buildings, manufacturing machinery and processes, and power grids. Military planners use simulations to assess large-scale, multidimensional staging and battlefield scenarios with such variables as personnel, weaponry, vehicles, portable infrastructure, communications systems, and supply chains.

NITRD modeling applications

But developing modeling and simulation capabilities for cutting-edge U.S. science and engineering remains one of the most technically difficult challenges in advanced computing. The more complex the phenomena to be modeled, the more demanding the software development issues. Current and FY 2004 NITRD research continues its focus on the advanced mathematical and computer-science underpinnings for scientific modeling and simulation. Recent NITRD achievements point to their increasingly critical role in sustaining U.S. technological preeminence.

Scientists at the National Center for Atmospheric Research (NCAR), with support from DOE/SC and NSF, in 2002 produced a high-resolution millennium-length global climate simulation. The 1,500-year simulation was generated using NCAR’s Parallel Climate Model, which dynamically couples the major components of Earth’s climate system, such as atmosphere, oceans, land, and sea ice. The simulation took 456 days to run on the IBM SP supercomputer at DOE/SC’s National Energy Research Scientific Computing (NERSC) facility. Among the findings was the discovery that the familiar climate mode of El Niño can change its activity substantially over the centuries, even when not influenced by outside forcing. As a result, the scientists cautioned that interpretations of changes in

g

f) In one of the largest molecular simulations yet achieved (106,000 atoms interacting over 5 million time steps), computational biophysicists at the University of Illinois have discovered a key mechanism enabling proteins called aquaporins, which make up the membranes surrounding cells, to transport large amounts of water – up to 250 liters daily in humans. For details, see page 51.
g) Visualization of scientific data begins with exacting mathematics. Cubes test curvature-based transfer functions in a synthetic data set from a quartic polynomial implicit function, serving to debug/demonstrate correctness of convolution-based measurements and show their effectiveness in a volume rendering context. Cube at right is Gaussian curvature.

Foundations for SCIENTIFIC LEADERSHIP

NEW WAYS TO 'SEE' AND UNDERSTAND

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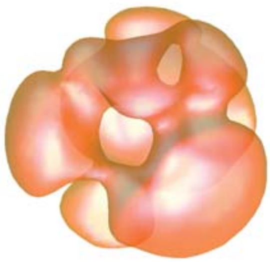

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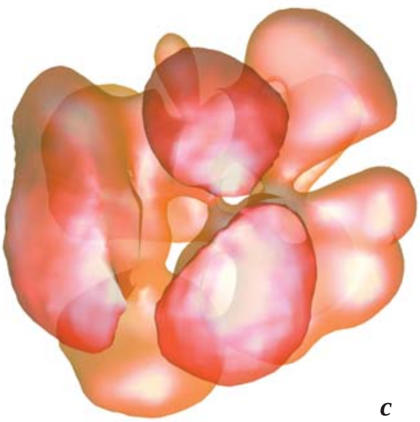

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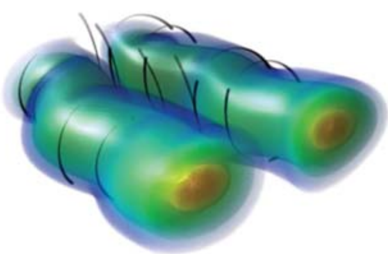

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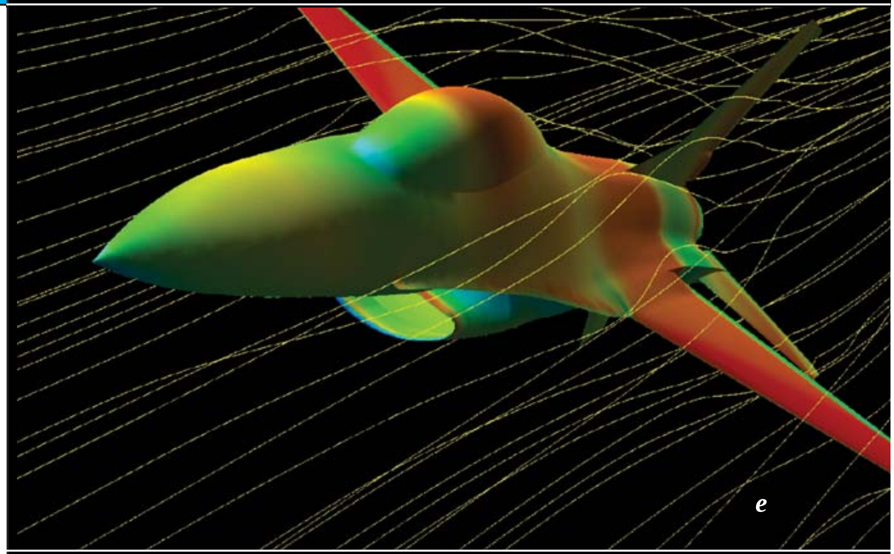

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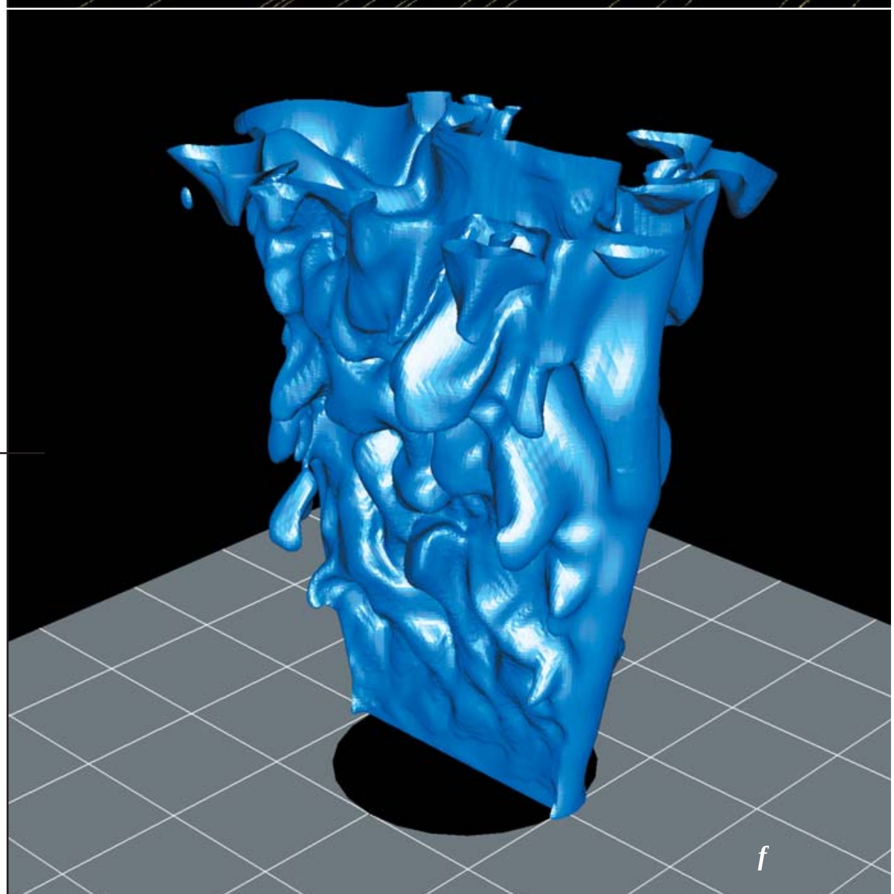


f

Stages of a supernova explosion over 50 milliseconds: ***a)*** *Initial implosion.* ***b)*** *In-falling gas approaches the core, where neutrinos heat and make the gas buoyant.* ***c)*** *Process causes enough convective energy transfer to create explosion.*

d) *University of California-Davis researchers are experimenting with new ways to visualize multidimensional data sets. Image renders isosurfaces, vorticity, and velocity of wakes.* ***e)*** *Image of F-16 flying at Mach .9 shows levels of stress on surfaces from highest (red) to lowest (blue). A University of Colorado researcher's innovative model integrating fluid dynamics and structural stress data evaluates "flutter" – a dangerous vibration in high-speed flight – in aircraft designs.*

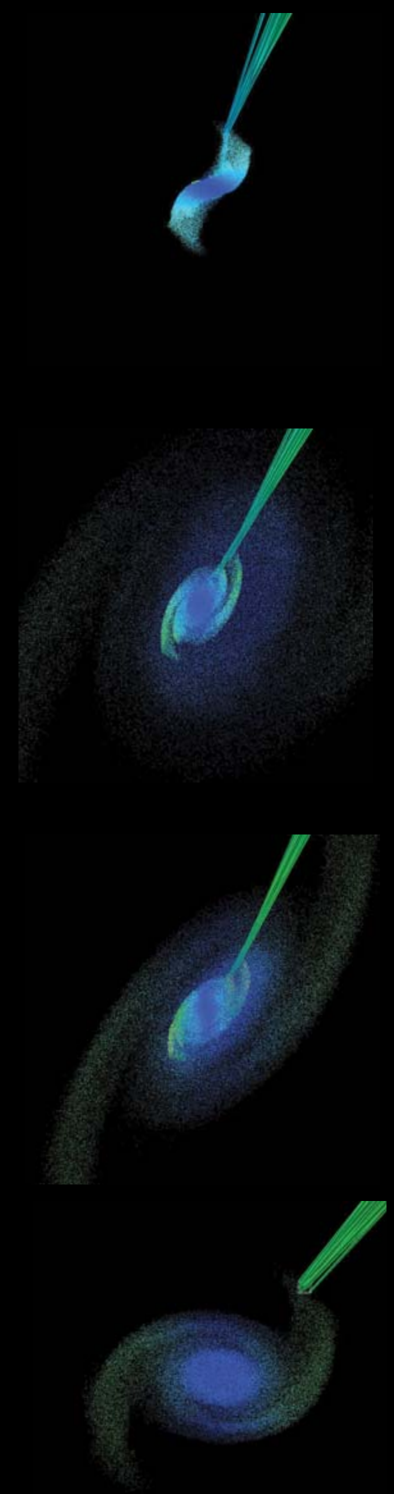
El Niño need to be evaluated with caution, and that physical mechanisms of these changes require further exploration.

The first 3-D simulations of the spectacular explosion marking the death of a massive star, called a supernova, were achieved by DOE/SC scientists in 2002. Such explosions, among the most violent events in nature, unleash power that can briefly outshine a galaxy of 100 billion stars. The work confirmed that the explosion process is critically dependent on convection, the mixing of the matter surrounding the iron core of the collapsing star. Understanding the nature of star deaths is considered a key to explaining the expansion of the universe. Supernova calculations are exceedingly computation-intensive because many processes, involving all four fundamental forces of physics, must be modeled for more than 100,000 time steps. Typical simulations (a million particles) took three months on the IBM SP at NERSC.

The Numerical Propulsion System Simulation (NPSS) developed by NASA scientists addresses one of the most costly and time-consuming elements of modern aviation manufacturing – testing the design, structure, and performance of jet engines. A first-of-its-kind tool for modeling and analyzing jet propulsion systems in a single package, NPSS can interact with and integrate externally generated data and design tools, and it allows geographically distributed teams to collaborate on simulations. This design advance was named one of the top 100 R&D achievements of 2002 by *R&D Magazine* and received the 2002 NorTech Innovation Award.

Researchers at the University of California-San Diego supported by NIH and NSF have developed a modeling technique that applies computational chemistry rather than "wet" laboratory methods to assess how well potential medications will work. Drug molecules bind to specific "receptor" proteins in the body, and pharmaceutical designers try to figure out where on the protein that binding will best occur. The computational model calculates the possible variations in a protein's shape and then tests the candidate drug's binding ability with all the variants, accounting for the molecular stretching and bending that can affect binding but are not captured in static models. This high-speed technique can be used with any drugs and proteins for which three-dimensional structural information exists – accelerating the search for alternatives to medications with severe side effects. Similar methods are helping immunologists identify the chemical triggers of immune response, a key step in the search for new vaccines.

A massively parallel structural dynamics software code named Salinas, developed by DOE/NNSA researchers for simulating the responses of structures to varying loads and stresses, earned a special 2002 Gordon Bell Award, the supercomputing field's top honor. The software supports the Federal nuclear stockpile stewardship program, which uses high-end computational capabilities to ensure the safety, security, and structural integrity of the Nation's nuclear weapons.



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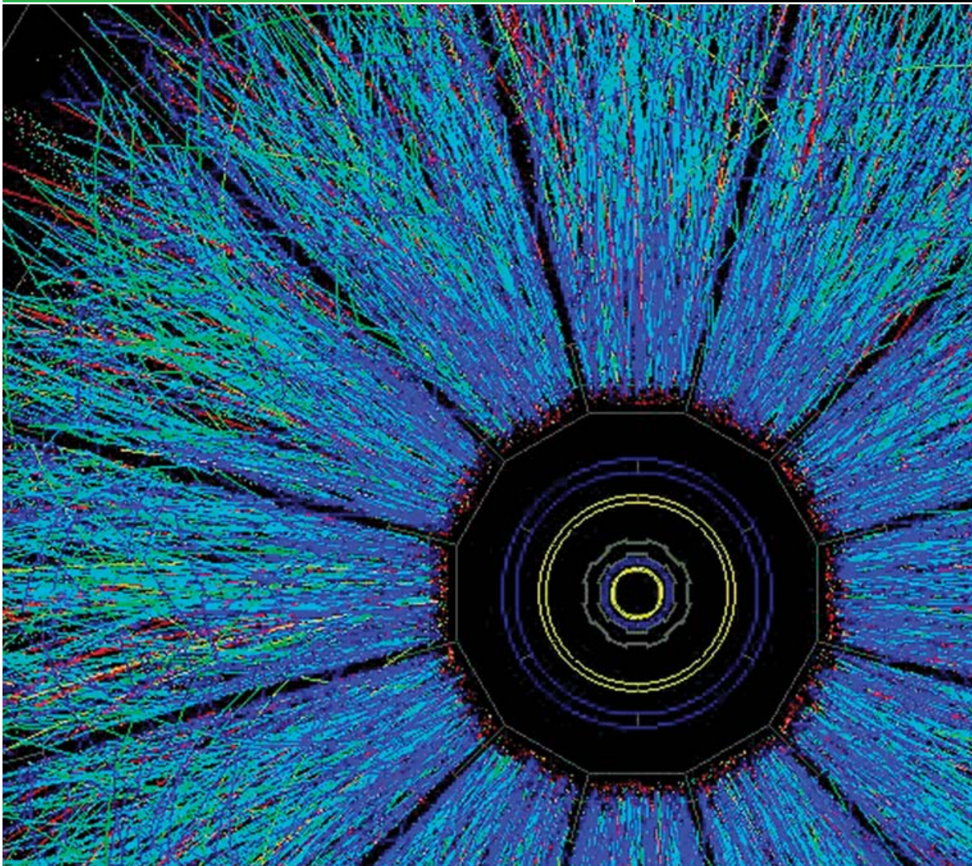
f) *The physics and chemistry of combustion, one of the most complex processes in nature, remain a major scientific challenge. DOE/SC scientists have developed the first fully resolved 3-D simulation of turbulent methane combustion (image at left), winning the 2003 SIAM/ACM Prize in Computational Science and Engineering.*

g) *Acceleration of concentrated particle beams is a core technique in the search to understand the elemental forms and properties of matter. Simulation shows formation of a halo around a single particle, a sign of incorrect injection of beamline into cyclotron.*

Foundations for
SCIENTIFIC LEADERSHIP

LARGE-SCALE SCIENTIFIC COLLABORATION



Never would I have dreamed in 1953 that my scientific life would encompass the path from DNA's double helix to the 3 billion steps of the human genome. The completion of the Human Genome Project is a truly momentous occasion for every human being around the globe.

James D. Watson, co-discoverer of the structure of DNA, during DOE/NIH double celebration in April 2003 marking the discovery's 50th anniversary and the successful conclusion of the decoding effort it made possible.

a) *Spray of subatomic particles produced by high-speed collision of gold ion beams in DOE/SC's Relativistic Heavy Ion Collider. A 1,200-ton instrument called the Solenoid Tracker at RHIC (STAR) records data from collision. High-end computation and data-sharing are critical in such unique experiments, enabling many scientists to reconstruct and visualize the sequence of events from the moment of impact and to analyze the data for evidence of new forms of matter – a central goal of high-energy physics research.*

The first great scientific triumph of this century – the decoding of the human genome announced in February 2001 – dramatically introduced the new era of large-scale collaboration enabled by computing and networking. When DOE/SC and NIH launched the Human Genome Project in 1990, the most powerful computers were 100,000 times slower than today's high-end machines, the private citizens using networks could send data at only 9600 baud (bits per second), and many geneticists did calculations by hand. The challenge – figuring out how the genetic instructions for life are organized in the four chemical compounds that make up the biomolecule deoxyribonucleic acid (DNA), called life's blueprint – was understood to be critical to the future of medical science. But the work was expected to take decades.

Ultimately, the international decoding effort, in which more than 1,000 scientists participated, became a showcase for the central role of IT in advanced research. The distributed teams of Human Genome Project researchers each computed pieces of possible chemical sequences and transmitted them over high-speed networks to the project's data repositories for other scientists to examine and use. Researchers devised new software tools that automated sequence computations and analyses. In a sign of the enormous IT-driven acceleration of the work, a June 2000 announcement of a "rough draft" of the genome noted that more than 60 percent of the code had been produced in the prior six months alone, at a rate of 1,000 bases (sequences of DNA's four nucleotides) per second around the clock. The total raw sequence calculations submitted numbered more than 22 billion.

Connecting people and resources

In every scientific domain today, investigating complex phenomena requires a great many minds, multiple skills, and state-of-the-art tools. Such research can be staggeringly data-intensive, often involving unique measurements generated by one-of-a-kind instruments. Just one collision experiment in an advanced particle accelerator, for example, produces millions of physics "events" per second, amounting to 40 or more terabytes of data all told, filling 8,000 high-capacity magnetic tapes. If the tapes were stacked, the pile would be 500 feet high. Such massive data sets exceed the capacity of all but the largest supercomputing systems to store or process.

