GRAND CHALLENGES: Science, Engineering, and Societal Advances Requiring Networking and Information Technology Research and Development

Interagency Working Group on Information Technology Research and Development

NOVEMBER 2003
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This definition is characteristic of humanity’s resolve to find solutions to challenges that go far beyond mere intellectual curiosity. It is embedded in humanity’s very nature to conquer new frontiers for social, economic, and political advancement. Information technology is an important element in conquering these frontiers.

Recognizing this role, the U.S. Government makes critical decisions about appropriate investments in IT R&D to help society forward both socially and economically. To inform that decision-making, in July of 2003, a group of leading Government technical program managers who participate in the Networking and Information Technology Research and Development (NITRD) Program completed their formulation of 16 illustrative science, engineering, and societal grand challenges. Addressing these grand challenges will require innovations in IT R&D.

The new NITRD illustrative grand challenges were formulated to stimulate current and future generations of NITRD and applications researchers. They are illustrative and not definitive or exhaustive because there are easily hundreds if not thousands of grand challenges that could be identified.

The NITRD illustrative grand challenges can be symbolically depicted as both a journey and a destination. The journey, which is likely to take more than a decade, is to a destination that lies far beyond current human understanding and capability. By describing these challenges, we intend to explain why IT R&D is important to society, justify why public investments in IT R&D are necessary and desirable, and galvanize the NITRD agencies and the IT R&D community to solve IT hard problems. Given the rapidly evolving nature of information technology, solutions to today’s grand challenges will fuel the grand challenges of tomorrow.

The NITRD Program’s illustrative grand challenges are:

Knowledge Environments for Science and Engineering
Clean Energy Production Through Improved Combustion
High Confidence Infrastructure Control Systems
Improved Patient Safety and Health Quality
Informed Strategic Planning for Long-Term Regional Climate Change
Nanoscale Science and Technology: Explore and Exploit the Behavior of Ensembles of Atoms and Molecules

“A Grand Challenge is a long-term science, engineering, or societal advance, whose realization requires innovative breakthroughs in information technology research and development (IT R&D) and which will help address our country’s priorities.”

—The 2003 NITRD Program Grand Challenge definition
Predicting Pathways and Health Effects of Pollutants

Real-Time Detection, Assessment, and Response to Natural or Man-Made Threats

Safer, More Secure, More Efficient, Higher-Capacity, Multi-Modal Transportation System

Anticipate Consequences of Universal Participation in a Digital Society

Collaborative Intelligence: Integrating Humans with Intelligent Technologies

Generating Insights From Information at Your Fingertips

Managing Knowledge-Intensive Dynamic Systems

Rapidly Acquiring Proficiency in Natural Languages

SimUniverse: Learning by Exploring Virtual Lifetime Tutor for All

This booklet provides an elaboration of each of the 16 illustrative NITRD grand challenges (henceforth referred to as grand challenges). They cover a wide spectrum of disciplines and sub-disciplines including education, the environment, health, the physical sciences, security, and transportation. For each grand challenge, there is a brief description, component challenges that require focus within the next decade, their relationship to national priorities, their potential benefits, IT hard problems that need solving in order to help realize the goals of the grand challenge, and indicators that will show that progress is being made in the intermediate term. These grand challenges are aligned with the missions of the NITRD agencies and address a vast array of broad societal goals.

The national priorities and the IT hard problems are the key pillars on which the grand challenges are structured:

- By describing the relationship between a grand challenge and national priorities, the grand challenge’s significance is connected to the highest aspirations of our country.

- The IT hard problems, whose solution the grand challenge requires, tie the grand challenge to core elements of information technology research and development and the NITRD Program.

These two sets of relationships are illustrated on pages 8 and 9.

Chapter 1 describes how and why these grand challenges were developed, chapter 2 explains the template used to describe the grand challenges, chapter 3 discusses the future of the grand challenges, and chapter 4 describes the grand challenges in detail.
1. INTRODUCTION

In November 2002, the Interagency Working Group on Information Technology Research and Development (IWG/IT R&D) of the National Science and Technology Council (NSTC), Executive Office of the President, established a Grand Challenges Task Force. The IWG/IT R&D, a body of leading Government experts who provide hands-on coordination of the multi-agency Networking and IT R&D (NITRD) Program, charged the Task Force with identifying a set of science, engineering, and societal challenges that will require innovations in IT R&D. The Task Force consisted of expert volunteers from ten NITRD agencies—AHRQ, DARPA, DOE/SC, EPA, NIH, NIST, NOAA, NSA, NSF, ODDR&E—plus FAA, OSTP, and the NCO/IT R&D (these acronyms are spelled out in Appendix 4).

1.1 CHARGE TO UPDATE THE HPCC GRAND CHALLENGES

The charge to formulate a set of NITRD grand challenges was specifically a call to update the list called for in the High-Performance Computing (HPC) Act of 1991 (PL. 102-192) that formally established the High Performance Computing and Communications (HPCC) Program. Through the HPCC Program, the U.S. Government coordinated multi-agency investments in developing and using high-performance computing systems and advanced networking technologies to meet the mission needs of the participating agencies and larger national goals. The Act’s objectives included to:

- Develop teraops (trillions of operations per second) computing systems
- Develop gigabit (billions of bits per second) networks
- Develop advanced algorithms and software
- Demonstrate innovative solutions to “grand challenge” problems using HPCC technologies

1.2 WHY HAVE NEW GRAND CHALLENGES?

Seven HPCC Program agencies identified 32 grand challenges (listed in Appendix 2). By the time of its formal conclusion in 1996, the HPCC Program had met both its programmatic and grand challenge objectives (see the HPCC Program’s FY 1996 annual report to Congress known as the Blue Book at http://www.nitrd.gov/pubs/blue96/).

The NITRD Program has succeeded the HPCC Program. The scope has been expanded to include all areas of information technology research and development, not just high-end computing and high-speed networking. This expansion has enabled the participating agencies to address a vastly broader range of information technologies and IT application challenges than in the HPCC Program and its grand challenges.

Recognizing that IT advances will enhance existing applications and enable new ones that can have an even greater impact on science, engineering, and society, the NITRD Grand Challenges Task Force developed a new definition of a grand challenge (found on page 2) and identified 16 illustrative grand challenges. These grand challenges are expected to yield significant breakthroughs of practical importance to mankind. As progress is made, these challenges can continuously evolve, be updated, and be replaced by new grand challenges.
2. CRITERIA AND TEMPLATE FOR FORMULATING THE NITRD ILLUSTRATIVE GRAND CHALLENGES

A set of criteria was established to guide the development of the grand challenges. These criteria are reflected in the template used in chapter 4 to describe the grand challenges and are explained below:

- Title
- Description of the Multi-Decade Grand Challenge
- Focus in the Next Ten Years
- Benefits
- Relationship to National Priorities
- Relationship to IT Hard Problem Areas
- Indications of Progress

2.1 TITLE

To stimulate multi-disciplinary thinking, the titles were crafted to reflect the Task Force’s goal that they challenge the intellectual aspirations of our country’s researchers beyond their understanding today or in the next decade. The list begins with physical science challenges in honor of their HPCC predecessors, followed by challenges that have strong human aspects. However, the list has not been prioritized by level of importance.