The NITRD agencies are leaders in envisioning and developing revolutionary IT capabilities to connect people in any location to such massive data sets, as well as to colleagues and computing resources, in secure high-bandwidth infrastructures for real-time scientific collaboration. In FY 2003, efforts funded by DOE/NNSA, DOE/SC, NASA, NIH, and NSF continue to build out the high-speed networks, terascale computing and petabyte storage resources, and advanced software for grid computing that enable large groups from all points of the compass to work together in a joint enterprise. In these leading-edge research environments, the NITRD community is exploring and prototyping technologies and methods for large-scale collaborative human activity that will become the norm for many American workers in the 21st century. Citing the cost-effectiveness of collaboration and resource sharing, businesses are already adopting NITRD-developed grid technologies to connect distributed teams and computing resources.

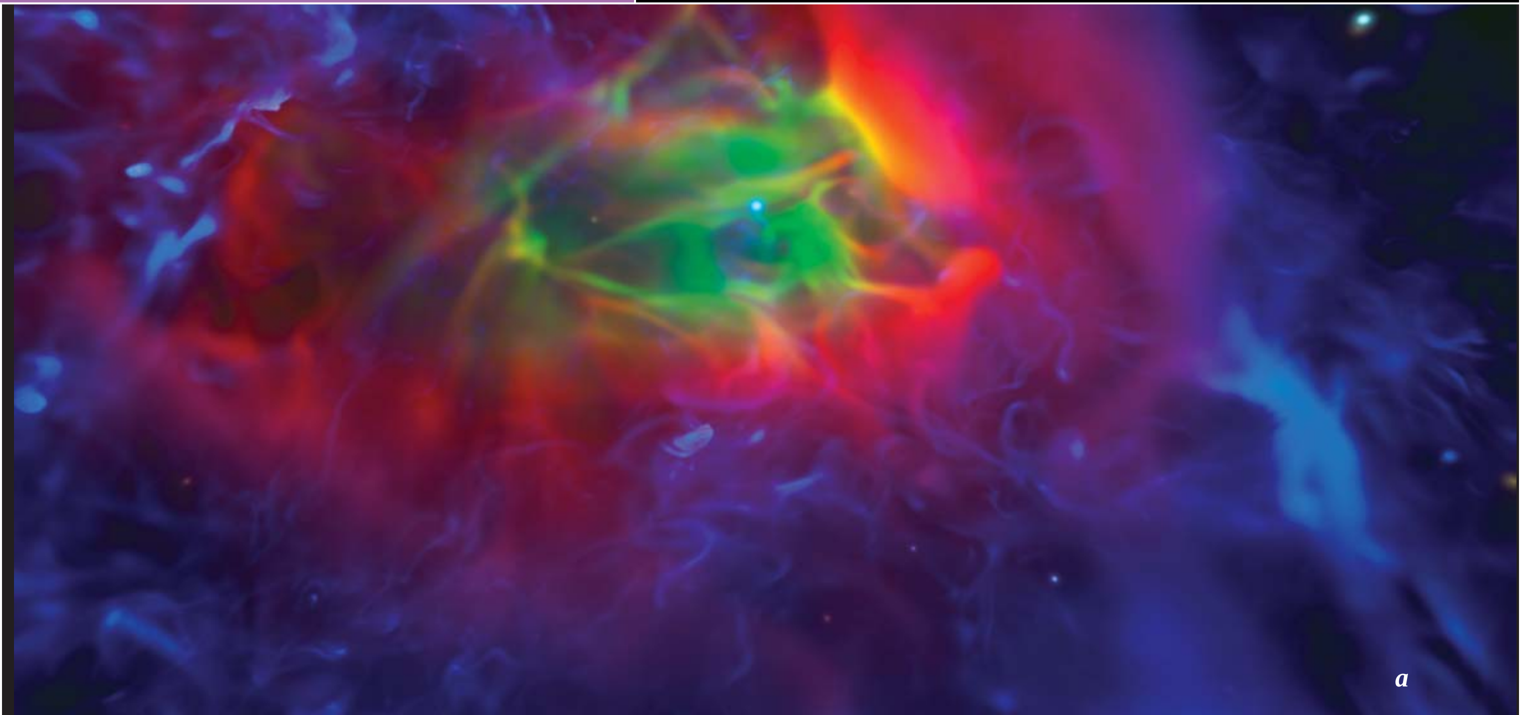
In a significant milestone for large-scale collaboration, NITRD-engineered high-speed networks (including DOE/SC's Energy Sciences Network, ESnet, and the NSF-sponsored TeraGrid and StarLight links) in February 2003 enabled an international team of particle physicists and corporate IT partners to set a new world network-speed record. The team sent 6.7 gigabytes of uncompressed data – the equivalent of four hours of DVD-quality movies – from Sunnyvale, California to Amsterdam, Netherlands in 58 seconds.

The High Performance Wireless Research and Education Network (HPWREN) sponsored by NSF at the University of California-San Diego uses advanced wireless capabilities to provide Internet links at educational institutions in remote sites, such as Native American communities. HPWREN is also prototyping a variety of distributed data-collection applications for high-speed wireless networking, including real-time measurement and multicasting of seismic events in southern California along the San Jacinto fault, wildfire tracking, and sensor networks for ecological monitoring in remote habitats.

b) *DNA molecule in liquid crystalline form.*
c) *Perspectives of HIV-1 protease, showing protease inhibitor indinavir in green. Red mesh represents computed solvent accessible surface, a key indicator of protein structure. Such computational modeling is greatly speeding the work of identifying the structures of the some 100,000 proteins in the human genome, which will enable new treatments for diseases like HIV.*

Foundations for SCIENTIFIC LEADERSHIP

WORKING ON THE GRID



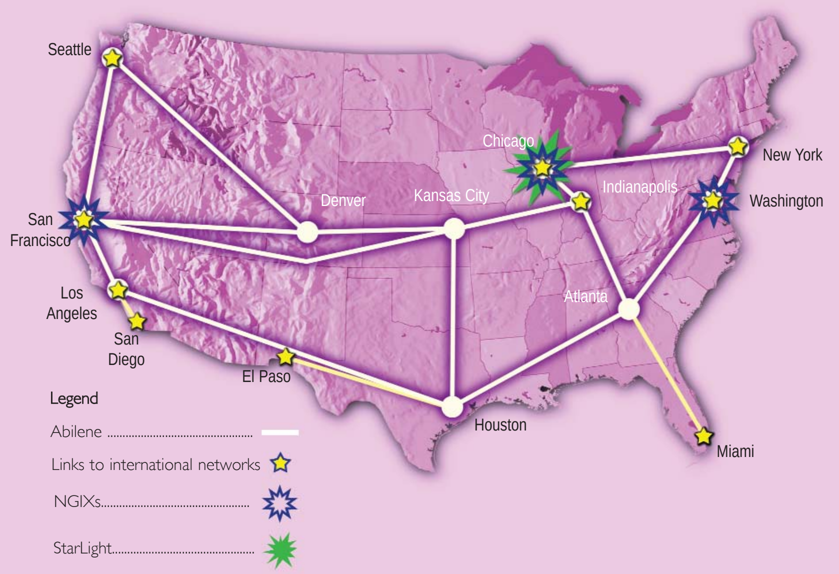
A Working Partnership

From the foundation of Federal R&D investments in networking technologies, a working partnership among the NITRD agencies, universities, and industry has developed a broadband infrastructure for research, providing connectivity not only to research facilities throughout the U.S. but to research networks around the globe. The optical backbone links (shown in white) are the Abilene network, supported by the Internet2 consortium of universities and partners Cisco, Nortel, and Qwest. The OC-192 backbone, able to transmit data at nearly 10 gigabits per second, connects to Federal research networks at Next Generation Internet Exchange Points (NGIXs, shown as blue stars). These Federal "peering" points transparently route traffic from one network to another. International exchange points to networks in Asia, Europe, and South America are shown as yellow stars. NSF's new StarLight facility (shown as green star) at the University of Illinois-Chicago adds to to these capabilities an advanced optical infrastructure and proving ground for network services optimized for high-performance applications.

The Federal research networks are:

DREN – Defense Research and Engineering Network, DoD
vBNS – very high-performance Backbone Network Services, NSF
NREN – NASA Research and Education Network
ESnet – Energy Sciences Network, DOE
BOSSnet – Boston-South Network, DARPA

U.S. HIGH-PERFORMANCE RESEARCH NETWORKS



a) Image of interstellar gas and dust opens 8-minute simulation of the solar system's birth developed for the Hayden Planetarium by a distributed multidisciplinary research team. The team used advanced computational techniques and grid technologies to share and work with nearly 7 terabytes of data, which ultimately were rendered into 70,000 high-resolution frames on the Blue Horizon platform at the San Diego Supercomputer Center. The processing took a day at a rate of 1.7 trillion operations per second.

The Globus software suite for grid computing – first developed by researchers in a joint effort by DARPA and DOE/SC and still being elaborated in the DOE/SC Science Grid, NSF's TeraGrid, and NASA's Information Power Grid – makes possible large-scale collaborative research frameworks in key domains of 21st century science. The NSF-funded National Virtual Observatory, for example, is developing grid-based tools to enable scientists for the first time to access and work with experimental data from more than 50 astronomical research facilities. The initiative aims to close the gap between the output of the international array of land- and space-based telescopes and sensors – now generating more empirical data annually than existed in the field of astronomy before 1980 – and the ability of researchers to make use of it.

Major IT vendors worldwide also are adopting the Globus Toolkit™, named "most promising new technology" of 2002 by *R&D Magazine.* The NITRD agencies are founding participants in the Global Grid Forum, the leading organization working to expand grid technologies for international scientific collaboration. A major related initiative in middleware research at NSF supports grid development by strengthening the underlying software technologies that make distributed computing possible.

IT frameworks for large-scale scientific collaboration being developed with NITRD support include:

DOE/SC

Collaboratory for Multi-Scale Chemical Sciences – Developing a Web portal and informatics infrastructure to enable sharing of validated data and collaborative investigation by researchers working in combustion science at scales from the atomic level to the macro level of turbulent combustion phenomena.

Earth System Grid II – Integrating storage, management, access, and collaboration technologies for massive data generated in DOE/SC climate research.

National Fusion Collaboratory – As the Administration moves to renew U.S. participation in development of the International Thermonuclear Experimental Reactor (ITER), this project is establishing secure frameworks for fusion scientists to work collaboratively with the massive data sets generated by the Nation's three large fusion facilities. The ensemble will include data repositories and advanced applications and collaboration software.

Particle Physics Data Grid (PPDG) – Creating high-bandwidth connectivity, storage and data access, and software tools for researchers in the most data-intensive of all the physical sciences. In a collaboration with NSF's Grid Physics Network, PPDG scientists have successfully simulated more than 1.5 million particle-collision events over a nationwide five-node grid.

NASA

Earth System Modeling Framework and Earth Observing System (EOS) testbed – In collaboration with DOE, NOAA, and NSF, this NASA effort has the ambitious goals of making the world's richest and most dynamic stores of scientific data about Earth both more accessible and more useful to a broad range of researchers. A central goal is to develop a single software framework that will enable researchers for the first time to integrate data from many different climate, weather, and environmental models. The testbed will create a data-storage and networking infrastructure to accommodate the growing volume of empirical data being generated by DOE/SC, EOS, NOAA, and the NSF-supported National Center for Atmospheric Research as well as tools to make the data accessible to the wider U.S. research community.

NSF

Geosciences Network (GEON) – In collaboration with the U.S. Geological Survey and the Geological Survey of Canada, this effort involving researchers from 13 universities is building digital libraries of high-quality geological information and integrated software tools for data access, analysis, modeling, and visualization. GEON will be a national resource for researchers, students, teachers, and the public.

Grid Physics Network (GriPhyN) – Using grid technologies to make the results of experiments at the world's largest experimental physics facilities accessible to the broader academic community.

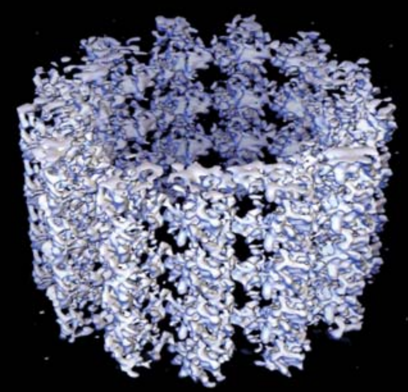
Network for Earthquake Engineering Simulation (NEESgrid) – Creating a high-performance infrastructure for real-time collaboration among the scientists and engineers who study earthquake dynamics in order to design materials and structures that reduce their threat to life and property. More details on page 27.

PROJECT URLs

Collaboratory for Multi-Scale Chemical Sciences (http://cmcs.ca.sandia.gov)
Earth System Grid II (http://www.earthsystemgrid.org)
Earth System Modeling Framework (http://www.esmf.ucar,edu)
Geosciences Network (GEON) (http://www.geongrid.org)
Grid Physics Network (GriPhyN) (http://www.griphyn.org/index.php)
National Fusion Collaboratory (http://www.fusiongrid.org)
Network for Earthquake Engineering Simulation (NEESgrid) (http://www.neesgrid.org)
Particle Physics Data Grid (http://www.ppdg.net)

Foundations for
SCIENTIFIC LEADERSHIP

BEING THERE: INSTRUMENTS AND VISUALIZATION



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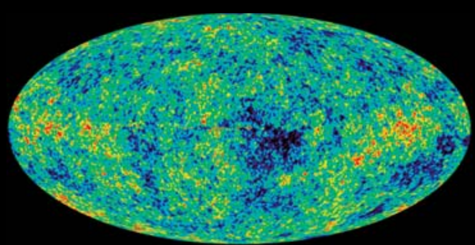

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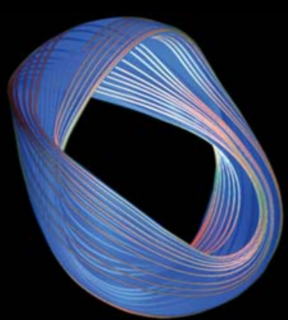

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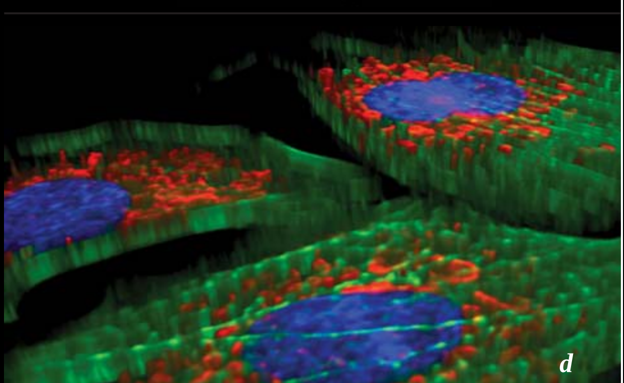

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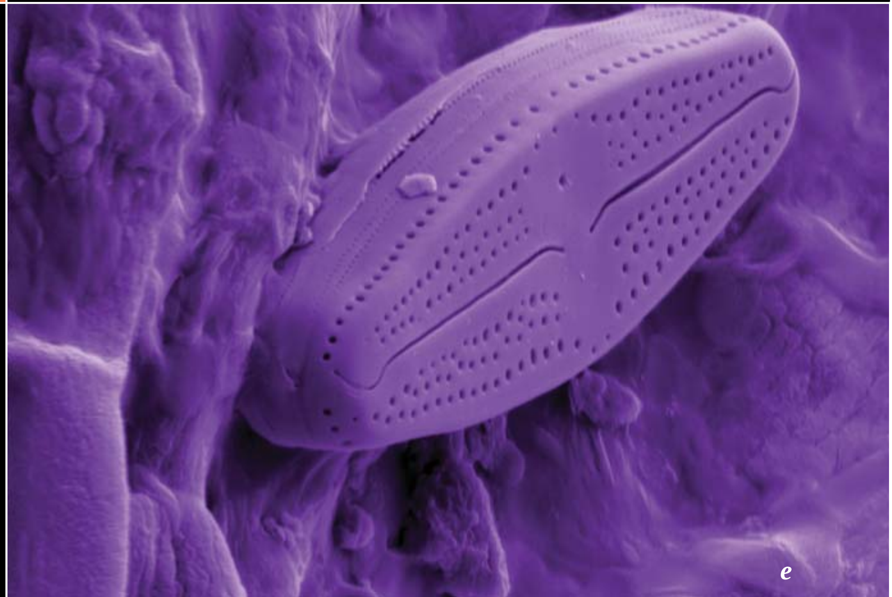

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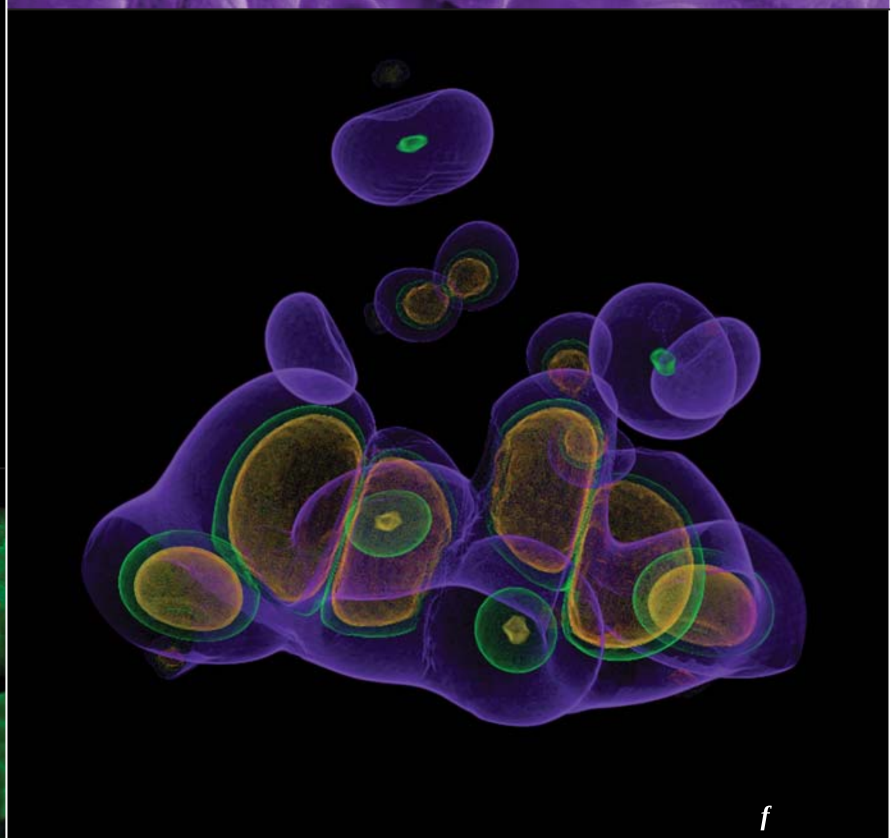
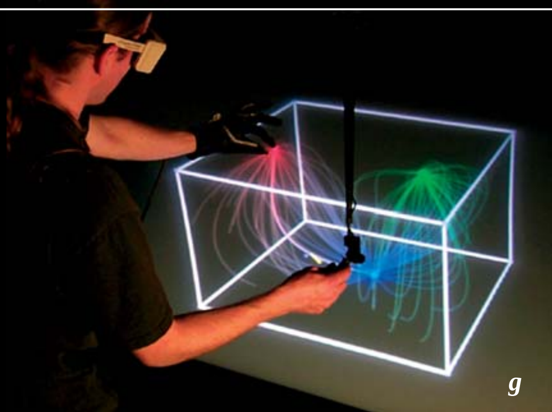
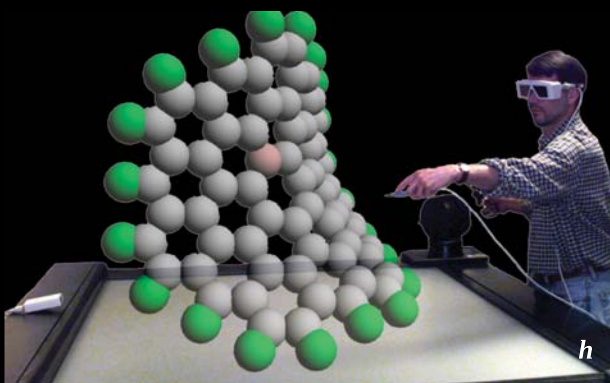