2.2 DESCRIPTION OF THE MULTI-DECADE GRAND CHALLENGE

The description articulates the challenge that the Task Force thinks is likely to be accomplished no sooner than ten years from now. However, given today’s normal rapid nature of technological advances and occasional serendipitous developments (such as the success of the Internet and the early success of the World Wide Web during the HPCC Program), these goals might be accomplished sooner. On the other hand, some of these grand challenges may not be accomplished even in half a century. Indeed, conceptual ideas similar to some of the NITRD grand challenges have already been subjects of decades of intensive research (natural languages is an example) and their descriptions here reflect advances that have been made to date.

2.3 FOCUS IN THE NEXT TEN YEARS

While keeping the longer-term grand challenge in perspective, certain aspects of the challenge have been identified for focused attention in the next ten years. Some of these focus areas were selected because they are particularly difficult and need to be tackled right away. For others, the knowledge and resources needed to address them are available today. Focus on these component challenges in the near term helps sustain focus on the longer-term grand challenge.

2.4 BENEFITS

The NITRD grand challenges can generate a vast array of social, economic, political, scientific, and technology benefits as their solutions are found. Common threads permeating these benefits include finding answers to complex questions that have long perplexed humanity, creating new disciplines of human inquiry and areas of multi-disciplinary collaboration, and developing and using new technologies.

2.5 RELATIONSHIP TO NATIONAL PRIORITIES

Working closely with officials at the White House Office of Science and Technology Policy (OSTP), the Task Force defined six
national priorities that reflect the country’s broad-based scientific, military, social, economic, and political values and goals. Each of the grand challenges strongly contributes to one or more of these national priorities:

- Leadership in Science and Technology
- Homeland and National Security
- Health and Environment
- Economic Prosperity
- A Well-Educated Populace
- A Vibrant Civil Society

While the NITRD grand challenges were structured within a national context, international collaborations and partnerships will be essential to successfully address many of the grand challenges, and all nations can benefit from the advances that are made.

Figure 1 (page 8) depicts relationships between the grand challenges and the national priorities. Each cell colored dark blue reflects an explicit relationship between a grand challenge and a national priority.

2.6 RELATIONSHIP TO IT HARD PROBLEM AREAS AND IT HARD PROBLEMS

IT hard problems areas are broad categories of topics of interest to the information technology research and development community and the NITRD Program. The Task Force identified 14 IT hard problem areas:

- Algorithms and Applications
- Complex Heterogeneous Systems
- Hardware Technologies
- High Confidence IT
- High-End Computing Systems
- Human Augmentation IT
- Information Management
- Intelligent Systems
- IT System Design
- IT Usability
- IT Workforce
- Management of IT
- Networks
- Software Technologies

Each grand challenge requires advances in several IT hard problem areas, as illustrated in Figure 2 (page 9). Each light blue cell indicates an explicit relationship between a grand challenge and an IT hard problem area.

For each IT hard problem area, the Task Force identified one or more illustrative IT hard problems (Appendix 1). Specific IT hard problems are identified in the write-up of each grand challenge. Progress towards the grand challenge will require breakthroughs or solutions to these IT hard problems. The IT hard problems are beyond our current understanding and capability, but intermediate progress toward accomplishing them will contribute to the grand challenge.

The IT hard problems span the breadth of the NITRD Program’s current investments. Given the fast moving nature of information technology R&D, the IT hard problems are likely to change over time, and the NITRD Program will evolve in response to these changes.

2.7 INDICATIONS OF PROGRESS

For a multi-decade activity such as a grand challenge, it is helpful to identify entities whose change over time indicates that progress is being made. These entities can be qualitative or quantitative in nature. Some of
the quantitative entities can nonetheless be difficult or impossible to measure (examples are reduced errors or reduced failures). Often the best, the most significant, or the most influential achievements are qualitative in nature, at least according to our current understanding. It could take decades to appreciate the impact of inventions or discoveries, for example. The indicators of progress for the NITRD grand challenges span this range.

3. FUTURE OF THE NITRD ILLUSTRATIVE GRAND CHALLENGES

The NITRD grand challenges are expected to change over time. Progress will be made. Goals will change. New challenges will emerge.

Twelve years have elapsed since the HPCC Program identified its grand challenges, and the NITRD Program or its successor may someday revisit its grand challenges with the intention of revising their definition and details.

In the meantime these grand challenges can guide technical program managers in NITRD agencies and policymakers in the Congress and the Executive Branch. They can serve as beacons for intellectual endeavors of current and future generations of students and researchers in universities and national and corporate laboratories across the country. Researchers wishing to reach beyond current limitations can build on the NITRD grand challenges in articulating their own visions.

The NITRD Program has a long history of collaboration and coordination across Federal agencies and with universities and corporations throughout the country, to which it attributes much of its success. Accomplishing the grand challenges’ goals is possible only by expanding these interactions.

Success in these grand challenges also requires international collaboration and cooperation, as illustrated by the following aspects of these grand challenges:

- Climate change, energy, human health, natural and man-made disasters, pollution, and transportation span national boundaries.
- Researchers, workers, teachers, and students live in different countries and/or speak different languages yet need to use unique scientific instruments or scientific data sets and need to communicate with each other both verbally and in writing. Some (emergency first responders and war fighters, for example) will also need to talk and listen to IT systems such as robots.
- The benefits of IT can be brought to remote areas both in the United States and around the world, and IT can be used to improve education, increase understanding of different cultures and societies, and build communities.
## FIGURE 1. RELATIONSHIPS BETWEEN THE ILLUSTRATIVE GRAND CHALLENGES AND THE NATIONAL PRIORITIES

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<tr>
<th>ILLUSTRATIVE GRAND CHALLENGES</th>
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FIGURE 2. RELATIONSHIPS BETWEEN THE ILLUSTRATIVE GRAND CHALLENGES AND THE IT HARD PROBLEM AREAS

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DETAILED DESCRIPTIONS OF THE NITRD ILLUSTRATIVE GRAND CHALLENGES
Description of the Multi-Decade Grand Challenge

- Organize and make broadly available distributed resources such as supercomputers, data archives, distant experimental facilities, and domain-specific research tools to enable new scientific discoveries and education across disciplines and geography

Focus in the Next Ten Years

- Understand the needs of scientists and how science is changing (for example, data sets are more complex and teams are more interdisciplinary)
- Increase access to computing systems, archives, instruments, and facilities
- Build on successful experiments:
  - Upper Atmospheric Research Collaboratory (UARC) and Space Physics and Aeronomy Research Collaboratory (SPARC)
  - Network for Earthquake Engineering Simulations (NEES)
  - Biomedical Informatics Research Network (BIRN)
  - National Virtual Observatory (NVO)

Benefits

- New discoveries across disciplines (for example, discoveries in one field can apply to other fields)
- Establish new fields of science and engineering

Relationship to National Priorities

- Leadership in Science and Technology
  - Help maintain U.S. leadership in a wide range of science, engineering, and technology disciplines
- National and Homeland Security
  - Safety and security will become increasingly dependent on advances in science and engineering
- Health and Environment
  - Improved water quality and human health
- A Well-Educated Populace
  - Boon to K-12, undergraduate, and graduate education
  - Boon to underdeveloped regions within the United States and around the world
- A Vibrant Civil Society
  - The social sciences and the humanities also use these environments (for example, museums make 3-D images of ancient artifacts)

IT Hard Problem Areas

- Algorithms and Applications
  - Modeling and simulation throughout science and engineering
- Complex Heterogeneous Systems
  - Control of science and engineering experiments
  - Embedded systems for science and engineering data collection and experiments
- Hardware Technologies
  - Mass storage technologies
  - Biological and nanoscale technologies applied to sensors
- High Confidence IT
  - Security
  - Reliability
  - Trust tools embedded in applications
  - Policy-enabled infrastructures (for example, protocols, policies, and mechanisms for sharing resources, and the embedding of scheduling in knowledge environments)

- High-End Computing Systems
  - HEC systems for applications that require computationally-intensive modeling and simulation

- Human Augmentation IT
  - Presence and awareness tools embedded in applications used in remote collaboration such as teleoperation

- Information Management
  - Creation and management of massive data and information repositories
  - Data analysis tools

- Intelligent Systems
  - Knowledge discovery in massive databases of archived knowledge

- IT System Design
  - Interoperability
  - Scalability of tools and environments as the number of users and sites increase

- IT Usability
  - Managing screen real estate to aid experimenters, data analyzers, and for chat facilities

- IT Workforce
  - Advanced IT for technicians

- Management of IT
  - Copyright restrictions to collecting and harvesting knowledge
  - Software and infrastructure standards

- Networks
  - Reliable, secure networks with differentiated services
  - Bandwidth for international collaborations

- Software Technologies
  - Software that recognizes different individual and group roles in science and engineering

Indications of Progress

- More users of distributed science and engineering environments
- More distributed science and engineering collaborations
- More scientists and engineers in remote parts of the country
- New tools and applications for more areas of science and engineering
- New science and engineering ideas and innovations
- Scientists and engineers achieve their goals more efficiently and effectively
- More “hands-on” science education in K-12 and undergraduate school
4.2 Clean Energy Production Through Improved Combustion

Description of the Multi-Decade Grand Challenge

- Improve the efficiency of the combustion of fossil fuels, which are the dominant source of energy in the United States
- Make our environment healthier by reducing greenhouse gas emissions

Focus in the Next Ten Years

- Optimize the design of combustion engines
- Improve catalysis—trapping of polluting gases produced by combustion engines—to minimize emissions
- Understand the impact of emissions on global climate

Benefits

- Improve the design of engines and turbines
- Reduce greenhouse gas build-up and global warming, which could result in rising ocean levels
- Improve human health by removing cancer-causing agents in by-products of combustion

Relationship to National Priorities

- Leadership in Science and Technology
  - Remain at the forefront in designing advanced simulation tools
  - Advance the science of combustion
  - Simulate an entire internal combustion engine
- National and Homeland Security
  - Reduce dependence on foreign oil
- Health and Environment
  - Reduce emissions of carbon and other pollutants
- Economic Prosperity
  - Fuel consumption has smaller demand on the economy
IT Hard Problem Areas

- Algorithms and Applications
  - Model the interactions of solids and gases, the moving boundary between them, and the changing geometries of an internal combustion engine
  - Incorporate complex nonlinear interactions of hundreds of chemical species in order to correctly predict pollutant production
  - Move from laboratory scale modeling (for example, table-top size engine burning pre-mixed fuel in a particular way with by-products measured by lasers) to modeling a diesel engine with complex geometry under less than laboratory-quality conditions, with 10 times more species and reactions, multiple time and space scales, and greater difficulty predicting soot and other by-products

- High-End Computing Systems
  - Research in high-performance computing systems architectures that support multiphysics applications with irregular memory access patterns

- Information Management
  - Coherent database of kinetic and thermo-chemical reactions developed from a large number of distributed sources of varying quality

- Management of IT
  - Sequester data in the general model from proprietary data that belong to different companies

Indications of Progress

- Accuracy of predictive models
- Technology transfer
- Increased fuel efficiency as tracked in CAFE standards
- Reduction in pollutant production
Description of the Multi-Decade Grand Challenge

- Ensure the continuous, safe operation of the Nation’s infrastructure systems such as the power grid, water supply, and transportation systems
- Protect against malicious attacks, physical failures, and complex cascading failures

Focus for the Next Ten Years

- Supervisory Control and Data Acquisition (SCADA) systems
- Transformation of legacy systems to capable, resilient IT-enabled infrastructures
- Coordinated decentralized supervisory control of new forms of distributed infrastructure such as air traffic control and transportation scheduling

Benefits

- Robust, survivable infrastructures that can provably withstand broad classes of malicious attacks and failures
- Higher capacity systems through refined management of safety margins
- Ability to isolate failures more easily, prevent widespread disruption, and reduce impact of failures

Relationship to National Priorities

- National Security
  - Information warfare
  - Military command, control, and communications
- Homeland Security
  - Critical infrastructure protection
- Economic Prosperity
  - Trustworthy infrastructure and energy independence
- A Vibrant Civil Society
  - Modern society requires reliable infrastructure
IT Hard Problem Areas

- Complex Heterogeneous Systems
  - Understand and balance simultaneous conflicting interacting requirements:
    - Tolerate failures (known as fault-tolerance)
    - Recover within time constraints
    - Maintain security while recovering from failures
  - Understand and control emergent (hard to predict) behavior in SCADA systems. Local interactions can lead to global-scale instability.

- High Confidence IT
  - Integrate security (authentication, access control, intrusion detection) into networked embedded systems where it has never existed
  - Establish a new paradigm of operating at acceptable levels through attacks. Shutting down to thwart attacks is not an option.