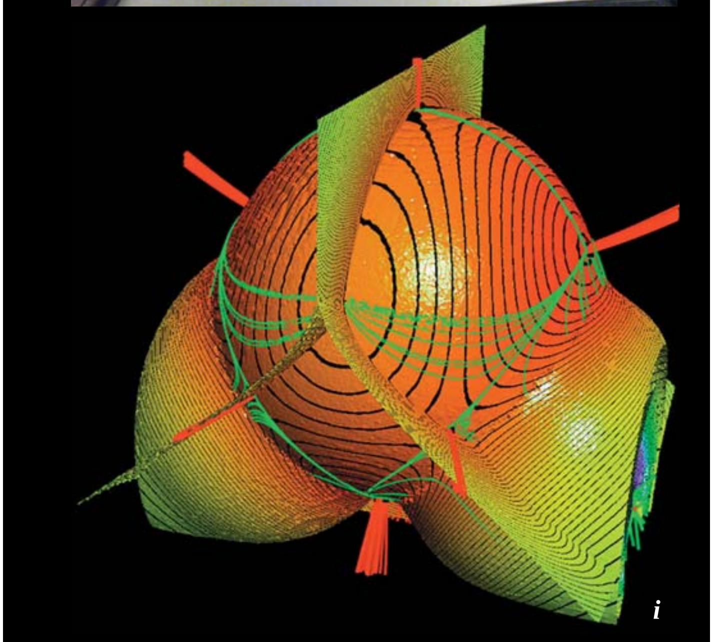
f

a) *From cryoelectron microscopy and image reconstruction, the most detailed view to date (8-angstrom resolution) of a microtubule, a weave of proteins in a cell's skeleton.*
b) *"Baby picture of the universe," made from microwave after-glow of the Big Bang – light that has traveled for 13 billion years.*

c) *To exploit nuclear fusion as a renewable energy source will require new knowledge about the properties of superheated gases, or plasmas. Scientists with the Center for Extended Magnetohydrodynamic Modeling, a DOE/SC collaboration of Federal labs and universities, are developing techniques to visualize plasma behaviors, such as the stable toroidal state shown.*







Information technologies pioneered in Federal research underlie the generation of highly sensitive diagnostic and research instruments now speeding advances throughout the sciences. These capabilities include the world's most powerful telescopes and instrumented satellites; magnetic-resonance imaging (MRI, which measures absorption of radio waves by tissue within a magnetic field), computed tomography (CT, an X-ray technique), and other non-invasive techniques for looking inside the body; electron, atomic-force, and other forms of microscopy and spectrometry that examine matter at the atomic level, and large-scale facilities that generate data about atoms by focusing concentrated light beams on them or creating high-speed particle collisions. All of these technologies are governed by IT hardware and software systems, with a top-layer software interface enabling human operators to manage the equipment and software components that translate measurements into digital data that can be displayed graphically.

Advanced visualization techniques developed through NITRD research have made it possible to render instrument data as high-resolution images in three dimensions, to show the dynamics of three-dimensional processes over time, to see and manipulate an image from all angles, and to generate sophisticated composites representing many layers of data.

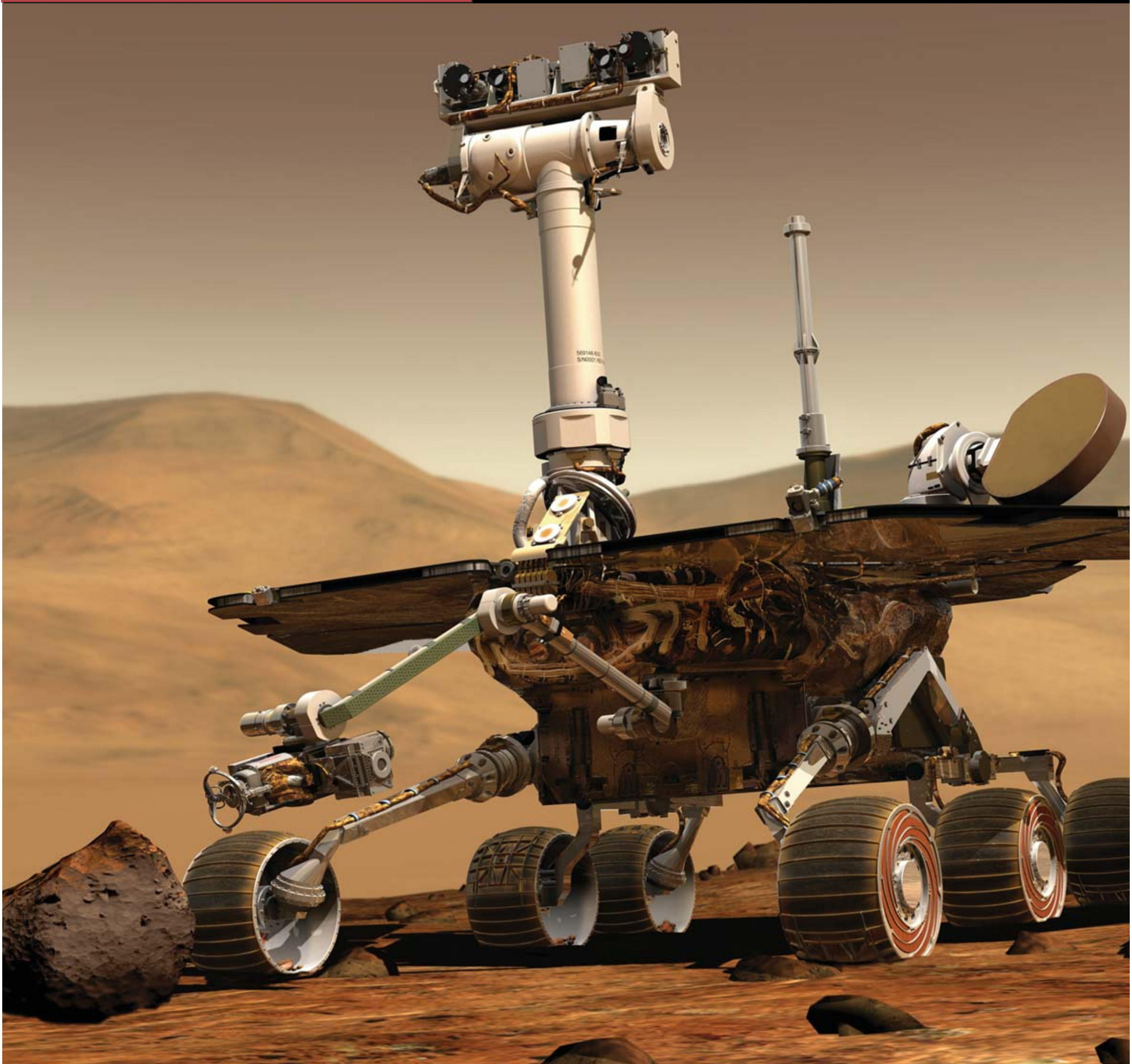
Like modeling and simulation techniques, visualizations of data generated by state-of-the-art instruments are providing not just scientists but students and the public with views of the intricacy of matter at scales too tiny or too vast to be seen any other way. In biomedical research, for example, imaging is rapidly expanding knowledge about proteins, the complex biomolecules that are life's core workforce. Investigation of their genetically determined shapes and functions is a top national research priority today. Scientists believe these molecules hold the keys to revolutionary new treatments for human diseases and those affecting other species.

Remarkable bits of software-driven engineering in atom-scale microscopy instruments even make it possible for users not just to see the invisible world of atoms and molecules, but to physically maneuver and experiment with them. These inventions, which include IT-guided optical "tweezers" and tiny probes, are helping propel a remarkable new science and technology of matter at the nano scale. (The prefix nano- means a billionth of, or 10^{-9}; a row of 10 hydrogen atoms is about one nanometer wide. For more about nanoscale science, please see page 24.)

d) *Computationally rendered image of specialized cardiac cells called myocytes that make hearts beat; cells are stained to show mitochondria (red), DNA (blue), and F-actin (green).* ***e)*** *Unidentified diatom sitting on a cockleburr seed. Details on page 52.*
f) *3-D data, like terrain, have a topology; image of fuel injected into chamber, from automated techniques for data analysis and transfer to show topologically equivalent regions (varying by color, opacity).*
g), h) *Virtual reality hardware and software technologies enable scientists to physically manipulate data-based 3-D structures. Details on page 52.*
i) *Water molecule – vector-field techniques show electronic charge density. Details on page 52.*

Foundations for SCIENTIFIC LEADERSHIP

BEING THERE: INSTRUMENTS AND VISUALIZATION



PHONE HOME: Communications with NASA's twin Mars Exploration Rovers, Spirit and Opportunity (launched June 10 and July 7, 2003, on their six-month, 34-million-mile journey) may benefit from the fact that Mars will be closer to Earth than at any time in the last 73,000 years. One-way transmission time will be 11 minutes, compared with 19 minutes during the 1976 Viking mission. In the agency's most elaborate deployment of IT capabilities to date, scientists and engineers are running the Mars mission using advanced hybrid networks, a new class of interactive collaborative

At the intersection of diagnostic devices, computer science and engineering, and medical practice, visualization technologies are also providing powerful new clinical tools. Physicians and surgeons can see exactly what form an individual patient's condition – such as broken bones, a tumor, or a vascular obstruction – takes inside the body and work with that information visually in considering approaches for treatment. A physician can custom-engineer prostheses, such as joint replacements, using computer modeling and then evaluate the designs in the context of a patient's particular anatomy.

Harvard University researchers supported by NIH and NSF are leading developers of such next-generation tools. Starting with the megabytes of data produced by CAT and MRI cross-sectional scanning, traditionally rendered as long sequences of 2-D grayscale images, the researchers computationally segment data representing the key anatomical features under diagnosis. Advanced visualization techniques translate the data into high-fidelity, 3-D color models of the features. These images from an individual patient can be layered with contextual information, such as the surrounding anatomical environment, the shape and position of the feature relative to statistical averages, and possible surgical routes. In neuroanatomy, one focus of the project, the imaging methods are especially useful in illuminating 3-D structural relationships not captured in a diagnostic scan. Brain surgeons are using the tools both in pre-planning and as guides in the operating room.

Long-distance investigation

Across the fabric of high-end connectivity woven of advanced networking and grid technologies for resource-sharing, NITRD-funded research is now linking researchers and students to the Nation's most advanced instruments for scientific and medical research and providing the computational and storage resources they need to work online. The Alpha Telescience Project, a collaboration of NSF's National Partnership for Advanced Computational Infrastructure (NPACI) and the NIH-sponsored National Center for Microscopy and Imaging Research, puts distant users at the controls of the center's high-voltage transmission electron microscope, with real-time streaming video to the desktop. An accompanying application allows the user to create a quick low-resolution version of any microscopic feature to see if it is of interest before deciding to acquire the full tomographic data. Telescience Project developers are prototyping an additional grid-enabled capability that will allow microscope users to generate 3-D tomographic images immediately via distributed parallel processing.

Making another kind of specialized resource – human expertise – more widely accessible is the focus of NIH efforts employing networking and telepresence capabilities for advanced medical training. Expertise in clinical medicine is more than intellectual; it also derives from "hands-on" experience in examining patients and performing surgical procedures. Researchers at Stanford University are using NITRD-developed "haptic" technologies – software and hardware tools for simulating the sense of touch – to help students experience surgical techniques over the Internet. A master surgeon at one location "traces" a surgical procedure with a haptic instrument connected to a computer, which translates the actions into software. A student at a remote computer receives a copy over the Net and, holding the haptic device, lets the software guide his or her hand several times. After a few practice tries, students rehearse the technique independently. These interactions can be stored and reused.

In addition to connecting users to unique resources, NITRD efforts connect distributed data-gathering instruments via networks delivering types and quantities of real-time empirical data that a lone scientist could not hope to amass in a lifetime. Remote-sensing, imaging, and wireless networking technologies developed by DARPA, DOE/SC, NASA, NIST, NOAA, and NSF support real-time monitoring systems for many domains of the national interest, such as air and water quality, rain acidity, drought and fire conditions, seismic and volcanic activity, and melting of the polar icecaps.

As a key weather-monitoring agency relied upon around the world, NOAA expects to collect an average of 2.5 terabytes of data daily from a global network of satellite-based sensors, 156 Doppler radars (a technology developed jointly by NOAA and NSF researchers), ocean vessels and buoys, radiosondes and surface observation stations, and makes much of the information publicly available online. NOAA's real-time observations are the mainstays of major U.S. sectors, including armed services' and civilian weather forecasting, emergency preparedness, aviation and ground transport, agriculture and fisheries, and recreation and tourism.

computing platform, and custom software tools for real-time distributed mission planning, rover remote control, data analysis, and imaging – all integrated to enable large-scale collaborative management of the intricate enterprise. The 400-lb. rovers are equipped with camera, microscopic imager, spectrometers, and robotic drilling arm to look for signs of life amid the red rocks.

Foundations for SCIENTIFIC LEADERSHIP

CROSSING BOUNDARIES – INTERDISCIPLINARY SCIENCE

Today the boundaries between all disciplines overlap and converge at an accelerating pace. Progress in one area seeds advances in another. New tools can serve many disciplines, and even accelerate interdisciplinary work.

Rita R. Colwell, Director, National Science Foundation, February 2003

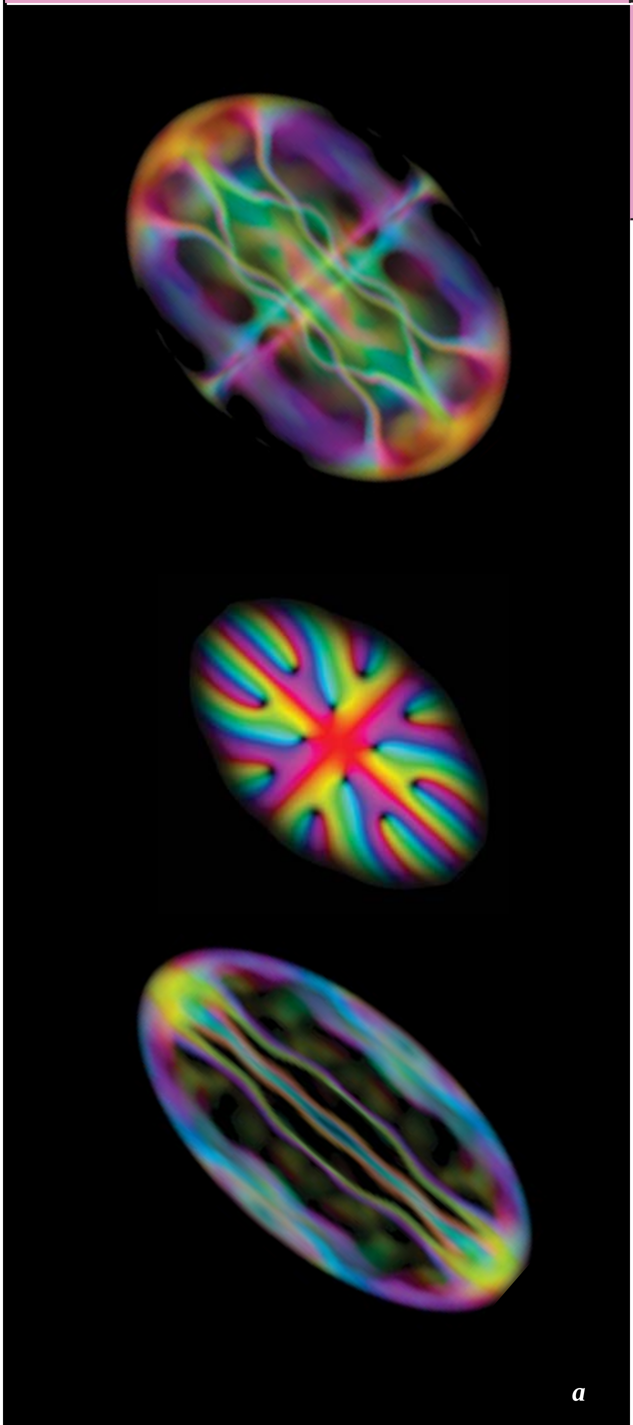
Such disciplinary interconnections, many scientists believe, will shape the scientific enterprise for the rest of this century, with teams of investigators tackling complex problems whose solutions call for knowledge, methods, and technical skills from a variety of fields. One early indicator of the trend: In 1990, only 6 percent of 1,600 researchers using DOE's synchotron light sources to study atomic particles were from the life sciences; today more than 40 percent of the more than 6,000 researchers using these instruments are bioscientists.