- Networks
  - Secure and survivable networks

Indications of Progress

- Decrease mean time to recovery (MTTR) to increase availability
- Fewer and smaller scale failures
### Description of the Multi-Decade Grand Challenge

- Improve patient care through safer evidence-based medicine and reduced medical errors
- Link patient information with medical knowledge to improve the decisions of health care providers and their patients

### Focus in the Next Ten Years

- Increase awareness of the magnitude of the problem of medical errors and potential solutions
- Establish uniform medical reporting requirements to enable analysis and feedback
- Collect and analyze medical error data to enable patient safety research
- Learn how to reduce errors in the health industry by studying other industries. For example, the airline industry requires pilots to report near misses.
- Educate the population about what questions to ask medical professionals

### Benefits

- Improved health care quality and patient recovery. For example, workers can go back to work more quickly and the elderly can live longer in their own homes
- A health care IT infrastructure that supports continuous improvements. Examples are bar-coded drugs, nursing use of time stamps, and use of radio frequency identification devices.
- Efficient use of health care resources
- Analysis system to monitor improvements while protecting confidentiality

### Relationship to National Priorities

- Health and Environment
  - Improved health of the American people and better use of resources
- Economic Prosperity
  - Improved quality of life

### IT Hard Problem Areas

- Algorithms and Applications
  - Modeling and simulation of medical errors
- High Confidence IT
  - Security and privacy for health information including authorization, authentication, biometrics, certification, encryption, and interfaces
- Human Augmentation IT
  - Scalable interoperable use of prompts, alerts, and reminders by doctors and patients
Information Management
• Data, information, and knowledge management to support evidence-based decision making
• Data mining and data warehousing to develop and enrich knowledge about patient safety

Intelligent Systems
• Human language technology such as common medical terminology to enable accurate communication and optimum decision making

IT System Design
• Interoperability of health information systems within hospitals, across providers, and among other stakeholders such as insurance companies, accreditation committees, and governments

IT Usability
• User interfaces that provide prompts, alerts, and reminders at the time and point of medical decision making
• Designs that vary for users of different skill levels and experience

Management of IT
• Public support for open source electronic health records to encourage innovative applications
• Economic, legal, policy, and social implications of the use of IT in patient safety

Networks
• Networking management, reliability, and scalability, to expand successful patient safety improvements nationally and internationally

Software Technologies
• Health information software requirements, engineering, and development
• Software reliability, performance, and quality assurance

Indications of Progress
• Reported medical errors first rise as reporting improves then fall in severity as more organizations systematically report errors
• Reduced mortality and illness due to medical errors
• New evidence-based tools for healthcare providers. For example, a clearinghouse for healthcare quality measures.
• Industry decisions about purchasing health care plans that incorporate patient safety research results
Description of the Multi-Decade Grand Challenge

- Provide decision makers with timely knowledge developed through comprehensive assessments of observations, models, and theories of the impacts of regional-level climate change to help them select the best adaptation and mitigation strategies.

Focus in the Next Ten Years

- Provide science-based information to inform the public debate about the effects of climate change and what to do about it.
- Reduce uncertainty in climate forecasts to enable common understanding and improve the prospects of consensus.
- Identify possible alternative futures and paths to those futures (global warming could cause ice to melt and ocean levels to rise and warrant reduced construction near ocean beaches).
- Improve decision-making in national and international arenas.
- Identify opportunities to manage the risks or mitigate the effects of climate change.

Benefits

- Improved long-term decision making based on predicted regional climate change.

Relationship to National Priorities

- Leadership in Science and Technology
  - Ability to predict climate change and evaluate alternative scenarios.
- Health and Environment
  - Viable health and climate.
- Economic Prosperity
  - Viable agriculture industry.
- A well-Educated Populace
  - Inform the public debate.

IT Hard Problem Areas

- Algorithms and Applications
  - Modeling of the environment including atmosphere, oceans, and biological systems under conditions of changing composition.
  - Scaling of algorithms, efficient parallelization, and communication among neighboring nodes.
- Hardware Technologies
  - Faster computers, access to results, and nanoscale data storage.
- High Confidence IT
  - Security.
  - Models that run for long periods of time on computers that do not crash.
High-End Computing Systems
- High-resolution regional climate models require massive computing power
- Access grids, data grids, and visualization grids for tighter coupling between the large distributed climate community and large but less distributed computing, storage, and visualization resources, and to enable regional models to access global climate data
- Ensembles may be run over grids

Human Augmentation IT
- Help humans “get their heads around” huge data sets

Information Management
- Access to and data warehousing, data mining, and knowledge management of multi-decade multi-disciplinary data sets

Intelligent Systems
- Automated ways of diagnosing and organizing data
- Assess data across multiple disciplines
- Multiple language access for the international arena

IT System Design
- Interoperability across diverse communities and diverse platforms
- Earth systems modeling framework portable to major architectures

IT Usability
- Interfaces that let users ranging from climate scientists to decision makers interact in ways that are natural to each group

IT Workforce
- Decision makers need to use advanced IT without becoming IT experts

Management of IT
- Database intellectual property issues
- Community moving toward open source due to small size of high-end computing market

Networks
- Sensor networks

Software Technologies
- Enable diverse community of researchers ranging from modelers to data managers to work together

Indications of Progress
- Accuracy of predictive models
- Technology transfer
- Broad agreement in national and international communities
- A viable economy in the 22nd century and beyond
4.6 **Nanoscale Science and Technology: Explore and Exploit the Behavior of Ensembles of Atoms and Molecules**

**Description of the Multi-Decade Grand Challenge**

- Predict what ensembles of atoms and molecules will do at the nanoscale
- Assemble ensembles of atoms and molecules into new devices

**Focus in the Next Ten Years**

- Simulate from first principles the fundamental behavior of ensembles of atoms and molecules
- Design and manufacture molecular scale devices
  - Apply physical properties to grow large quantities of self-organizing nanoscale materials by chemical reactions (examples are nanotubes and nanowires)
  - Fabricate these materials into useful devices
  - Detect and correct faults in nanoscale materials
- Nanoscale computers
  - Distributed control of processing elements in nanoscale computers—the many small unsophisticated elements will need to synchronize with each other directly rather than have a central clock
  - Understand and apply nanoscale signal transport to nanoscale computer I/O

**Benefits**

- A second Industrial Revolution

**Relationship to National Priorities**

- Leadership in Science and Technology
  - Ability to predict nanoscale behavior and manufacture reliable nanoscale devices
- National and Homeland Security
  - “Smart dust”—simple nanoscale sensors that blanket a battlefield to monitor movement of troops or pathogens and enable commanders to better plan attacks
- Health and Environment
  - New pharmaceutical drugs, new microbes for environmental remediation, etc.
- Economic Prosperity
  - New materials and devices with new magnetic properties, greater strength, etc.
IT Hard Problem Areas

- Algorithms and Applications
  - Modeling and simulation to understand the transition between nanoscale and microscale behavior, which will enable the application of novel emergent nanoscale behavior to devices with 1,000 to one million atoms

- Hardware Technologies
  - Nanoscale technologies
  - Denser storage

- High-End Computing Systems
  - Nanoscale technologies applied to high-end computing systems

- Human Augmentation IT
  - Materials to augment human capabilities (an example is clothing that camouflages by changing color)

- IT System Design
  - Continue to decrease component size

- Networks
  - Development of sensor networks

Indications of Progress

- Number of atoms in nano-object whose properties can be predicted
- Length of time that a nanoscale device can be simulated
- Density of storage media
- Development of designer materials and pharmaceuticals
4.7 **Predicting Pathways and Health Effects of Pollutants**

**Description of the Multi-Decade Grand Challenge**

- Better understand how pollutants are transported and transformed in the environment
- Predict how pollutants reach people and how they affect human health

**Focus in the Next Ten Years**

- Better understand the movement of pollutants across boundaries (for example, transfer through skin) and how pollutants are transformed in the body
- Better predict the response of genes, cells, organs, and people to pollutants

**Benefits**

- More efficiently and effectively identify and reduce health risks
- Quicker approval for use of safe new compounds
- Reduced need for laboratory animal testing

**Relationship to National Priorities**

- **Leadership in Science and Technology**
  - Advance scientific learning about health risks and develop technologies to address them
  - Help maintain U.S. leadership in genomics, toxicology, and environmental science

- **National and Homeland Security**
  - Better respond to disasters such as mass releases of dangerous chemicals

- **Health and Environment**
  - Reduced environmental health risks

- **Economic Prosperity**
  - Faster approval for materials determined to be of low rather than high risk (for example, a low-risk pesticide)

**IT Hard Problem Areas**

- **Algorithms and Applications**
  - Modeling and simulation of the environment, people, and their interactions
  - Communication between simulations of different scales such as pollutant effects in cells vs. organs

- **Complex Heterogeneous Systems**
  - Environmental sensors need IT advancements

- **High Confidence IT**
  - Protecting the privacy of human health data
High-End Computing
- Grid computing
- Make HEC systems more usable by making codes run more efficiently on different architectures

Human Augmentation IT
- Visualize modeling and simulation results to see patterns in complex datasets
- Better collaboration among people of different disciplines and in different locations

Information Management
- Holistic approach to different disciplines and their data (alternative is custom programming)
- Manage and store large data sets for long periods of time so that the data can be read decades from now
- Data mining to find new patterns or new information (for example, examine health and environmental data to identify risks of exposure to pollutants)

Intelligent Systems
- Generate and represent new knowledge to be shared and integrated across disciplines

IT Usability
- Human computer interfaces and interactions with data collection tools (such as gene chip arrays), the data they produce, and data analysis of complex data sets

IT Workforce
- Environmental scientists such as biologists need to use advanced IT without becoming IT experts
- Interdisciplinary interactions between IT specialists such as computer scientists and non-IT specialists who depend on IT such as biologists, chemists, ecologists, economists, and meteorologists

Networks
- Grid R&D to make distributed IT resources easily usable by non-specialists

Software Technologies
- Build systems of models (for example, chemical, environmental, skin, and inside the body) that interact in well-defined manners
- Model development by non-software engineers

Indications of Progress
- Reduced health risks
- Reduced cost and time to screen chemicals for harmful effects
- Better predictions of sub-populations that are sensitive to pollutants
Description of the Multi-Decade Grand Challenge

- Locate and assess the source and level of natural (earthquakes, hurricanes, etc.) or man-made (chemical, biological, and radiological hazards) threats, and respond rapidly to minimize loss of life and property

Focus in the Next Ten Years

- Heating, ventilation, and air conditioning (HVAC) and water systems able to identify and respond to meteorological, weather, chemical, biological, and radiological hazards
- Networks of semi-autonomous robots for hazard removal
- More accurate predictions of micro effects of natural and man-made threats

Benefits

- Increased safety and security of the environment with reduced susceptibility to threats
- Safety and security of public infrastructure and physical systems such as water supply, communications lines, air terminals, office buildings, etc.
- Safer technologies for hazard removal

Relationship to National Priorities

- National and Homeland Security
  - Minimize the impact of terrorists threats or attacks
- Health and the Environment
  - Safer environment
- Economic Prosperity
  - Better quality of life
  - Fewer disruptions with less impact on the economy
IT Hard Problem Areas

- **Algorithms and Applications**
  - Modeling and simulation for:
    - Threat assessment, location, and response
    - Predicting earthquakes, floods, tornados, etc.
    - Complex physical systems in real time (for example, airflow in an airport terminal)

- **Complex Heterogeneous Systems**
  - Heterogeneous sensors, networks, and computing systems
  - Distributed control of networks of autonomous and semi-autonomous robotic responders

- **High-End Computing**
  - Faster architectures for demanding modeling and simulation

- **Human Augmentation IT**
  - Collaboration and visualization technologies for responders

- **Information Management**
  - Asynchronous collecting and processing of large numbers of independent data streams

- **Intelligent Systems**
  - Reasoning, cooperating robotic responders

- **Networks**
  - Deploy, manage, and monitor large-scale dynamically reconfigurable networks of heterogeneous detectors
  - Fault-tolerant sensors and robots, enabling systems to survive and recover

Indications of Progress

- Network size and richness of topology
- Mean time to detection, location, and response
- Ability to model smaller-scale natural disasters (wind shear, for example)
Description of the Multi-Decade Grand Challenge

- Analyze long-term transportation needs and alternative solutions and their costs
- Design, construct, operate, and maintain an integrated multi-modal transportation system that is safer, more secure, more efficient, and has higher capacity than today

Focus in the Next Ten Years

- Facilitate commuter and traveler time, cost, and safety
- Analysis of long-term needs and costs (for example, compare the cost of building and maintaining subway systems to the cost of building and maintaining highway systems and highway vehicles)
- Intelligent vehicles that maintain safe distances
- Automated highway systems that increase capacity
- Intelligent passenger screening systems
- City-wide timing of traffic lights to enable higher capacity and fast, effective reaction to accidents
- Synchronized scheduling of public transportation systems (airplanes, trains, subways, and buses) so more people can get to their destinations faster

Airplanes controlled by pilots rather than air traffic control centers, to increase airspace and airport capacity
- Faster trains (bullet and magnetic levitation)
- Innovative transportation systems such as SegWay™, unmanned air vehicles (UAVs), and highly-automated personal air vehicles
- Integrate modes (for example, subways that go to train stations and airports with on-demand service)
- Standards for software-centric transportation systems to enable faster safety and security certification

Benefits

- Travelers save time and have increased flexibility in scheduling travel
- Governments expend fewer resources on building, maintaining, and securing our transportation systems
- Improved safety due to reliable and intelligent transportation system
- Lower insurance rates as the system becomes safer

Relationship to National Priorities

- Health and Environment
  - Minimize the impact of vehicle pollution on human health and the environment
  - Decrease consumption of gas and oil
- Economic Prosperity
  - Lower commercial and government cost of moving people and goods
  - More productive economy due to less time spent commuting and traveling
IT Hard Problem Areas