Scientists traditionally have tried to understand Earth's environment by taking sample observational measurements – such as of water tables, rainfall, cloud cover, air flows and temperatures, ocean currents, vegetation and animal distributions, photosynthesis rates, polar ice thickness – and theorizing about how all these factors fit together. In this century, advanced information technologies will make it possible to see how such influences work together and to develop deeper knowledge of the environment as a complex system of systems interacting with and affected by humans.

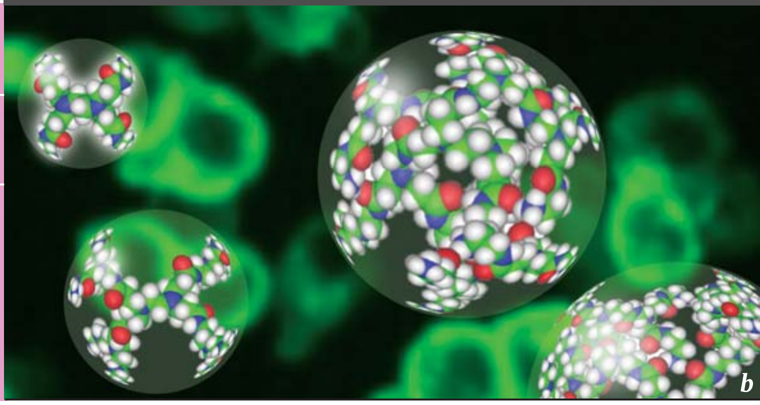
Complexity in biological systems

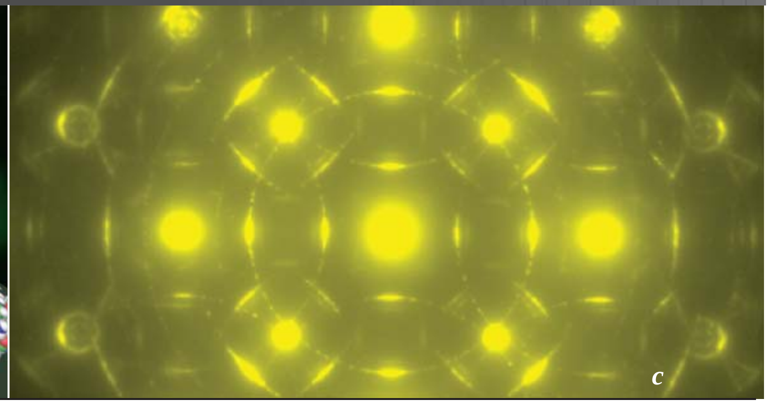
A major NSF initiative, Biocomplexity in the Environment, is funding a wide range of multidisciplinary efforts to map biocomplexity systemically, from the genetic and submolecular scale to macroclimatic forces and effects of human activities. Researchers at the University of North Carolina, for example, have developed a real-time environmental scanning system that couples chemical-detection technologies with tomographic mapping capabilities to compute pollution maps covering large geographic areas. The maps can depict multiple chemicals at once, a significant factor in examining chemical constituents and dispersal of industrial and agricultural residues.

The emerging field called chemical genetics depends on IT capabilities for rapid discovery of microscopic research tools that will



a) Bose-Einstein Condensate (BEC), a new form of matter demonstrated by NIST researcher Eric Cornell and colleagues, earning them a 2001 Nobel Prize in Physics. BEC is created when atoms are supercooled to an almost motionless state. Simulation images show unique vortical patterns formed by BEC (bright areas indicate lower atom density) in quantum trapping experiments.





narrow the gap between what bioscientists are learning about human proteins and applications of these findings in clinical medicine. Chemical genetics aims to identify small molecules that either activate or deactivate protein functions. Researchers can use these "molecular probes" to more quickly analyze how proteins malfunction in such diseases as cancer, multiple sclerosis, and Parkinson's. Harvard University chemists sponsored by NIH's National Cancer Institute have created ChemBank, an online repository of small-molecule chemical structures and properties and accompanying IT analysis tools for biologists to contribute to and use. The Harvard lab is systematically identifying molecular probes in an automated screening process that uses imaging and software tools to capture data on the effects of various small molecules on protein behavior.

How the other half lives

In DOE/SC's Genomes to Life program, hundreds of Federal, industry, and university researchers from the biological, environmental, physical, and computing sciences are engaged in a long-term effort to extend IT-based genetic research methods to the world of microbes. These tiny organisms, which make up more than 50 percent of Earth's total biomass, control biogeochemical cycles and affect soil productivity, water quality, and global climate.

In that sophisticated biomachinery – which can use even toxic wastes as energy sources and can produce such diverse energy products as hydrogen and methane – scientists see means for developing clean energy, removing excess carbon dioxide from the atmosphere, and remediating contaminated environments left as a legacy of the Cold War. The research is applying "high-throughput" computational methods developed in the Human Genome Project to identify microbial proteins and their functions. But it will also require computing power and tools far beyond today's levels to develop data about and analyze the behavior of large microbial systems and colonies, as well as their multiscale, multidimensional interactions with the environment.

Scientists with multiple skill sets

Even the work of individual scientists – such as Surya Mallapragada, an Iowa State University researcher named one of the world's top 100 technical innovators for 2002 by *Technology Review* – highlights the multidisciplinary flow of contemporary science. In research supported by DOE and NSF, the materials chemist and chemical engineer is combining biomolecular chemistry, advanced IT capabilities, and nanotechnology in a technique to regenerate nerve cells, which are not amenable to methods used with other types of cells. On an ultrathin (a few thousandths of an inch) biodegradable polymer film that she and her team engineered, the researcher uses digitally controlled laser and ion-reactive etching instruments to make grooves a few microns (millionths of a meter) deep. The grooves are then coated with protein and Schwann cells (which in the body form nerve cells' myelin sheath) and peripheral nervous system axons are placed in each sheath-like groove. The axons have grown at a rate of three or four millimeters daily, and Mallapragada has successfully applied the technique to regenerate sciatic nerves in rats. She is examining how to extend the concept to central nervous system cells, such as those of the optic nerve, which pose even more difficult regeneration problems.

***b)** University of Michigan researchers are experimenting with dendrimers – spherical polymer molecules with a uniquely consistent branching chemical structure – as vehicles for identifying diseased cells, reporting their location, and delivering targeted therapies. Details on page 53.*

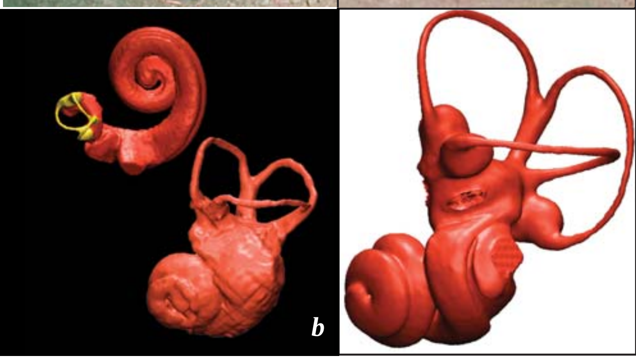
***c)** DOE/SC-funded work at the University of Illinois Center for Microanalysis of Materials aims to understand the electrical properties of nanoscale heterostructures such as layered oxide thin films for future electronics.*

Foundations for
SCIENTIFIC LEADERSHIP

CROSSING BOUNDARIES – NANOSCALE SCIENCE AND TECHNOLOGY

A biological system can be exceedingly small. Many of the cells are very tiny, but they are very active. They manufacture various substances, they walk around, they wiggle, and they do all kinds of marvelous things – all on a very small scale. Also, they store information. Consider the possibility that we, too, can make a thing very small which does what we want – that we can manufacture an object that maneuvers at that level.

Richard Feynman, 1959 speech, "There's Plenty of Room at the Bottom"



Interdisciplinary science is perhaps most dramatically displayed in the new field of nanotechnology, where, as OSTP Director John H. Marburger puts it, "the notion that everything is made of atoms finally becomes operational."

Nanotechnology, with IT as both a major driver and an enabler, is developing at the intersection of materials science, engineering, physics, chemistry, and biology. With dimensions of only a few billionths of a meter, nanoscale structures are typically investigated with advanced IT capabilities that enable scientists to see and manipulate individual atoms and molecules as well as simulate nanostructural dynamics with mathematical precision. The NITRD agencies, which pioneered tools for nanoscience through research on next-generation semiconducting and superconducting materials, chip architectures and microfabrication processes, MEMS devices, optoelectronic/photonic technologies, and visionary molecular computing concepts, remain at the forefront of nanoscale discovery. DARPA, DOE/SC, EPA, NIH, NIST, NSA, and NSF are core participants in the National Nanotechnology Initiative, an Administration R&D priority for FY 2004 as is the NITRD Program.

Nanotechnology research leads in many long-term directions, including custom-designed materials with properties unlike any we know today, revolutionary techniques for combating disease and maintaining health, and ultra-miniaturization of computing and other mechanical and electronic systems. But the nanoscale realm holds many mysteries. We do not yet understand, for example, how the laws of physics operate in nanoscale structures – their behavior cannot be predicted from physics at the macro scale. Even so, nanotechnology promises an extraordinarily diverse range of innovations ahead, as suggested in the following examples of current research advances.

In work awarded the top honor of the International Conference on Computational and Experimental Engineering and Sciences, a NASA computational nanoscientist and his team have engineered a process to fabricate carbon nanotubes – the strongest new material yet devised, with the ability to be either a semiconductor or a metal – and have successfully demonstrated nanotubes in semiconductor logic circuits. The goal of this and related research is nanoscale computing, sensing, telecommunications, and avionics components to radically reduce the weight and scale of spacecraft. The versatile nanotubes are also being used in strong lightweight polymer composites for structural applications. NASA studies indicate that replacing aluminum aircraft structure with carbon nanotube composites could reduce the dry weight of large commercial aircraft by 80 percent, with a 25 percent reduction in fuel use.

Biomolecular motors

One of the most astonishing areas of nanoscale discovery is molecular biology, where scientists, such as those in the Genomes to Life effort, are trying to understand how the work of life actually gets done at Feynman's "bottom" level. Like tiny vehicles, many types of protein physically move or transport subcellular material. Following on the new

a) *Elaborate lab technologies and data mining enabled NSF-supported researchers to identify a protein – glucose-6-phosphate isomerase, necessary to initiate pregnancy in ferrets – that also plays a role in cancer metastasis.* ***b)*** *An international team, using visualization software developed for NIH's "Visible Human" data, has discovered a secret of whales' and dolphins' swimming skill – 3-D image reconstructions from CT scans of early and contemporary skulls show even the earliest cetaceans had mammals' tiniest semicircular canals for their size. Left to right, dolphin, early whale, bushbaby.*

knowledge about proteins' complex shapes, investigators are examining "biomolecular motors," proteins that change shape to generate force, or torque, in order to carry out tasks.

In an elegant application of electron microscopy and IT-driven optical tweezer techniques, researchers funded by DOE, NIH, and NSF have not only measured in real time the power of a biomotor but demonstrated what may be a key mechanism of viral infection. The research showed that bacteriophage phi-29 – a virus that destroys soil bacteria – packs large amounts of its DNA into its external shell, called a capsid, a space about 6,000 times smaller than the DNA's normal volume. The packing action requires 57 to 60 piconewtons of force – which the researchers describe as the equivalent of lifting six aircraft carriers if scaled up to human dimensions. The internal pressure generated in the capsid is 60 atmospheres – about 10 times the pressure in a champagne bottle. The researchers propose that, like a champagne cork, the compressed viral DNA, which cannot replicate unless it enters a host cell, explodes into the healthy cell to which the virus has attached.

Getting themselves together

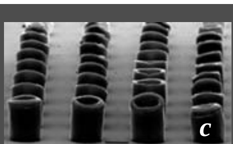
Another facet of nanoscale molecular research examines how both organic and inorganic atoms and molecules organize themselves into larger structures. Understanding what scientists call "self-assembly" is a critical step toward the ability to custom-design novel materials for such uses as targeted delivery of drugs and therapies inside the body, protective coating and encapsulating, imaging, and automated microfabrication. Advanced IT techniques have confirmed the fantastically intricate lattice structures formed by inorganic atoms and molecules such as in metal alloys. But self-assembly processes in organic matter, governed by genetic instructions, are less well understood. NSF-supported researchers in February 2003 reported a milestone in such work, achieving a self-assembled liquid crystal lattice of 255,240 atoms in branching molecules called dendrons, which make up the protein coat around viruses. The result, published on the Web site of the journal *Science,* was not only the most complex organic structure yet created via self-assembly, but also the first organic compound to assume an intricate structural form previously seen only in metals.

Revolutionary computing devices

Just as IT is critical to the future of nanotechnology, nanoscale science is seen as the means of surmounting IT's "red brick wall" – the approaching physical limit to the miniaturization of chip architectures, and thus to advances in computing speeds. The NITRD Program encompasses research in biomolecular chemistry and quantum physics as potential sources of revolutionary computation and data-storage technologies. One gram of DNA, for example, stores the equivalent of 10^8 terabytes of digital data – about ten thousand times the capacity of today's largest mass storage systems. In 2002, University of Southern California researchers funded by DARPA, NASA, NSF, and the Office of Naval Research achieved a notable biocomputing success, using DNA molecules to reach the correct answer to a computational problem with 20 variables and more than a million possible solutions. Previous DNA experiments had solved problems with a maximum of nine variables. "This landmark study," said *Science,* "proves that molecular computation is not a far-fetched possibility but a quickly evolving discipline that may have major impact on more established disciplines such as biotechnology."

Quantum IT research begins with the fact that subatomic particles (atomic nuclei, photons, electrons, etc.), which follow the unique laws of quantum mechanics, exist – in computing terms – partly in both the binary 0 and 1 states at the same time. In theory, a particle's superposed quantum states, called "qubits," could provide the basis for exponentially higher calculation speeds than are possible in the binary world.

In 2001, NIST researcher Eric A. Cornell and two other Americans shared the Nobel Prize in Physics for proving the existence of a near-motionless atomic state – the Bose-Einstein Condensate – that had long been theorized but not achieved empirically. Since the evanescence of quantum states (they disappear in quadrillionths of a second as atoms spin and move) is a fundamental barrier to quantum computing, the ability to generate the low-energy Bose-Einstein state marked a significant advance. NIST and Massachusetts Institute of Technology researchers have proposed a quantum computer design based on this work. DARPA, DOE/SC, NASA, NSA, and NSF researchers also are exploring ways to exploit nanoscale phenomena in quantum information systems.



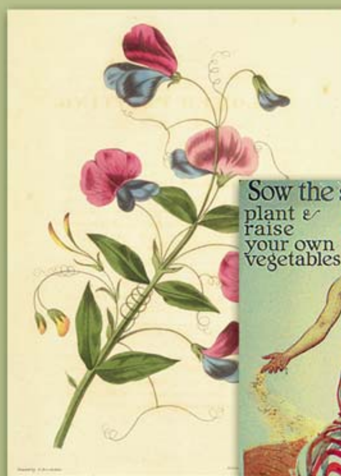
c) Carbon nanotubes, made with NASA fabrication technique. Each tube is about 100 nanometers wide. ***d)*** *In biomolecular motor built by Cornell University researchers, adenosine triphosphate (ATP) enzyme powers nickel propeller at 8 revolutions per second. Post is 200 nanometers tall, propellers about 750 nanometers long.*

Foundations for
RESEARCH AND LEARNING

SHARED KNOWLEDGE. SHARED RESOURCES

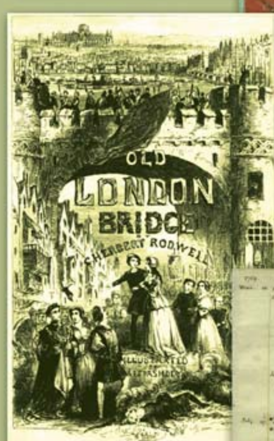
There is a growing mountain of research. ... The investigator is staggered by the findings and conclusions of thousands of other workers – conclusions which he cannot find time to grasp, much less to remember, as they appear. ... Professionally, our methods of transmitting and reviewing results of research are generations old and by now are totally inadequate for their purposes.

Scientist Vannevar Bush, in a 1945 *Atlantic Monthly* article proposing "Memex," a configurable device for information storage and retrieval



b) Frontispiece from "A new treatise on flower painting, or, Every lady her own drawing master," by George Brookshaw (1818). Digital Library for the Decorative Arts and Material Culture, University of Wisconsin. (http://libtext.library.wisc.edu/DLDecArts/)

c) World War I poster from American Women's History: A Research Guide, a Web resource developed by Ken Middleton, a librarian at Middle Tennessee State U. (http://www.mtsu.edu/~kmiddlet/history/women/wh-intro.html)



d) 19th century engraving from Tufts University's Bolles Collection on the history of London. Can be accessed through the NSF-supported Perseus Digital Library of materials on the history of Western culture. (http://www.perseus.tufts.edu)

e) March 1769 entry in Thomas Jefferson's Monticello garden book notes planting of peach, pear, cherry, apple trees. Massachusetts Historical Society digital archive is supported by Congressional Save America's Treasures program. (http://www.thomasjeffersonpapers.org)

f) Signed handwritten score of "Star Dust," from the Hoagy Carmichael Collection at Indiana University, the composer's alma mater. (http://www.dlib.indiana.edu/collections/hoagy/)

a

a) *Cuneiform tablets, one of humankind's earliest data storage and information management technologies (ca. 3300- 2000 B.C.), and new translation research are focus of the Cuneiform Digital Library (http://cdli.ucla.edu).* *Details on page 53.*

g

g) *Thomas Edison films in Open Video Project include first America's Cup race, Cushing/Leonard boxing match (right). (http://www.open-video.org)*

Today, more than half a century after Vannevar Bush described information overload in a data-intensive world, high-performance networking, computing, and information-management technologies are making possible the far-reaching support system for human thought that he envisioned. Although they rarely make news themselves, the diversified digital libraries of core knowledge developed through NITRD agency investments have become a necessary, and invaluable, resource for rapid innovation, not only in research but in education and training, medical practice and health care, heavy industry and manufacturing, pharmaceutical design, business-to-business technologies, agriculture, and many other fields of endeavor.