- Algorithms and Applications
  - Modeling and simulation of current and evolving transportation systems
  - Better optimization of transportation

- Complex Heterogeneous Systems
  - Sensors and actuators embedded in highway systems, vehicles, etc., to maintain safe distances between vehicles of different sizes and under various weather conditions

- High Confidence IT
  - Available, reliable, safe, secure air traffic, highway, railway, and shipping systems
  - Smart cards to authorize and authenticate transportation system personnel

- Information Management
  - Data mining of transportation system information for increased safety and security

- Intelligent Systems
  - Intelligent vehicles

- IT System Design
  - Integration of diverse transportation systems

- IT Usability
  - Address a vast range of operator and user needs

- Management of IT
  - Standards
  - Certification of systems and procedures

- Networks
  - Reliable, secure mobile networks
  - Faster, small, light-weight sensor networks

- Software Technologies
  - Software for developing and operating integrated transportation systems

Indications of Progress

- Reduced time and cost to validate and verify IT components of transportation systems
- Reduced time and cost to certify new technologies
- Reduced time and cost for system-level certification and accreditation
Description of the Multi-Decade Grand Challenge

- Conduct scientific experiments to understand the broad politico-socio-economic-technical impact of increased human use of constantly changing digital technologies. These experiments can address questions such as:
  - What is the impact on people who are left out?
  - Should digital participation be universal?
  - What kind of technologies should be deployed?
  - Does digital information work everywhere?
  - What are the public policy implications?

Focus in the Next Ten Years

- Longitudinal studies of socio-technical transformation such as at Blacksburg (Virginia) Village
- Map global social transformation (such as in homes, educational institutions, communities, and from e-business)
- Understand intended and unintended consequences of a digital society

Benefits

- Potential for all to participate
- Better predict human behavior in a digital society and intended and unintended consequences
- Maximize intended consequences such as enhanced economic productivity, and better, faster innovation and knowledge creation
- Minimize unintended consequences such as the digital divide and personal identity theft
- Optimize societal transformations

Relationship to National Priorities

- Leadership in Science and Technology
  - Broader participation in science and technology
- National and Homeland Security
  - Strong social networks to enhance trust and security
- Health and Environment
  - New knowledge about healthcare
- Economic Prosperity
  - Productive industries, e-commerce, skilled workforce
- A Well-Educated Populace
  - More people can use IT in their learning
  - More on-line learning institutions
- A Vibrant Civil Society
  - Tight communities with strong social networks
  - On-line voting
**IT Hard Problem Areas**

- **Algorithms and Applications**
  - Model digital societies and transformations

- **Complex Heterogeneous Systems**
  - Complexity and emergent behavior may be similar in IT and social systems

- **High Confidence IT**
  - Security, privacy, and trust

- **High-End Computing Systems**
  - Universal participation will be over the grid

- **Human Augmentation IT**
  - Increase human sensory bandwidth, for example by equipping into the ears of the blind to take in what eyes do

- **Information Management**
  - Research in domains such as digital libraries and museums is central

- **Intelligent Systems**
  - Better care for more of the elderly through a wide variety of remote intelligent technologies (for example, smart homes and computers that talk)

- **IT System Design**
  - Society will in part drive IT evolution and the IT evolution will change society

- **IT Usability**
  - Technologies to enable universal participation

- **IT Workforce**
  - Workforce skilled in analyzing sociological impact of the transition to a digital society

- **Management of IT**
  - Open source to help fulfill needs
  - Intellectual property and copyright issues

- **Networks**
  - Mobile networks to enhance universal participation
  - Last mile problem
  - Planning that acknowledges that the fabric of civil society and the fabric of the IT infrastructure are intertwined

- **Software Technologies**
  - New programming methods that let programmers design for properties such as privacy or surveillance
  - A science of software that obeys Moore’s Law, which states that computing performance roughly doubles every 18 months while chip size, power, etc., remain constant
  - Composability of software modules developed by different organizations

**Indications of Progress**

- Better anticipate consequences
- Better understand how unintended consequences emerge and develop remediation strategies
Description of the Multi-Decade Grand Challenge

- Understand how people, (software) agents, robots, and sensors (PARS) contribute to a collaboration
- Understand the structural complexity of PARS collaborations (for example, teams, networks, or hierarchies into which the PARS components can self-organize)
- Design architectures in which PARS components self-organize for optimal concerted social/physical/technological actions useful to society (for example, manage a crisis, perform surgery, or teach children)

Focus in the Next Ten Years

- Distributed intelligence
- Knowledge representation, management, fusion, and synthesis
- Science of coordination (for example, centralized versus decentralized organization) and division of labor
- Science of collaboration
- Mixed human-computer initiative with adjustable autonomy. (For example, either a person or a robot can start an action, but who is the decision maker? How does one override the other? If a robot detects life-threatening information, how does it alert the human to flee?)
- Understand and interpret implicit signals. (Computers have been explicit but humans have affects (emotions) that they reveal in facial expressions or tone of voice, for example. How do agents and robots read these affects, and how do they respond differently when conveying commands, suggestions, hints, or urgency?)
- Empirical experiments (for example, how humans and robots interact in a crisis or disaster)

Benefits

- Ability to rapidly convene coalitions to respond to crises or massive failures of systems such as the electrical power grid
- Smart homes, hospitals, highways, classrooms, schools, etc.
- Remote health care monitoring and care delivery
- Dramatic increase in productivity of the service economy
- Manufacturing at the intersection of mass production (making it cheaper, thereby benefiting the manufacturer) and customization (benefiting the consumer)

Relationship to National Priorities

- Leadership in Science and Technology
  - Distributed entities on the Internet or the grid organized to collaborate (for example, robots in Antarctica)
- National Security
  - War fighters and information technologies coordinate and collaborate
- Health and Environment
  - Health infrastructure (for example, fill prescriptions online)
  - Telemedicine (sensors in homes, hospitals, diagnostic sensors, etc.)
  - Smart aids for the elderly
- Economic Prosperity
  - Increase productivity along value chain of manufacturers and service providers
A Well-Educated Populace
- Pedagogical agents for individual students or student teams
- Collaborative learning environments
- Lifelong learning
- Integrated research and education
- Teachers and students remotely control instruments such as advanced telescopes and microscopes

A Vibrant Civil Society
- Distributed communities with common interests

IT Hard Problem Areas
- Algorithms and Applications
  - Model interactions between humans and intelligent technologies
- Complex Heterogeneous Systems
  - Implement interactions and decision making among people, agents, robots, and sensors
  - Control of interactions with physical systems
- High Confidence IT
  - Data and information security
- Human Augmentation IT
  - Augment human cognition and augment reality with input from agents, robots, and sensors
  - Collaboration environments and tools
- Information Management
  - Knowledge management for distributed intelligence
  - Natural languages for communication between humans and intelligent technologies
- Intelligent Systems
  - Cognitive systems aware of context and human affects
- IT System Design
  - Self-organizing architectures
  - Interoperability
- IT Usability
  - User interfaces developed from knowledge of human behavior and human interaction with agents, robots, and sensors
- IT Workforce
  - Train non-IT specialists to work with agents, robots, and sensors
- Management of IT
  - May need open source if humans and robots write different software components
- Networks
  - Mobile networks (such as for crises or disasters)
  - Reconfigurable networking to support ad-hoc alliances
  - Reliability and scalability
- Software Technologies
  - May need new programming languages

Indications of Progress
- Time savings
- Improved outcomes
- Better, faster scientific discovery
- Achieve goals of larger scale in selected domains than are possible today
Description of the Multi-Decade Grand Challenge

- Rapidly and spontaneously retrieve accurate insights:
  - Locate information from multiple text sources, archived databases, image archives, and sensor streams for a person or team solving a problem
  - Identify and organize connections between disparate pieces of information
  - Validate or refute hypotheses and overcome human biases about hypotheses

Focus in the Next Ten Years

- Automate the collection of metadata, which are data about data (for example, description of fields in a database and how the data were collected and processed) as the data are collected
- Develop taxonomies (classification in an ordered system to indicate relationships)\(^1\) for information in different forms (text, images, video, time series, etc.)

Benefits

- More rapid decision making
- Greater accuracy due to using multiple sources and points of view
- Faster progress in science through understanding the implications of individual findings and linking findings together
- More national and international interdisciplinary cooperation and discovery (for example, globally connect people who generated related results, identify researchers in similar fields)

Relationship to National Priorities

- Leadership in Science and Technology
  - More rapid scientific discovery across disciplines
- National and Homeland Security
  - Better insights into crises as they happen
  - Assessment of intelligence data
- Health and the Environment
  - Integrate public health data
  - Understand the ecosystem
- Economic Prosperity
  - New products and processes and more efficient supply chains due to understanding and analyzing information more efficiently
  - Making good information more readily available is essential to today’s Information Economy

IT Hard Problem Areas

- Complex Heterogeneous Systems
  - Rapidly collect, analyze, and draw conclusions about information from multiple sources such as SCADA systems and networks of sensors

- High Confidence IT
  - Confidentiality of proprietary information

- Information Management
  - Comprehensive ability to find and analyze information on disparate topics, from disparate sources, and of varying quality
  - Preservation of metadata

- Intelligent Systems
  - Automated tools that either start with an initial hypothesis and look for supporting evidence or look for alternative hypotheses and find data and information to support or refute such hypotheses
  - Automated tools to analyze information and identify causal relationships
  - Analyze and present information in multiple languages

- IT Usability
  - Interact with a wide variety of users who have a wide variety of inquiries and presentation preferences

- Networks
  - Ad-hoc networking
  - Sensornets

Indications of Progress

- Standard information retrieval metrics such as precision (the proportion of retrieved items that are relevant) and recall (the proportion of relevant items that are retrieved)

- Time to perform a task

- Ability to understand something better

- Industry interest in adopting these technologies to improve productivity
Description of the Multi-Decade Grand Challenge

- Establish management practices that enable knowledge-intensive organizations to use structured global collections of knowledge to make complex decisions that result in rapid reconfiguration of processes, and rescheduling and redeployment of resources, to respond quickly to changing circumstances.

- Maintain stability and achieve peak performance in knowledge-intensive organizations characterized by uncertainty and constant change.

Focus in the Next Ten Years

- Simulate knowledge-intensive environments involving hundreds of complex interacting agents.

- Validate simulations with real organizational data (for example, instrument parts of organizations to see if theory underlying simulations holds true).

- Develop and evaluate new real-time information systems for knowledge-intensive environments.

- Catalogue lessons learned to identify best practices for managing dynamic environments.

Benefits

- Organizations function more smoothly.

- Best use of resources.

- Peak performance during times of constant change.

Relationship to National Priorities

- National and Homeland Security
  - Reengineer intelligence agencies to handle uncertainty and change.

- Health and Environment
  - Help hospitals better respond to emergencies.

- Economic Prosperity
  - Increase organizational productivity.

IT Hard Problem Areas

- Algorithms and Applications
  - Model change in knowledge-intensive environments.

- Complex Heterogeneous Systems
  - Rapid reconfiguration and rescheduling of human and machine resources.
  - Information sharing and distributed decision-making in organizational hierarchies.
- High Confidence IT
  - Intelligence agencies need data and information to be stored in a secure fashion, retrieved in a timely manner, and transported safely and correctly.

- High-End Computing Systems
  - Intelligence agencies have some of the most demanding knowledge-management needs, which require high-end computing.

- Human Augmentation IT
  - Improve complex decision making through augmented cognition and augmented reality, collaboration, and visualization of large knowledge collections

- Information Management
  - Scalable distributed processing and storage

- Intelligent Systems
  - Collaborative knowledge discovery, retrieval, representation, and integration to make inferences
  - How do we best gather, represent, and share knowledge about sources, designs, scheduling, customer profiles, process status, energy, and geo-politics?

- IT System Design
  - Maintain system stability and predictability when everything is in flux
  - Best mechanisms for negotiating protocols (plug-and-play is still a dream)

- IT Usability
  - User interfaces for displaying complex structured knowledge

- IT Workforce
  - Understand workflow rules (which may be hidden)

- Management of IT
  - Intellectual property issues
  - Open source issues

- Networks
  - Reconfigure networks (people everywhere need access to networked devices on the fly)

- Software Technologies
  - This new area may require new software languages, etc.

Indications of Progress
- Improved decision making
- Meet deadlines
- Integrate and balance change and stability
- Quicker reaction times
4.14 Rapidly Acquiring Proficiency in Natural Languages

Description of the Multi-Decade Grand Challenge

- Develop computational models of how people acquire language
  - Use acquisition modeling, along with empirical data, to understand first language acquisition by children and later acquisition of other languages
  - Use acquisition modeling to advance understanding of the structure of languages and how they relate to human cognitive processes

- Use best models of acquisition to develop tools
  - Use acquisition models to develop courses and computerized tutoring systems for language learning
  - Apply knowledge from acquisition models to develop advanced machine translation and automated language information extraction

Focus for the Next Ten Years

- Develop and test partial models of language acquisition phenomena

- Merge partial models into a unified model of language acquisition

- Experiment with different learning models (such as reinforcement, evolutionary, clustering, and supervised) to develop an overall natural language learning model

Benefits

- Better understanding of how people learn languages and similar skills

- Better ways of teaching—both automatically and via individualized human instruction

- Systems to help immigrants acquire English proficiency

Relationship to National Priorities

- Leadership in Science and Technology
  - Maintain U.S. leadership in linguistics, cognitive psychology, and artificial intelligence

- National and Homeland Security
  - Translation devices, language data mining, language training, intelligence gathering