Digital collections take many forms. Some are built and managed by a single organization in one location; others are actually Web-based frameworks and protocols that enable users to access widely distributed digital archives. Materials can include images and animations, software, sound, and video as well as data and texts. In addition, NITRD-sponsored research originated the IT capabilities that make it possible for people to discover the information they need, organize it, and work with it on their desktops. These technologies – for example, Web browsers; search engines; data-mining, analysis, and management tools; metadata frameworks (information that helps users understand the origin and nature of a digital record); data display and manipulation tools; and language translation methods – provide the technical foundations for a universal digital knowledge system.

But the work is far from finished. Research across the NITRD agencies continues in FY 2003 and FY 2004 on substantial technical issues – such as interoperability among file formats, indexing protocols, and interfaces; data management, storage, and validation; networking bottlenecks; and long-term preservation – that impede development of digital libraries. These efforts reflect urgent demand in every field for deep reservoirs of sharable knowledge to maximize the value of existing findings and enhance the potential for significant advances. Some examples of NITRD digital-library achievements and works in progress:

E-PRINT Network – DOE manages the world's largest "one-stop shopping" site for preprint reports in science and technology. These papers by scientists on their unpublished research in progress are fundamental resources for the U.S. research community. The E-PRINT Alerts feature allows users to specify their interests and receive notification as relevant new information is added. Scientific papers in biology, chemistry, computer science, engineering, environmental sciences, materials science, mathematics, physics, and other areas of interest to DOE are included. (http://www.osti.gov/preprints/)

E-Specimens – NSF-funded projects at the University of Texas at Austin provide online access to libraries of biological specimens. The DigiMorph specimen library is an archive of X-ray-computed tomography data whose animations and details are used in research labs and classrooms around the world. The e-Skeletons Project lets users examine the bones of a human, gorilla, and baboon and information about them in an osteology database. (http://www.digimorph.org/ and http://www.eskeletons.org/)

NO ORDINARY TABLE

The significance of sharing resources is highlighted when the resources in question are costly specialized research facilities, such as this multi-ton "shake table" under construction at the University of Nevada at Reno as part of NSF's Network for Earthquake Engineering Simulation (NEES). Only a small number of universities have built the structurally fortified labs equipped with unique heavy machinery required to shake experimental loads on such tables with the forces of an earthquake. Yet, other than measuring damage after a real event, shake tables have been the principal scientific tool for studying how to design structures to withstand quakes.

Using high-end computing and broadband networking capabilities, the NEESgrid will enable earthquake engineering researchers nationwide to observe and participate in these experiments in real time, make use of data stored in a common archive, and share advanced modeling and simulation software to study earthquake impacts and design resilient structures.

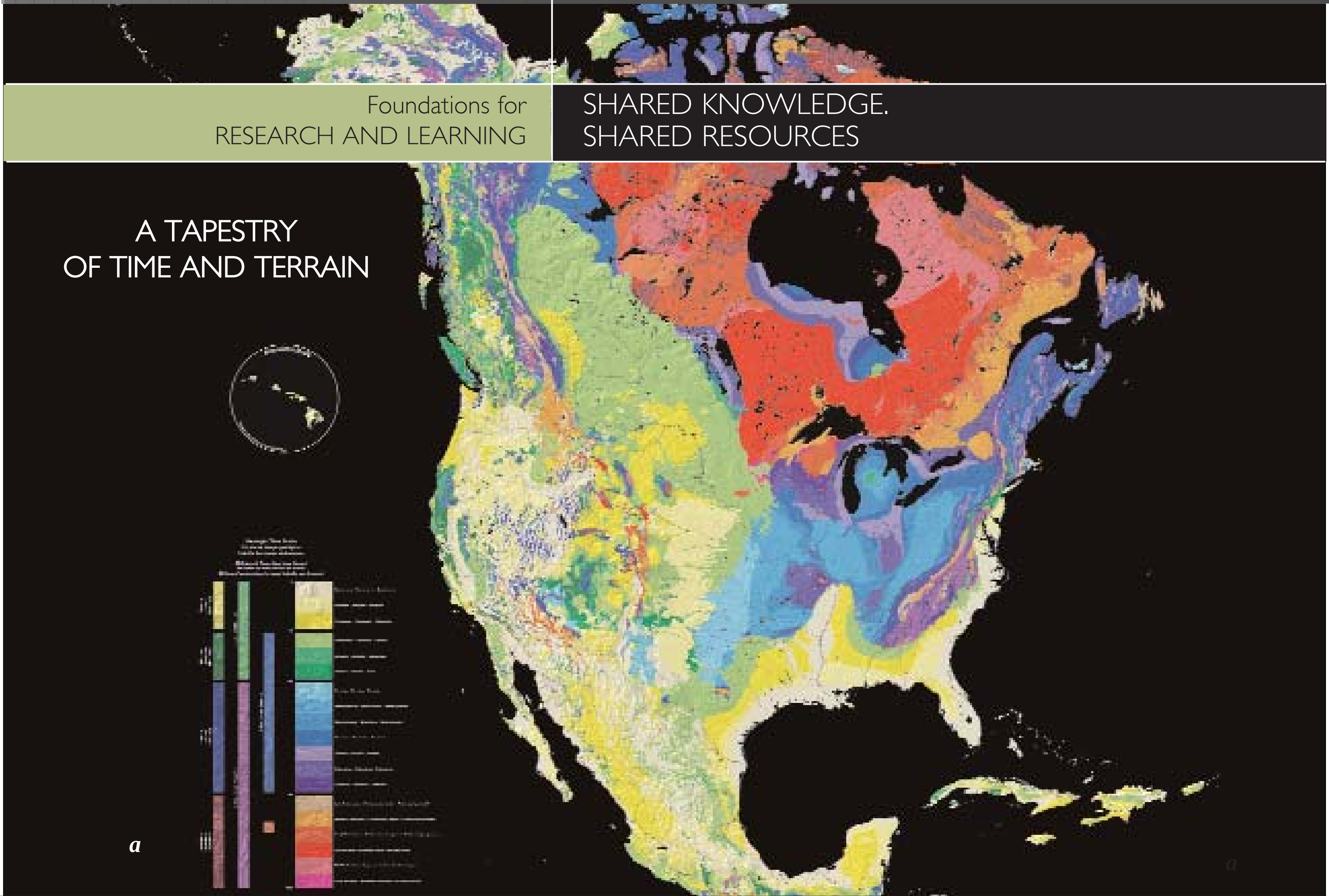
Head of Herrerasaurus ischigualastensis, oldest known dinosaur, from Upper Triassic Period. Discovered in Argentina in 1959. Image from Digimorph collection, University of Texas.

Spiders"R"Us, a University of Arizona Artificial Intelligence Laboratory program, is developing next-generation search-agent tools for knowledge discovery on the Web. (http://ai.bpa.arizona.edu/spidersrus/)

Foundations for RESEARCH AND LEARNING

SHARED KNOWLEDGE. SHARED RESOURCES

A TAPESTRY OF TIME AND TERRAIN



Digital libraries supported by the NITRD agencies are making vast stores of cultural, educational, technical, and scientific information available to the public

a) A new online resource for students, teachers, and the public, the U.S. Geological Survey's Tapestry of Time and Terrain interactive map merges the most accurate and detailed agency data on the topography and geology of North America. Users can explore the geological history of mountain formation, river erosion and deposition, glaciation, volcanic action, and other processes over 26 billion years. Details on page 53. (http://tapestry.usgs.gov)

GenBank and related databases – The National Library of Medicine's National Center for Biotechnology Information maintains public, searchable databases of the genomic sequences submitted in the Human Genome Project, the current draft of the genome, and completed genomic sequences for 800 other organisms. Scientists from around the world continue to upload new data to GenBank as they refine the original human draft sequences or develop sequences for other species. The Web site provides a variety of tools for working with the databases as well as archives of related information, such as a catalog of inherited human disorders. (http://www.ncbi.nlm.nih.gov/)

International Children's Digital Library – In this NSF-supported effort, the University of Maryland, the Internet Archive, and international partners are developing a library of 10,000 children's books from 100 cultures and new technologies to serve young readers. The library will serve children ages 3 to 13 worldwide. (http://www.icdlbooks.org)

NASA Cosmic Collection – In a large-scale technology transfer, the agency has released more than 500 NASA-designed software programs as publicly available open-source resources. The software, used in such fields as chemistry, aerodynamics, and engineering design, is being made available online by the OpenChannel Foundation. (http://www.openchannelfoundation.org)

National Guidelines Clearinghouse™ and National Quality Measures Clearinghouse™ – These online archives established by AHRQ provide a unique national resource for medical clinicians and health-care professionals, amassing for the first time comprehensive databases of the codified treatment knowledge, formal practice guidelines, and evidence-based quality indicators that have been developed by medical, health-care, and government organizations in clinical medicine. The guidelines clearinghouse, a partnership with the American Medical Association and the American Association of Health Plans, contains guidelines on diseases and conditions, treatments and interventions, source organizations, and related resource documents. Users can apply an online software utility to compare the contents of various guidelines. The quality measures clearinghouse provides objective summaries of quantitative measures of clinical performance (such as hospital pneumonia rates) developed by organizations throughout the health-care field. Software enabling users to compare measurement information is also provided. (http://www.guideline.gov/) and (http://www.qualitymeasures.ahrq.gov/)

National Science Digital Library – In FY 2004, NSF-funded work will continue on development of a comprehensive collection of core knowledge, teaching materials, and learning resources for nationwide high-school and college-level education in the sciences, technology, engineering, and mathematics. (http://www.nsdl.org/)

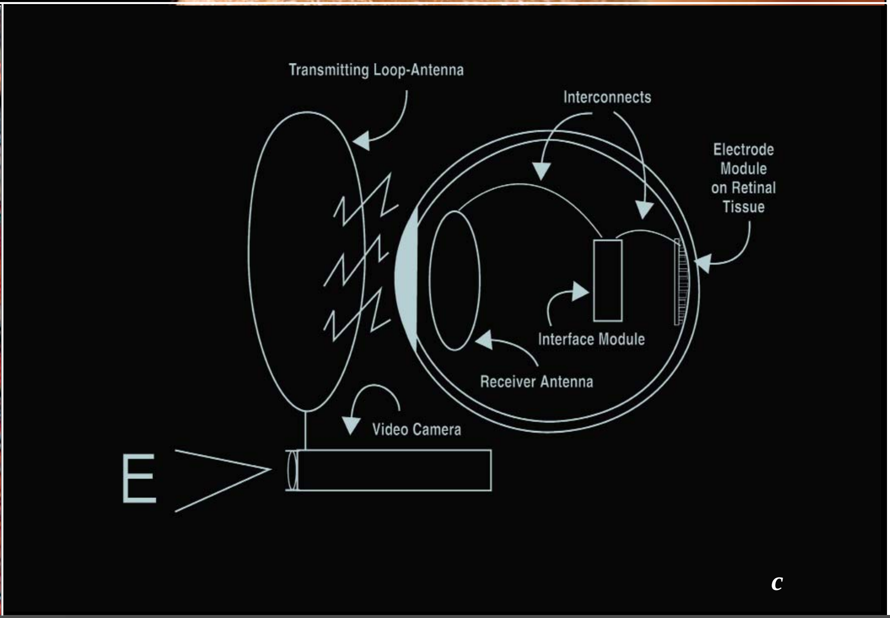
NIST Data Gateway – Through one online portal, users can access more than 80 NIST-developed databases of fundamental scientific information and validated reference data on topics ranging from atomic spectra, chemistry, mathematics, and physical constants, to calibration and manufacturing standards, product design, properties of materials, and thermophysical data. (http://srdata.nist.gov/gateway/)

Protein Data Bank (PDB) – As the international repository for 3-D data on the structures of biological macromolecules, the PDB is playing a critical supporting role in current research on the complex shapes and activities of proteins and their relationships to causes and mechanisms of disease. Funded collaboratively by DOE/SC, NIH, NIST, and NSF, this free interactive resource – accessed some 50 million times in 2002 – enables researchers to find and download validated structural data on more than 10,000 individual proteins generated with several techniques (X-ray crystallography, nuclear magnetic resonance imaging, and computational modeling). Researchers can also submit results of their own work to the collection. (http://www.pdb.org)

PubMed – The world's largest online collection of contemporary scientific literature related to the biomedical sciences and medicine, this public resource established and managed by NIH's National Library of Medicine contains 12 million abstracts from 4,500 journals. In FY 2003, it will be searched more than 400 million times. (http://www.ncbi.nlm.nih.gov/entrez/)
MEDLINEplus, a companion online library designed especially for consumers, will approach 100 million searches. (http://www.medlineplus.gov)

Foundations for 21st CENTURY SOCIETY

EDUCATION, TRAINING, TECHNOLOGIES, OPPORTUNITIES



a) *NASA hyperspectral imaging technologies capture fine-grained information about surface features and vegetation. Scientific farming methods now incorporate imaging to regulate cultivation and improve yields.*

b) *Funded by DOE/SC, a public-private collaborative team is developing tiny MEMS technologies to restore vision. Eye diseases such as macular degeneration damage the rods and cones that convert light into electrical messages to the brain.* ***c)*** *In prototype, a video camera, which could be attached to glasses, transmits signals via loop antenna to MEMS devices inside the eye that stimulate retinal nerves.*

> Information and communication technology are having a profound effect on the way of life of people in many different cultures throughout the world. No other technology in the past has spread so rapidly and with such transforming effect. ... The transformation of societies around the globe is just beginning.
>
> John H. Marburger III, Director of OSTP, March 2003

Innovation emerges in many forms and across all walks of life, supported by access to education, rich sources of information and ideas, and enabling technologies. The following examples suggest the breadth of this diversity.

A man with a plan

In the 1990s, a North Dakota farmer had an idea about how to help fellow farmers in his region cost-effectively improve the productivity of their land. With technical support from NASA, Montana State University, and the University of Minnesota, he created Agri ImaGIS, the first Web-enabled provider of satellite remote-sensing imagery and analysis software for precision agriculture across the U.S. and Canada. Clients log on to www.SATshot.com, where they download the free AI/Satshot Viewer, based on NASA imaging software customized by the farmer and university colleagues for the agricultural application. Through partnerships with major satellite companies, the Agri ImaGIS site lets users select the exact coordinates of the near-infrared imagery they wish to purchase, download the package, then apply the software to mine the images for information, pinpointing areas of high or low productivity indicated by vegetation density and vigor, soil condition, and moisture levels. A tool called Map ImaGIS enables users to build base maps of their fields and boundary lines, which they can overlay with zone-management information such as variable watering, seeding, and fertilization metrics.

Diagnostic alert

At the University of Pennsylvania Medical School, physicians treating critically ill patients on ventilators who are at high risk of pneumonia have tested a handheld "acoustic nose" sensor array as an early-warning device for detecting the disease. Traditional diagnostic X-ray and bacterial culture methods can take several days. The "nose," a technology developed by researchers at the NSF-supported Center for Neuromorphic Systems Engineering at the California Institute of Technology, clearly distinguished between patients who were infected and those who were not. Now being commercialized by Cyrano Sciences, Inc. of Pasadena, the "Cyranose" sensor array of carbon-black/polymer composites, which can be tailored to detect any type of chemical vapor, interacted with molecules in patients' exhaled breath to produce a unique electrical response displayed as a dot pattern on a computer screen. Rather than prescribing antibiotic treatments to all at-risk patients as a precaution, doctors could give antibiotics only to those signaling infection while awaiting confirmation from the more time-consuming tests, said the doctor who directed the study.

Life-saving IT network

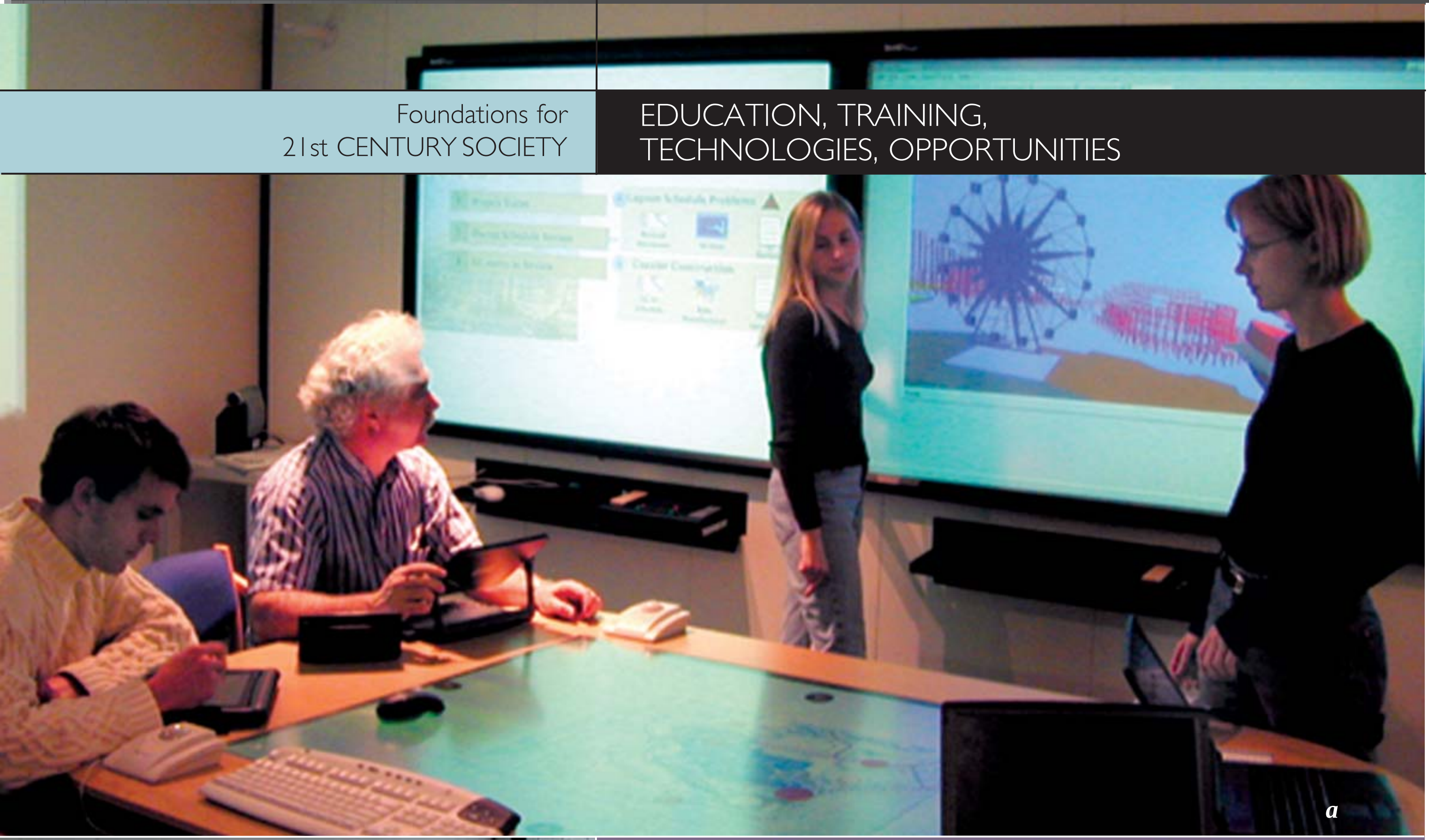
In 2002, 171 Americans were rescued in personal aircraft and marine emergencies through an IT-based international search-and-rescue alert network co-supported by NOAA, the Coast Guard, the Air Force, and NASA. The Cold War-era program, started in 1982 by the U.S., Canada, France, and Russia, now includes 36 countries and operates around the clock, relaying radio-beacon distress signals picked up by U.S. and Russian satellites and a network of ground computer stations to a central facility for location analysis and on to the nearest rescue teams. All told, the COSPAS-SARSAT system (see page 54 for acronym details) has rescued some 14,500 people worldwide, including 4,500 Americans. Following a request by NOAA to the Federal Communications Commission, as of July 1, 2003, outdoor adventurers anywhere in the continental U.S. are also authorized to carry 406-megahertz personal locator beacons (PLBs). Unlike personal aircraft and vessels, which are required to carry such equipment, citizens who want COSPAS-SARSAT protection on wilderness trips are urged to register their PLBs with NOAA to speed rescue operations if they are needed.

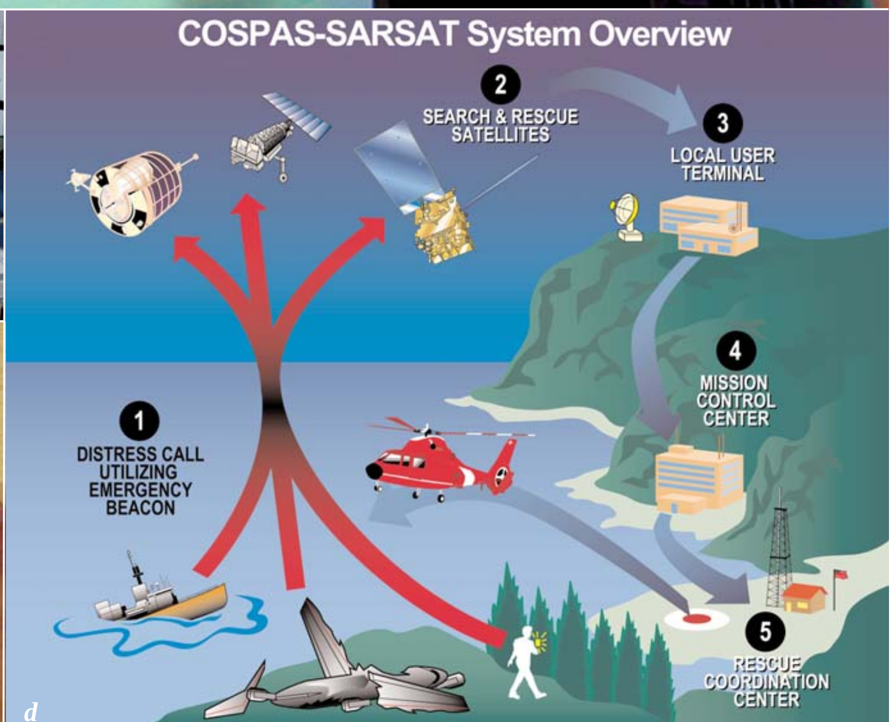
A father's software discovery

An 11-year-old New York girl named Jen, confined to her home by spinal muscular atrophy, a severe form of muscular dystrophy, now uses the family computer to communicate with friends, surf the Web, and connect to school lessons because her father came across some free software developed by DARPA- and NSF-supported

Foundations for 21st CENTURY SOCIETY

EDUCATION, TRAINING, TECHNOLOGIES, OPPORTUNITIES



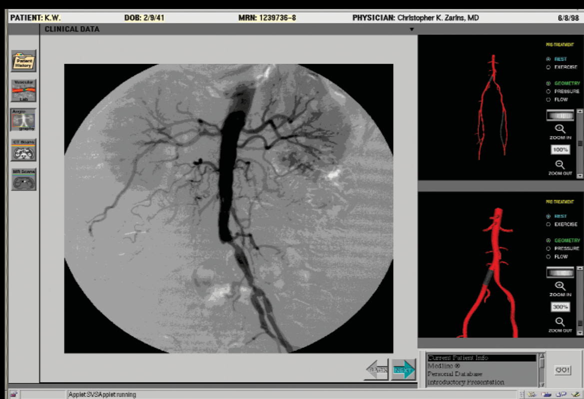


b) NSF's QuarkNet initiative with DOE brings high-school physics teachers and students to Fermi National Accelerator Laboratory (Fermilab). Last summer, Fermi scientists helped teachers build a cosmic ray detector.

c) NASA's new braille book about astronomy was evaluated by students at the Colorado School for the Blind.

d) Schematic shows operation of NOAA COSPAS-SARSAT international search-and-rescue network, which has saved thousands of lives.

a) Students of researcher Terry Winograd (second from left) test capabilities of interactive workspace called "iRoom" in NSF-funded project at Stanford University to investigate the future roles of advanced technologies in collaborative work.



e

f

researchers at Carnegie Mellon University. The two pieces of software, designed as part of a project looking at new uses for personal digital assistants (PDAs) in conjunction with desktop computers, are posted on the Web for any interested parties to "beta test." One turns a PDA into a remote keyboard and mouse; the other enables the user to create shortcut buttons on the PDA to automate computer processes. Jen, who has good fine motor control, finds the PDA's pencil stylus and touch-screen capabilities easy to use. As a result of her father's serendipitous discovery, the CMU team is working on ways to make the technology even more helpful to people with physical limitations.

Lights that talk

At Boston's Spaulding Rehabilitation Hospital, researchers funded by NIH and NSF have demonstrated a technology that uses the flickering of ordinary fluorescent lighting to transmit information to PDAs with photocells carried by patients, alerting them to appointments, room locations, and other useful in-patient details. The invention, which enabled even patients with traumatic brain injuries to navigate autonomously, won a 2002 R&D 100 Award and is being marketed by Talking Lights, LLC of Boston.

Next-generation microprocessors

A research team at DOE laboratories has transferred to the chip industry a microprocessor fabrication technology that is considered the next generation in chip-making, capable of producing processors tens of times faster than today's and memory chips with 40 times the storage capacity. The new lithographic technology uses extreme ultraviolet light (EUVL), which has 10 times shorter wavelengths than plain ultraviolet light (UVL). EUVL can etch a far greater number of features on each chip than is possible with current UVL techniques. The industry consortium that will further refine the prototype under a cooperative research and development agreement is headed by Intel and includes Advanced Micro Devices, IBM, Infineon, Micron Technologies, and Motorola. In February 2003, the DOE team was awarded the laboratories' Excellence in Technology Transfer award for its accomplishment.

***e)** NASA researchers work with Stanford Medical School cardiac specialists to apply agency fluid-dynamics modeling technologies to create innovative surgical planning tools that enable physicians to view and analyze patient blood flows and blockages.*

***f)** High-school students assemble an electronic logic board at Fermilab.*

E-gov: Streamlining services for citizens

Across the Federal government, new structures to improve citizen services and streamline operations are arising today from the foundations of IT R&D. Under the Administration's E-Government Strategy, agencies are moving rapidly toward two ambitious goals: quick, easy, and secure online access for citizens to government services and information, and a radical reduction in internally duplicative record-keeping, transactional, and information-processing systems through coordinated development of IT standards and procedures. (See http://www.egov.gov/.)

In April 2003, for example, DoD and the Department of Health and Human Services announced that they would adopt the framework of the highly regarded Veterans Administration (VA) electronic health-records system as a key step toward a secure national health information infrastructure. The VistA system (Veterans Health Information Systems and Technology Architecture), with its Enterprise Single Sign-On developed by NIST for the VA, is considered a leading example of a patient-centric, secure health-records infrastructure that improves care and reduces paperwork.

E-gov projects are also working toward IT-based simplification of Federal procurement, grant-making, and benefits systems. The NITRD Program is supporting E-gov technical activities to ensure universal citizen accessibility to services and to build state and local government and private-sector partnerships around the program's goals. In addition, NSF's Digital Government program supports a variety of technical R&D efforts to develop new technologies that expand public access to government services at all levels (http://www.diggov.org/).

In a grassroots collaborative project, digital archivists from NITRD agencies and others have created a highly visible symbol for a more user-oriented government – a new Web portal called science.gov that organizes in one place, by category and alphabetically, links to the national treasure of scientific and technical information in the online archives of 10 Federal science agencies (http://www.science.gov). Other FY 2003 E-gov developments include a free online Federal tax-filing system, used by several million people in its first season, and a Web portal called regulations.gov, through which citizens can access the texts of proposed rules and submit comments (http://www.regulations.gov).

NITRD support for human development

When minds can expand, new ideas – and inventions – flourish. For that reason, one ongoing focus of NITRD research is technologies to help all people enhance their individual capacities and skills. Assistive technologies and devices developed from NITRD-funded research in robotics, speech recognition, voice activation, multimodal interfaces, and wireless remote-control systems are making it possible for people of all ages with disabilities to participate more fully and independently in society.

NITRD research investments play a direct human-capital role in the national interest, underwriting the advanced education and training of tomorrow's top-level U.S. technological workforce and supporting the work of today's IT research leaders. NITRD agencies also support the Nation's main training programs to expand IT talent pools in such strategic fields as bioinformatics, cybersecurity, and advanced scientific computing.

The NITRD agencies actively champion innovation in science, mathematics, engineering, and technology education, encouraging use of their online archives for educational purposes and providing special Web sites with learning activities for children and young adults. NSF, unique among the agencies in its broad mission to advance U.S. research and education across the sciences, supports fundamental investigations of human cognitive development and innovative IT applications for education and training at every level. NASA's Learning Technologies Project develops advanced multimedia curricula for teachers to use to engage students in grades K-14 in the excitement of Earth and space sciences.

An emerging area of NITRD research sponsored by NSF – interdisciplinary studies of the social, economic, and workforce implications of IT – is developing baseline empirical findings and new knowledge that will help policymakers and citizens better evaluate and make informed decisions about IT applications in 21st century society. This work is exploring such topics as effects of new information technologies in work, education, commercial, and research environments; barriers to IT careers for women and minorities; intellectual property and information privacy issues; citizen participation in the digital society; and human values in technology design.

THE NITRD AGENCIES: RESEARCH DIRECTIONS

AHRQ – the Agency for Healthcare Research and Quality – focuses on research into state-of-the-art IT for use in health care applications such as computer-based patient records, clinical decision support systems, and standards for patient care data, information access, and telehealth.

DARPA – the Defense Advanced Research Projects Agency – is focused on future-generations computing, communications, and networking as well as embedded software and control technologies, and human use of information technologies in national defense applications such as battlefield awareness.

DOE/NNSA – the Department of Energy National Nuclear Security Administration, Advanced Simulation and Computing (ASCI) – was established to develop new means of assessing the performance of nuclear weapon systems, predict their safety and reliability, and certify their functionality through high-fidelity computer models and simulations.

DOE Office of Science is exploring, developing, and deploying computational and networking tools that enable researchers in the scientific disciplines to model, simulate, analyze, and predict complex physical, chemical, and biological phenomena important to DOE. The Office also provides support for the geographically distributed research teams and remote users of experimental facilities whose work is critical to DOE missions. FY 2004 is the fourth year of the Office's Scientific Discovery through Advanced Computing (SciDAC) initiative, which is focused on the next generation of scientific simulation and collaboration tools for the scientific areas that are the focus of DOE research.

EPA – the Environmental Protection Agency – has the IT research goal of facilitating multidisciplinary ecosystem modeling, risk assessment, and environmental decision making at the Federal, state, and local levels, and by other interested parties, through advanced use of computing and other information technologies.

NASA – the National Aeronautics and Space Administration – is extending U.S. technological leadership to benefit the U.S. aeronautics, Earth and space science, and spaceborne research communities.

NIH – the National Institutes of Health – is applying the power of computing, both to manage and analyze biomedical data and to model biological processes, in its goal to develop the basic knowledge for the understanding, diagnosis, treatment, and prevention of human disease.

NIST – the National Institute of Standards and Technology – is working with industry and with educational and government organizations to make IT systems more useable, secure, scalable, and interoperable; to apply IT in specialized areas such as manufacturing and biotechnology; and to encourage private-sector companies to accelerate development of IT innovations. It also conducts fundamental research that facilitates measurement, testing, and the adoption of industry standards.

NOAA – the National Oceanic and Atmospheric Administration – is an early adopter of emerging computing technologies for improved climate modeling and weather forecasting, and of emerging communications technologies for disseminating weather forecasts, warnings, and environmental information to users such as policymakers, emergency managers, industry, and the general public.

NSA – the National Security Agency – is addressing some of the most challenging problems in the country in computing, storage, communications, networking, and information assurance in order to help ensure our national security.

NSF – the National Science Foundation – supports basic research in all NITRD areas, incorporates IT advances in science and engineering applications, supports computing and networking infrastructure for research, and educates world-class scientists, engineers, and IT workforce.

ODDR&E – the Office of the Director, Defense Research & Engineering, Department of Defense – manages the University Research Initiative, which focuses on IT R&D for Department of Defense applications, research infrastructure, and science and engineering education.

Other Federal agencies participate in networking and information technology research and development, and coordinate with NITRD activities, using funds that are not budgeted under the program.

FY 2004 AGENCY RESEARCH PLANS BY PROGRAM COMPONENT AREA (PCA)

The long-term research agenda of the NITRD Program is embodied in agency activities designed to achieve critical agency mission goals. It is through steady year-by-year progress toward those goals that far-reaching advances emerge, as the early sections of this FY 2004 Blue Book attest. The following summary of agency FY 2004 research plans by PCA suggest current high-priority areas of investigation, such as R&D in high-end computing architectures, the Grid, middleware, cognitive systems, quantum technologies, modeling and simulation, visualization, networking (optical, wireless, mobile, adaptive, scalable, networked sensors, modeling and management, scalability), software in many dimensions (specification, engineering, testing, software for embedded systems, software-enabled control, cost issues), large scale digital libraries, the Web, speech and language translation, assistive technologies, collaboration technologies, assurance, dependability, robustness, security, standards, IT infrastructure for research, social and economic issues.

High End Computing Infrastructure and Applications (HEC I&A)

NSF: Terascale cyberinfrastructure; grid resource management; application of high-performance computing for science and engineering research

NIH: Creating models and visualizations for both basic and applied science sciences

NASA: Develop terrestrial information grid with numerous geographic locations containing resources including computing, networking, data, and instruments (both fixed and mobile) to solve problems of interest to the NASA aerospace, earth science, and space science enterprises

DOE Office of Science: Partnerships for terascale science

DOE/NNSA: Innovations in high-end systems architecture and software, and in visualization techniques to enable modeling and simulation for U.S. stockpile stewardship

NIST: Creating models and visualization for basic sciences (e.g., physics) and applications (e.g., building structure and material strength)

NOAA: Development and dissemination of modeling frameworks and tools for parallelizing geophysical fluid dynamics equations for the research and development of advanced weather and climate models and the resources to support these applications

EPA: Paradigms, techniques, and tools for modeling complex environmental phenomena – such as interactions of air, water, and soil – and for analyzing simulations' sensitivities and uncertainties

High End Computing Research and Development (HEC R&D)

NSF: Systems software, middleware, software environments, libraries, visualization, data management, and algorithms for heterogeneous distributed high-end systems; quantum and biological concepts

DARPA: High Productivity Computing Systems; polymorphous architectures; networked embedded sytems; biocomputational systems; cognitive computing systems

NASA: Simulated autonomous science exploration; collaborative science and engineering technologies; biomolecular probe for disease detection and astronaut health monitoring; Intelligent Vehicle Health Management system; advanced methods to assist in complex, distributed mishap investigation; prototype Concept Design and Risk Tool that identifies, tracks, and trades risks

NIH: Bioinformatics; computational biology; tools for determining 3-D molecular structures; visualization and analysis of images from instrumentation data

DOE Office of Science: Scalable mathematical algorithms and software infrastructure (operating systems, component technologies, optimal mathematical solvers) for terascale modeling and simulation applications

DOE/NNSA: Science and engineering innovations in high-speed computation and visualization to enable supercomputer modeling and simulation for U.S. nuclear stockpile stewardship

NSA: Collaborations with high-end systems manufacturers; operating system and programming language improvements; fundamental technologies for special-purpose devices (optical interconnects, power controls, cooling, switches, and design tools); computer memory interconnects performance; fundamental physics of quantum information systems

NOAA: Earth System Modeling Framework; improved climate and weather models via enhanced Modular Ocean Model, Flexible Modeling System, and Scalable Modeling System; high-performance scalable systems

NIST: Research in quantum computing, secure quantum communication, optimization and computational geometry, photonics, nanotechnologies, optoelectronics, and new chip designs and fabrication methods

ODDR&E: University-based research in novel information processing, including quantum communications and memory

Human-Computer Interaction and Information Management (HCI & IM)

NSF: Innovative IT applications for learning; stochastic models of human interaction with computing systems; interactive multimodal devices and assistive technologies; technologies for collaborative work; development of new online collections of scientific and educational resources; research in architectures, tools, and technologies for digital libraries; preservation of digital records; knowledge discovery, analysis, and visualization in multiscale, heterogeneous data sets; multilingual access to audio archives

DARPA: Rapid, two-way, natural language speech translation interfaces and platforms; rich, accurate, automatic speech-to-text transcription; multilingual detection, extraction, and summarization of information; augmented cognition

NIH: Modeling and simulation tools for exploring biomedical data; aggregatation and management of large-scale data resources for the medical community

NASA: Use neuro-engineering to develop and integrate technologies for task management, enhanced cognitive performance of teams; model knowledge use in context of work; develop "smart" software and autonomous devices; novel algorithms and software tools for extraction and visualization of very-large-scale, multisource data sets

DOE Office of Science: Integrated set of software tools for scientific collaboratory environments; research in software and infrastructure to manage very-large-scale data, instrumentation, and research results; integration of massive, heterogeneous data sets

NIST: Evaluation methods to measure relevance of content extraction; metrics, standards, and testing to advance technologies for access to and use of multimedia information; measuring performance of robotic and intelligent systems; pervasive computing and "smart spaces"; study of modes for effective human-robot communication

NOAA: Collaborative tools and information management techniques for distributed research and collaboration

ODDR&E: University-based research in computer-assisted tutorial systems; reasoning across data with diverse measures of uncertainty; representations of uncertainty for decision making

AHRQ: Information management to enable studies of health care and delivery system effectiveness; supports research in tools to enhance patient safety by reducing medical errors; funds studies of IT methods enabling providers to share information with patients; established and maintains both the National Guidelines Clearinghouse and the National Quality Measures Clearinghouse™ with detailed online information about health care metrics

EPA: Prototype tools to support evaluation of results from diverse environmental models

Large Scale Networking (LSN)

NSF: Support expansion of Extensible Terascale Facility providing high-end computing and networking infrastructure for colleges and universities; continue National Middleware Initiative to develop common enabling middleware and domain-specific cybertools for grid computing; fund development of discipline-based networks for collaboration; research in cybersecurity technologies

NIH: Distributed biology resources, knowledge management and discovery, training and education, telemedicine, re-engineering the clinical research enterprise

DARPA: Adaptive networking; network modeling and simulation

NASA: Distributed operation of advanced aerospace simulation; distributed access for computational modeling and simulation of the Earth's environment; networking for seamless access to ground, air, and space-based distributed computing, information, and knowledge

DOE Office of Science: Collaboration applications development, distributed applications environments, high-performance network facilities for science

NSA: Wide-area optical networking including optical transparency, dense wavelength division multiplexing (DWDM), physical-layer transmission impairments, and high data-rate signal encoding

NIST: Sensor interfacing and networking for interoperability and integration, cybersecurity, security and effectiveness of wireless and ad hoc networks

NOAA: Networking to support real-time access to environmental data and information; innovative data access including Web-based tools and agents; support for visualization and collaboration; network tools for crisis management

ODDR&E: Adaptive protocols for mobile wireless networks; scalable optical networking; and mobile wireless, scalable, peer-to-peer networking

AHRQ: Supports practice-based research networks of primary care physicians across the U.S. and an online medical journal of patient safety incidents including root cause analyses

Software Design and Productivity (SDP)

NSF: Empirical software engineering research; continuous change management of component-based software; profiles and patterns of software evolution; strategic software design to move from a risk-driven to a value-driven development model

DARPA: Model-based integration of embedded software; software-enabled control

NIH: Software investigations in support of biomedical computing applications

NSF/NASA: Cooperative program in Highly Dependable Computing and Communication Systems Research for projects to design, implement, test, evolve, and certify dependable, cost-effective software-based systems, using a new NASA testbed facility to evaluate research findings on real-world hardware and software artifacts

NASA: Automated software engineering methods, including technologies and tools for embedded and robotic devices; specification using Bayesian techniques; experimental evaluation of software

DOE/NNSA: Create common software development/execution environment for all Advanced Simulation and Computing (ASC, formerly ASCI) high-end platforms that supports end-to-end ASC application needs for robustness and scalability as well as I/O, storage, and visualization needs

NIST: Develop a common reporting format for sharing usability data with consumer organizations; determination of software quality using automated and knowledge-based methods; with industry partners, plan shared manufacturing business-to-business interoperability testbed; improve software engineering processes and the profession's development through international cooperation in defining its body of knowledge

NOAA: Develop a component-based modular research model of the geophysical environment

ODDR&E: University-based research in software model checking for embedded systems; real-time fault-tolerant network protocols

High Confidence Software and Systems (HCSS)

NSF: Innovative research in trustworthy computing, including scientific principles for construction of high-confidence systems, component technologies, composition and decomposition methods, modeling and analysis techniques, design tradeoffs between security and performance; safety, security, and privacy for Internet-enabled systems; real-time distributed, embedded, and hybrid systems; fault-tolerance approaches for critical infrastructure protection

DARPA: Self-regenerative systems (natural robustness through biological metaphors, self-rejuvenating software, scalable redundancy, diagnosis and healing, and probabilistic measurement and validation)

NIH: Assurance methods and technologies for life-critical medical devices and telemedicine applications; reliability, privacy, and security of medical data and IT infrastructures for research

NASA: Software design for safety, including development of High Dependability Software Consortium with leading universities and industry for improving methods and techniques to achieve very high reliability in mission-critical software; artificial intelligence and formal methods techniques for specification, automated fault detection, and validation

NSA: Research in secure network management, secure switched network technologies, and advanced research in cryptography (key management, algorithms); advanced research in high-confidence software and system technologies (formal specification, synthesis, and verification tools and techniques, domain-specific languages, reliability engineering, and functional programming); and continuing advanced research in securing end-user systems (security middleware such as the security-enhanced operating system LINUX kernel, Object Request Brokers)

NIST: Security technologies for critical infrastructure protection; standards, methods, and metrics in authorization and authentication, including biometric techniques; tools for NIST's advanced encryption standard; with NSA, support the National Information Assurance Partnership to promote cost-effective international standards for software evaluation, testing, and certification; conformance testing for adherence to standards

ODDR&E: University-based research on Decision Making under Information Uncertainty

Social, Economic, and Workforce Implications of IT and IT Workforce Development (SEW)

NSF: Support for fundamental research on the complex processes of adaptation and interchange between society and new information technologies, including studies of large-scale technologies for collaboration and information integration in research, education, and work; human values in IT design; impacts of IT on socio-technical systems such as markets, professions, and communities; human aspects of cybersecurity and system vulnerabilities; technologies and tools for independence throughout life; and computational approaches in the economic, social, and organizational sciences. Development and evaluation of IT applications in education and training; research on barriers to IT careers for women and minorities; multidisciplinary research opportunities for students

NIH: Support opportunities for IT training, especially in bioinformatics; individual and program grants for advanced IT R&D training for health professionals

NASA: Foster public-private collaborations to develop advanced technologies, such as interactive, virtual-presence, and immersive environments and interfaces to remote instruments, that integrate agency science and engineering capabilities to strengthen K-12 science and mathematics education in alignment with national education standards

DOE Office of Science: Computational Science Graduate Fellowship Program, a nationwide competitive program to train the next generation of leaders in computational science for DOE and the Nation

Agency NITRD Budgets by Program Component Area

FY 2003 Budget *Estimates* and FY 2004 Budget Requests (dollars in millions)

Agency	High End Computing Infrastructure and Applications (HEC I&A)	High End Computing Research and Development (HEC R&D)	Human Computer Interaction and Information Management (HCI & IM)	Large Scale Networking (LSN)	Software Design and Productivity (SDP)	High Confidence Software and Systems (HCSS)	Social, Economic, and Workforce (SEW)	Totals
NSF (2003) estimates	*211.7*	*76.0*	*128.8*	*109.0*	*53.4*	*63.8*	*65.9*	*708*
NSF (2004) requests	218.1	97.9	125.3	103.4	55.0	59.9	74.0	734
NIH	*77.1*	*37.8*	*93.1*	*128.8*	*6.8*	*3.7*	*12.1*	*359*
NIH	87.6	41.7	99.0	132.2	9.2	3.7	12..2	386
NASA	*35.2*	*26.0*	*40.8*	*12.6*	*55.8*	*34.7*	*4.2*	*209*
NASA[a]	45.9	34.6	67.1	28.9	59.2	24.2	6.7	267
DARPA		*109.8*	*42.9*	*17.6*	*58.6*	*3.2*		*232*
DARPA		108.5	78.4	18.2	13.3	4.0		222
DOE Office of Science	*98.4*	*37.3*	*16.2*	*28.7*			*3.5*	*184*
DOE Office of Science	88.9	51.3	16.4	30.0			3.5	190
AHRQ			*6.4*	*5.2*				*12*
AHRQ			32.0	25.0				57
NSA		*51.3*		*2.1*		*28.1*		*82*
NSA		21.3		1.9		28.1		51
NIST	*3.5*		*6.2*	*3.2*	*7.5*	*2.0*		*22*
NIST	3.5		6.2	3.2	7.5	2.0		22
NOAA	*13.5*	*1.8*	*0.5*	*2.8*	*1.5*			*20*
NOAA	13.5	1.8	0.5	2.8	1.5			20
EPA	*1.6*		*0.2*					*2*
EPA	1.6		0.2					2
ODDR&E		*3.6*	*2.0*	*4.7*	*1.0*	*0.7*		*12*
ODDR&E								
Subtotals	*441.0*	*343.6*	*337.1*	*314.6*	*184.6*	*136.2*	*85.6*	*1,843*
Subtotals	459.1	357.1	425.1	345.5	145.7	122.0	96.4	1,951
DOE/NNSA	*40.5*	*37.5*		*13.5*	*31.3*		*4.4*	*127*
DOE/NNSA	41.5	37.3		14.4	32.8		4.4	130
DISA						*6.1*		*6*
DISA			46.2	13.2		6.1		66
TOTALS[b]	*481.5*	*381.1*	*337.1*	*328.1*	*215.9*	*142.3*	*90.0*	*1,976*
TOTALS[b]	500.6	394.4	471.3	373.3	178.5	128.1	100.8	2,147

Notes:

[a] NASA FY 2004 budget reflects full cost

[b] These totals include discrepancies from what appears in the President's FY 2003 and FY 2004 budgets due to a combination of rounding and shifts in program estimates

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Participation in Federal NITRD Activities

The following are criteria developed by the multiagency IT research program that agencies considering participation can use to assess whether their research activities fit the NITRD profile.

NITRD Goals

Assure continued U.S. leadership in computing, information, and communications technologies to meet Federal goals and to support U.S. 21st century academic, industrial, and government interests

Accelerate deployment of advanced and experimental information technologies to maintain world leadership in science, engineering, and mathematics; improve the quality of life; promote long-term economic growth; increase lifelong learning; protect the environment; harness information technology; and enhance national security

Advance U.S. productivity and industrial competitiveness through long-term scientific and engineering research in computing, information, and communications technologies

Evaluation Criteria for Participation

Relevance of Contribution

The research must significantly contribute to the overall goals of the Federal Networking and Information Technology Research and Development (NITRD) Program and to the goals of one or more of the Program's seven Program Component Areas – High End Computing Infrastructure and Applications (HEC I&A), High End Computing Research and Development (HEC R&D), Human Computer Interaction and Information Management (HCI & IM), Large Scale Networking (LSN), Software Design and Productivity (SDP), High Confidence Software and Systems (HCSS), and Social, Economic, and Workforce Implications of Information Technology and Information Technology Workforce Development (SEW) – in order to enable the solution of applications problems that address agency mission needs and that place great demands on the technologies being developed by the Program.

Technical/Scientific Merit

The proposed agency program must be technically/scientifically sound and of high quality and must be the product of a documented technical/scientific planning and review process.

Readiness

A clear agency planning process must be evident, and the organization must have demonstrated capability to carry out the program.

Timeliness

The proposed work must be technically/scientifically timely for one or more of the Program Component Areas.

Linkages

The responsible organization must have established policies, programs, and activities promoting effective technical and scientific connections among government, industry, and academic sectors.

Costs

The identified resources must be adequate to conduct the proposed work, promote prospects for coordinated or joint funding, and address long-term resource implications.

Agency Approval

The proposed program or activity must have policy-level approval by the submitting agency.

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Image Credits and Technical Descriptions

Page ii

Wing scale of a Monarch butterfly. Image by Scott J. Robinson, Imaging Technology Group, Beckman Institute for Advanced Science and Technology, University of Illinois, Urbana-Champaign

Robinson comments: A wing scale is what makes a butterfly or moth feel slick when you handle it by the wings. Scales are tiny and fragile – they're easily dislodged from the wing. Being so loose, they are notoriously difficult to photograph, because they cannot easily be electrically grounded. They readily charge up with electrons, producing horizontal streaks, or worse, that can ruin an image. Even my image has some evidence of charging in it.

Single scales vary in size but can be about 180 microns (micrometers) long by 70 microns wide and maybe 15 or 20 microns thick. For comparison, a human red blood cell can be 8 to 14 microns across, and a rod-shaped bacterium is often 2 microns long. The image size is about 10.7 megabytes.

The microscope is a Philips/FEI environmental scanning electron microscope (SEM) with a field emission electron gun (XL30 ESEM-FEG). The ultra-high-definition option is something we've had for only a few months. It required a new high-end video card and software that allows us to collect images with many more lines per frame than previously possible – enabling us to enlarge images without making the scan lines visible to the viewer. With older SEMs, we used film, but the film had to be exposed, line by line, to the signal from a small high-definition TV monitor. Now we take digital images, without film and without the extra monitor, but we still have to depend on line-by-line assembly of the image.

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Visualizations by Chris Henze, NASA Advanced Supercomputing Division

Henze comments: The high-resolution GCM runs on a "half-degree" computational grid: The dimensions are 576 (east-west) x 361 (north-south) x 32 (up-down) = 6.65 million gridpoints. I'm plotting the dynamical variable "q," which is the specific humidity. This is the ratio of the mass of water vapor to the total mass of air in a parcel, and it varies from about 2 to 25 g/kg as you go from the poles to the equator. For the images, I integrated q in the vertical direction across all 32 model layers – that's the white swirly stuff. Note that the specific humidity is not the same as cloud cover – clouds are not directly resolved by large-scale models like this one. The continental background shows various surface and vegetation types provided by the GCM's "land surface model." The distinct light-gray area in the arctic regions, and north of Antarctica, is sea ice. I also calculated the gradient of the surface pressure and used this in a bump map to produce relief shading. This is largely obscured by q, but you can see shadows in high-gradient areas like the Andes.

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Simulations by Phil Smith, Rajesh Rawat, and James Bigler, Center for the Simulation of Accidental Fires and Explosions (C-SAFE). Images courtesy of the Scientific Computing and Imaging Institute at the University of Utah

The authors comment: These simulations of the spread of a fire in a 10-meter heptane pool were performed on a 300^3 uniform computational mesh, using sophisticated highly scalable radiation and turbulence models to show the temperatures from 250^3 and 300^3 data sets. From the simulation data generated by C-SAFE, the real-time ray tracer software can visualize multiple time steps of the fire using direct volume rendering. The time-dependent data are visualized using a flip book- style animation to show the progression of the fire. The simulations capture the fine vortical structures formed at the base of real large-scale fires and also the roll-up of vortices observed in real fires. [NOTE: Full-color versions of these images showing temperature variations in red, yellow, and gray are viewable in the Web gallery of the Scientific Computing and Imaging Institute at the University of Utah (http://www.sci.utah.edu/galleries_front.html).]

Pages 4-5

a) U.S. Air Force photo by Staff Sgt. Shane A. Cuomo

b) U.S. Air Force photo by Staff Sgt. Jeremy T. Lock

c) DoD photo by Chief James Krogman, U.S. Navy

d) U.S. Air Force photo by Master Sgt. Terry L. Blevins

e) U.S. Air Force photo by Tech Sgt. Richard Freeland

f) Image courtesy of Sea-Viewing Wide Field-of-View Sensor (SeaWIFS) Project, NASA/Goddard Space Flight Center, and ORBIMAGE

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a) Photo by Randy Montoya, DOE/SC

b) Image courtesy of U.S. EPA Scientific Visualization Center; research principal investigator Dr. Alan Huber

c) Image courtesy of IBM Business Consulting Services

d) Image by Christopher L. Barrett, National Infrastructure Simulation and Analysis Center

Pages 8-9

Visualization by Chris Henze, NASA Advanced Supercomputing Division

Henze comments: This image is from work I'm doing with Gwen Jacobs at Montana State University. The research area is neurobiology, or neuroinformatics, or neurophysiology, etc. We are investigating the cricket cercal sensory system, which works roughly as follows: On the hind end of the cricket (or any orthopteran) are two antenna-like structures called cerci. Each cercus is covered with approximately 1,000 fine hairs that are deflected by impinging air currents. Each hair is mechanically constrained to move in a plane, and when it does so a transducer at its base creates electrical signals in an associated sensory neuron. The axons from all the sensory neurons project in an orderly fashion into the abdomen of the cricket, where they form a three-dimensional "neural map," whose global excitation patterns correspond to global movement patterns of the entire ensemble of receptor hairs.

The neural map is "read" by interneurons, whose intricate dendritic arbors (input branches) form synapses (electrical connections) with the sensory neurons. There are far fewer interneurons than sensory cells, and many of them are "identified," which means they can be found reproducibly – with largely the same branching pattern – in any cricket. Each identified interneuron receives input from a substantial volume of the three-dimensional neural map, and by a computational process it converts this time-varying spatial pattern into a sequence of action potentials, or "spikes" – essentially a bitstream. These bitstreams can represent simple air movement parameters, such as direction or velocity, or they may represent complex features like vortices shed from the wings of an approaching predatory wasp. The processing and representation of information about the environment in terms of neural activity is the essence of "neural coding" and "neural computation."

The image shows an identified interneuron (named "10-2"). Gwen collected the geometric information ("morphometric data") for the identified interneurons by painstaking 3D microscopy. The 3D location and diameters of every branch point or place where the diameter changes (about 10,000 such segments here) are recorded. Here I've colored each segment by four stripes – red-black-white-black – partly for fun, but partly to visualize the extent of each segment. This is important because we are constructing electrical models of these cells, and the models' accuracy is dependent on the segment lengths.

Pages 10-11

a), b), c), d) NOAA Geophysical Fluid Dynamics Laboratory

e) Visualization by National Center for Supercomputing Applications; model and data by Carl Cerco, Environmental Laboratory, Engineer Research and Development Center, U.S. Army Corps of Engineers, in partnership with EPA Chesapeake Bay Project

f) Visualization by Emad Tajkhorshid, Peter Nollert, Morten O. Jensen, Larry J. W. Miercke, Joseph O'Connell, Robert M. Stroud, and Klaus Schulten, Theoretical and Computational Biophysics Group, Beckman Institute for Advanced Science and Technology, University of Illinois, Urbana-Champaign

Tajkhorshid explains: The image illustrates the results of computer simulation of a protein complex that forms channels in the membranes surrounding cells of bacteria, plants, and higher animals, including man. The simulation describes the protein complex (four identical proteins forming the complex) in a membrane made of 320 lipid molecules (bright red) immersed in more than 17,000 water molecules (blue). The system includes 106,000 atoms the motion of which has been calculated, dividing time into 5 million small steps. For each step the forces between all 106,000 atoms needed to be calculated. The computer simulations of these proteins, conducted at the NIH-funded Resource for Macromolecular Modeling and Bioinformatics, are a prime example of advances in biomedical computing. The computations not only for the first time simulated completely the transport of materials across the membranes of living cells in full detail, but also answered questions that had puzzled biomedical researchers for many years.

The simulated protein, called aquaporin, forms membrane water channels that can transport water efficiently across cell membranes. In the human body, more than ten different types of aquaporin have been found. These proteins play critical roles in control of water in various organs, and in kidneys conduct large volumes of water, concentrating urine through reabsorption of more than a bathtub (200-250 liters) of water every day. Impaired function of aquaporins is associated with several common diseases, such as diabetes insipidus and congenital cataracts. Although each single protein provides an independent conduit for water transport, water channels form tetramers (sets of four) in the membrane. These proteins are shown as rods of four different colors in the image.

The main puzzle was how aquaporins conduct water very quickly and in large amounts, but prevent any electrically charged molecules, in particularly protons, the smallest charged atom, from participating in the flow. If charges would move along, cells would loose their electrical potential that provides the energy fueling for many cellular processes. To prevent such discharging, the import and export of water needs to be very carefully screened against charges; the ensuing problem is what one witnesses at border crossings where careful screening necessarily leads to slow traffic. But somehow aquaporins manage screening against protons without any traffic delay.

The solution to the puzzle was revealed by a combination of observation and calculation, where calculation showed the key detail: The flow of water molecules through the channel was found to arise with water molecules streaming fast, but always in single file through a narrow channel, as shown in the figure for one of the four channels by highlighting water molecules (small blue elements in center). During their passage, the water molecules are forced to line up all in the same direction and rotate in the middle of the channel by 180 degrees before they continue their path. This orientation of the flowing molecules turned out to be the basis of an extremely strict selectivity that prevents the discharge of electrical charge through a proton current.

g) Simulation images by Gordon Kindlmann, courtesy of the Scientific Computing and Imaging Institute at the University of Utah

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a), b), c) Michael S. Warren, Los Alamos National Laboratory, DOE/SC

d) Image generated by Aleksander Stompel, courtesy of Visualization and Computer Graphics Group, Center for Image Processing and Integrated Computing (CIPIC), University of California, Davis

e) Image by Charbel Farhat, University of Colorado, Boulder

f) Simulation by John B. Bell and Phillip Colella, Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory, DOE/SC

g) Andreas Adelmann and Cristina Siegerist, Lawrence Berkeley National Laboratory, DOE/SC

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a) STAR Project, Brookhaven National Laboratory

b) Image courtesy of Michael W. Davidson, Florida State University

c) Image by Dr. Jiri Vondrasek, Macromolecular Crystallography Laboratory, National Cancer Institute. Courtesy of HIV Protease DataBase, NIH and NIST

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a) Visualization by David R. Nadeau and Erik Engquist, San Diego Supercomputer Center, University of California, San Diego. Data by Stuart Leavy and Bob Patterson. National Center for Supercomputing Applications, Urbana-Champaign; Ryan Wyatt, Clay Budin, Mordecai Mac Low, and Li, Norman, Heitsch, and Oishi, Hayden Planetarium, American Museum of Natural History, New York; Tom Abel, Pennsylvania State University, and John Hawley, University of Virginia

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Pages 18-19

a) Kenneth Downing and colleagues, Lawrence Berkeley National Laboratory, DOE/SC

b) NASA/Wilkinson Microwave Anisotropy Probe Science Team

c) Center for Extended Magnetohydrodynamic Modeling, DOE/SC

d) Perspective views of rat ventricular myocytes rendered by Alex DeCastro at the San Diego Supercomputer Center using NPACI Scalable Visualization Tools. The work is from John W. Adams, Amy L. Pagel, Christoper K. Means, Donna Oksenberg, Robert C. Armstrong, Joan Heller Brown, Department of Pharmacology, University of California, San Diego.

e) Image by Don Appleman, Imaging Technology Group, Beckman Institute for Advanced Science and Technology, University of Illinois, Urbana-Champaign (http://www.itg.uiuc.edu)

Appleman comments: The original image is black & white (gray scale), because it was made using a HiVac Environmental Scanning Electron Microscope (ESEM), which produces images with electrons rather than photons, and therefore does not capture color information. I later colorized the image.

"HiVac" refers to "high vacuum." The ESEM pumps the air out of the chamber that holds the sample so that air molecules will not interfere with the electron beam. The magnification was 13,199x. The reason the diatom is unidentified is that there are over 10,000 varieties of diatom. I can tell you that this is a "pennate" diatom, but as I am not a marine biologist, I cannot narrow it down further. The holes in the hard, outer silica shell of the diatom allow the soft internal parts of the diatom to contact the environment. When the diatom dies, the silica shell is left behind. That's what is shown here.

f) Image generated by Gunther Weber, courtesy of Visualization and Computer Graphics Group, Center for Image Processing and Integrated Computing (CIPIC), University of California, Davis

g) Image courtesy of Scientific Computing and Imaging Institute, University of Utah

Institute researchers comment: Visualization by means of a computer monitor is only the first step in presenting information to the viewer. Three-dimensional displays are one of the next steps and provide a much more realistic rendering of physical space. SCI Institute investigators seek to provide even more complete interaction with data by making use of additional sensory input and control mechanisms. Specific examples include the use of position and motion tracking devices, three-dimensional cursors, and "data gloves" that provide intuitive ways of merging the user and image spatial domains. We also employ "haptic" feedback devices that generate physical forces in the user's hands based on the material properties of the data sets under examination. The goal of this research is a complete immersion of the user into the data to provide more intuitive, efficient, and synergistic interaction than is possible with conventional visualization techniques.

By doing a good job with design and implementation, we hope to achieve bounded error interaction, where a single bound describes the combined system errors throughout the workspace. Ultimately, we want our system to be capable of quantifying the synergistic effects through user studies.

Our software architecture is an integration of custom components and commercial application program interfaces (APIs). The individual software components communicate via shared memory and UDP messages to the application process. The two custom software components are the Synergistic Data (SD) Library and the Virtual GL (VGL) Library. The SD Library provides visualization methods, haptic rendering methods, data set support, and interface widgets. The VGL Library provides the device and display management for virtual environment rendering. We currently use SensAble's GHOST API for basic PHANToM interface and NCSA's Vanilla Sound Server (VSS) for simple audio-reinforcement feedback.

Our very first demonstration using the prototype system was an analytic simulation of an electrostatic point charge field. We have two sources (red and green spheres) and one sink (blue sphere) in this field. In the image, a researcher explores the electrostatic point charge field on the Visual Haptic Workbench. Streamlines show the global structure of the field, colored by proximity to the charge sources (red and green spheres) and charge sink (blue sphere). A bounding box widget shows the extents of the data set. The streamspheres between the red and blue spheres are locally advected in both directions from the local interaction point, shown as a purple proxy widget and yellow force vector to the left of the PHANToM stylus.

h) Image by Chris Henze, NASA Advanced Supercomputing Division

Henze explains: "Virtual mechanosynthesis" (VMS) is a computational steering facility that couples an ongoing molecular dynamics simulation with a virtual-reality environment. The molecular dynamics part uses the "Brenner potential," which is an empirical reactive bond order force field specifically parameterized for hydrocarbons. The "reactive" part means you can make or break atomic bonds. The virtual-reality environment consists of a headtracked active stereo display (the glasses I'm wearing have high-speed shutters that alternately block one eye or the other – allowing different left and right eye views, with stereo disparity; the glasses also have a sensor – the wire appearing to come out of my ear – that relays my head position to the graphics engine so I can change the view appropriately), a six-degree of freedom handtracked input device (essentially a 3-D mouse, the wand in my left hand), and a haptic (force feedback) device (black device in my right hand). The total effect is that you can float around in 3-D and grab and rearrange atoms, and they respond "realistically." So you can try to build things and the molecular dynamics keep you honest – insofar as the dynamics are accurate, you should only be able to build physically plausible structures. This facility allows nanotechnologists to explore structures on an atomic scale, to rehearse and debug complicated assembly sequences, and in general to develop chemical intuition.

In this mock-up, I'm manipulating a piece of hydrogen-terminated graphite. The gray spheres represent carbon atoms, and the green spheres around the edge are hydrogens. I've just inserted the pink atom (another carbon, but colored pink because I'm hanging on to it) into the graphite sheet, creating a seven-membered ring (a septagonal defect) that gives rise to negative curvature (potato-chip, or saddle-like).

i) Image by Chris Henze, NASA Advanced Supercomputing Division

Henze comments: This is a visualization of quantum chemistry data. It is a portrayal of a water molecule. The surfaces are separation and attachment surfaces (precisely analogous to those in fluid flow fields) in the gradient field of the Laplacian of the electronic charge density. The black stripes are contour lines in the Laplacian field (clearly indicating that the surfaces are *not* isosurfaces). The green and red lines are streamlines showing the stable and unstable (respectively) manifolds of saddle points in the gradient field.

Following ideas of Richard Bader, we are trying to understand the electronic structure of matter by applying vector field topological techniques to the charge density of atoms and molecules. The Laplacian of the charge density is a measure of its curvature, or “lumpiness” – and its structure reveals a wealth of chemical behavior.

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Illustration by NASA Jet Propulsion Laboratory/Cornell/Daniel Maas/ Maas Digital LLC

Pages 22-23

a) Visualizations by David Feder and Peter Ketcham, NIST

b) Image by Paul Trombley, Center for Biologic Nanotechnology, University of Michigan

Nicholas W. Beeson, senior research associate in the NIH-supported work, comments: This image is a composite of several sources. The background green is a microscopic image of living cells stained with a fluorescent dye. Overlaying it are computer-generated models of the PAMAM dendrimer, which were used to guide our initial synthetic work three years ago. These models depict generations 3 to 5 of the dendrimer. Then our graphics artist overlaid these models with a highlighting semi-transparent sphere. The final image is an artist’s conception of how the nanodevice targets cancer cells.

We are currently testing a nanodevice in mice with cancer. This nanodevice recognizes cancer cells, enters them, and then delivers a chemotherapeutic agent (an anti-cancer drug). Since the anti-cancer drug never gets to any of the healthy cells, the systemic toxic effects of the drug are greatly reduced (the mice do not lose their hair). Since the anti-cancer drug is specifically delivered to cancer cells, the tumor is greatly reduced in size. The nanodevice work has progressed to the point where we are conducting our third set of animal trials. We are seeing a 100-fold improvement in therapeutic index. The therapeutic index is a combination of reduced toxicity and increased efficacy. In short, the mice receiving our nanodevice are not showing toxic effects, and their tumors are dying.

There is much testing yet to do, but we have in hand a real nanodevice that performs a biomedical function.

c) Image by J.C. Lee, Sungkyunkwan University, Suwon, Korea, courtesy of the Center for Microanalysis of Materials, Seitz Materials Research Laboratory, University of Illinois, Urbana-Champaign

Pages 24-25

a) U.S. Fish and Wildlife Service

b) Images by F. Spoor, University College, London, using Voxel-man

c) NASA Advanced Supercomputing, NASA Ames Research Center

d) Image courtesy of Montemagno Research Group/Cornell University

Pages 26-27

a) Image by Nissen, H., Damerow, P. and Englund, R. (1991) _Frühe Schrift und Techniken der Wirtschaftsverwaltung im alten Vorderen Orient : Informationsspeicherung und -verarbeitung vor 5000 Jahren_. Bad Salzdetfurth [Germany]: Franzbecker, pp. 92-93. Courtesy of Cuneiform Digital Library, University of California, Los Angeles

CDLI staff comments: This large tablet, known as Erlenmeyer 152, is an account of workmen from the Southern Mesopotamian city of Umma (modern Tell Jokha, Iraq), from the time of the Third Dynasty of Ur (ca. 2036 B.C.). A fuller description and translation of this text can be found in the electronic publication, Englund, R. “The Year: “Nissen returns joyous from a distant island”,” _Cuneiform Digital Library Journal_ 2003:1, §21 (http://cdli.ucla.edu/Pubs/CDLJ/2003/CDLJ2003_001.html).

b) Image courtesy of Digital Content Group, University of Wisconsin-Madison Libraries. Copyright 2000 © Board of Regents of the University of Wisconsin System

c) Image courtesy of Todd Library, Middle Tennessee State University

d) Image courtesy of Digital Collections and Archives, Tufts University

e) Image courtesy of the Coolidge Collection of Thomas Jefferson Manuscripts, Massachusetts Historical Society. The “Thomas Jefferson Papers: An Electronic Archive” project is supported by the Save America’s Treasures program established by Congress in 1999.

f) Image courtesy of the Hoagy Carmichael Collection, Indiana University Digital Library, Bloomington, Indiana. Project supported by the Federal Institute of Museum and Library Services.

g) Images courtesy of the Open Video Project, Interaction Design Laboratory, School of Information and Library Science, University of North Carolina at Chapel Hill

No Ordinary Table: Image courtesy of Large-Scale Structures Laboratory, University of Nevada, Reno

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a) North America Tapestry of Time and Terrain compiled by Kate E. Barton, David G. Howell, and José F. Vigil, U.S. Geological Survey, Department of the Interior

Vigil comments: The North America Tapestry of Time and Terrain is a product of the U.S. Geological Survey in the 2003 Geologic Investigation series (I-2781). The map was prepared in collaboration with the Geological Survey of Canada and the Mexican Consejo Recursos de Minerales.

This cartographic Tapestry is digitally woven from a geologic map and a shaded relief image. This digital combination reveals the geologic history of North America through the interrelation of rock type, topography, and time. Regional surface processes as well as continent-scale tectonic events are exposed in the three dimensions of space and the fourth dimension, geologic time.

The geologic map carries two types of information - the age of surface or near-surface bedrock and the type of rock. The topographic map started as a digital elevation model (DEM), a data file containing measurements (spaced at a 1-kilometer interval) of height of the land surface above sea level. From that we prepared the shaded relief map, produced using Spatial Analyst extension with HILLSHADE command in ArcGIS. Vertical exaggeration is 10x. The bedrock and relief maps were merged by computer to form the Tapestry.

The geology was generalized from the forthcoming Geologic Map of North America, compiled by John C. Reed (USGS) and John O. Wheeler (Geological Survey of Canada) for the Decade of North American Geology and sponsored by the Geological Society of America. Geologic map data were processed and reprojected in ArcINFO geographic information system (GIS) software. The shaded relief map, derived from a DEM contributed by EROS Data Center, provides the underlying cartographic structure. The two component maps were

Image Credits and Technical Descriptions, continued

georeferenced to one another using GIS software, and the final images were combined using graphics software. Scale: 1:8,000,000; Projection: Lambert Azimuthal Equal Area.

The colors on the main Tapestry represent different ages of the bedrock that makes up North America. For example, the various rocks that form the ancient Canadian Shield are shown in shades of red. For some areas, we do not know exactly when the rocks formed, but only a general range of likely ages. We have grouped these rocks of uncertain age into broad categories, so that instead of representing a brief geologic Period, they are assigned to an Era or combination of Eras.

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a) Satellite image courtesy of NASA Earth Science Enterprise

b) Photo by Randy Montoya, DOE/SC

c) Sandia National Laboratories, DOE/SC

Pages 32-33

a) Image courtesy of Interactivity Lab, Computer Science Department, Stanford University

b) Photo by Thomas Jordan, Fermi National Accelerator Laboratory Education Office, DOE/SC

c) Photo courtesy of NASA and Colorado School for the Deaf and the Blind, Colorado Springs, Colorado

d) COSPAS-SARSAT schematic courtesy of NOAA

[NOTE: Reflecting its Cold War origin, COSPAS stands for Cosmicheskaya Sistyema Poiska Avariynich Sudov (Space System for the Search of Vessels in Distress). SARSAT stands for Search and Rescue Satellite-Aided Tracking.]

e) Screenshot of ASPIRE software courtesy of Cardiovascular Biomechanics Research Laboratory, Division of Vascular Surgery, Stanford University

f) Photo by Pote Pothongusan, Cape Henry Collegiate School, Virginia Beach, Virginia

Abstract

The Federal agencies that participate in the Networking and Information Technology Research and Development (NITRD) Program coordinate their IT research activities both to support critical agency missions and to maintain U.S. leadership in advanced computing, networking, and information technologies. The NITRD Program's collaborative approach enables agencies to leverage strengths, avoid duplication, and increase the interoperability of research accomplishments to maximize the utility of Federal R&D investments. This Supplement to the President's FY 2004 Budget summarizes FY 2003 NITRD accomplishments and FY 2004 plans, as required by the High-Performance Computing Act of 1991.

The report highlights in particular the end results of NITRD research – innovative applications of information technologies in every sphere of the national interest, from national defense and homeland security to advanced scientific and engineering research, business and industry, education, and health care.

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Congress requires information concerning non-U.S. high-performance computing and communications funding activities. In FY 2003, DARPA was the only NITRD agency that entered into grants, contracts, cooperative agreements, or cooperative research and development agreements for information technology research and development with either 1) a company other than a company that is either incorporated or located in the U.S. and that has majority ownership by individuals who are citizens of the U.S., or 2) an educational institution or nonprofit institution located outside the U.S. DARPA funded an IT research-related award of $1.075 million to Cambridge University, Cambridge (UK). In FY 2003, no NITRD procurement exceeds $1 million for unmanufactured articles, materials, or supplies mined or produced outside the U.S., or for manufactured articles, materials, or supplies other than those manufactured in the U.S. substantially all from articles, materials, or supplies mined, produced, or manufactured in the U.S.

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