- A Well-Educated Populace
  - Use both a first language and later languages more effectively

- A Vibrant Civil Society
  - Better human language communication
IT Hard Problem Areas

- **Algorithms and Applications**
  - Model how languages link to knowledge and model learning of languages

- **Complex Heterogeneous Systems**
  - Robots respond to natural language input
  - Multi-language systems

- **Human Augmentation IT**
  - Assist people who have learning disabilities or linguistic handicaps
  - Assist people with problems in acquiring non-native languages

- **Information Management**
  - Create and manage large corpora of latitudinal language learning data for testing acquisition models

- **Intelligent Systems**
  - Sharpen knowledge of machine learning and how different types of machine learning can be combined to learn languages
  - Convert large unstructured human language databases to structured databases (for example, to enable successful searching)

- **IT Usability**
  - Computer interfaces that adapt to user input

Indications of Progress

- Models that show how the human world view is structured by language and how language structures world view

- Better model-based systems for teaching languages

- Improvements in information extraction from natural language data

- Databases that track facts (what, why, how, when, where, who?)

- Industry uptake of language acquisition models and the language models they imply
Description of the Multi-Decade Grand Challenge

- Learn about our world and beyond by exploring what happens in interoperable plug-and-play learning modules that simulate various aspects of the universe
  - Modules have various levels of expertise and assume various levels of user knowledge
  - Can be used by people of all ages and expertise

Focus in the Next Ten Years

- Initial modules for biological systems (for example, blood or digestive system), weather, and planetary system
- Modules for grade school through graduate school and for lifelong learning

Benefits

- More effective learning environment
- Inexpensive resources available to all learning institutions
- Evens out the education system across the country

Relationship to National Priorities

- Leadership in Science and Technology
  - Train the next generation of researchers and workforce
- Health and Environment
  - Simulation helps people better understand the effects of disease and the effects of pollutants in the environment
- Economic Prosperity
  - A better educated citizenry contributes more to society
- A Well-Educated Populace
  - All of society benefits from educated citizens

IT Hard Problem Areas

- Algorithms and Applications
  - Simulation of all systems in the universe
- Human Augmentation IT
  - Visualizations of simulations
- IT System Design
  - Robust self-evolving, self-maintaining, interoperable modules
- IT Usability
  - Interfaces for different levels of expertise
  - Maximize the time spent interacting with content, not with the interface
- Software Technologies
  - End user programming so that non-professional users can create their own simulations and modules

Indications of Progress

- Number of modules contributed to SimUniverse
- Number of SimUniverse users
- Improved standardized test scores
- Increased number of masters degrees and PhDs in science and technology
- New scientific discoveries
- Increased quality in scholarly papers
Description of the Multi-Decade Grand Challenge

- A personal tutor that understands what a user knows and does not know, provides just-in-time tutoring as needed, adapts to a user’s learning style and knowledge level, and is initiated by either the user or the tutor

Focus in the Next Ten Years

- Employ a model of the user (strengths, weaknesses, preferred learning methods) and machine learning to tailor a general-purpose tutor for a variety of knowledge domains and expertise that can adapt to the user’s capabilities and learning needs from birth

- Identify and begin work on topics such as:
  - Practical how-to training for the workforce. For example, computer skills for novices to experienced users, learning new software languages by building on languages one already knows, or a refresher to maintain skills.
  - Foreign languages. For example, develop a tutor that can teach Spanish to people ranging in age from 3 to 103.

Benefits

- A better educated populace
- Customized learning environments at lower cost

Relationship to National Priorities

- Economic Prosperity
  - Just-in-time training
- A Well-Educated Populace
  - Better educated workforce
- A Vibrant Civil Society
  - All of society benefits from educated citizens

IT Hard Problem Areas

- Algorithms and Applications
  - User modeling
- Human Augmentation IT
  - Context-aware information delivery
- Information Management
  - Adding in new content modules
- Intelligent Systems
  - Understand human cognition
  - Human language technology
- IT System Design
  - Evolve the tutor to new platforms with little user involvement
- IT Usability
  - Adaptable user interfaces for different levels of user expertise

Indications of Progress

- Improved productivity
- Increased participation in community activities
- Increased understanding of other cultures and societies
- Increased return on investment for education funding
APPENDIX 1: ILLUSTRATIVE IT HARD PROBLEMS CATEGORIZED BY IT HARD PROBLEM AREAS

For each IT hard problem area, the Grand Challenges Task Force identified one or more illustrative IT hard problems. Progress toward the grand challenges will require breakthroughs or solutions to these IT hard problems. Specific examples are given in the description of the grand challenges in chapter 4.

Algorithms and Applications
- Modeling and simulation

Complex Heterogeneous Systems
- Adaptive scheduling and control
- Complex systems/emergent behavior
- Control of physical systems including scientific experiments and SCADA systems
- Distributed decision making
- Embedded systems including actuators, sensors, and MEMS
- Robotics

Hardware Technologies
- Biological technologies
- Nanoscale technologies
- New mass storage technologies
- Quantum technologies

High Confidence IT
- Data and information security
- High confidence middleware
- High confidence open source
- Reliability
- Safety
- Security including authorization, authentication, biometrics, certification, encryption, interfaces, and protocols
- Software assurance

High-End Computing Systems
- Grid computing
- High-end computing architectures, systems software, and applications software
- Use of biological, nanoscale, and quantum technologies in high-end computing systems

Human Augmentation IT
- Augmented cognition and augmented reality
- Collaboration technologies
- Visualization
Information Management
- Asynchronous collection and processing of independent data streams
- Coherent databases developed from distributed data of varying quality
- Data and information management
- Data mining and data warehousing
- Distributed processing and storage
- Metadata creation and use
- Preservation

Intelligent Systems
- Cognitive systems
- Context-aware computing and autonomic networks to add more intelligence to IT systems
- Human language technology
- Knowledge discovery, representation, and integration

IT System Design
- Architecture
- Graceful evolution
- Hardware/software co-design
- Interoperability
- Preservation

IT Usability
- Human/computer interaction including user interfaces
- Universal accessibility

IT Workforce
- Advanced IT for non-IT specialists
- Interdisciplinary interaction
- IT workforce issues

Management of IT
- Intellectual property issues
- Open source issues
- Standards
- Technology transfer

Networks
- Ad-hoc networking/reconfigurable networking
- Grid
- Mobility
- Network middleware
- Networking management, reliability, and scalability
- Sensor networks

Software Technologies
- Programming environments
- Programming languages
- Software requirements engineering, software development methods and tools, and software engineering
- Systems software and middleware
APPENDIX 2: THE HPCC PROGRAM’S GRAND CHALLENGES

NSF

- Aerospace
  - Coupled field problems
  - Computer Science
  - Machine learning
  - Parallel input/output (I/O) methods for I/O-intensive grand challenges

- Environmental Modeling and Prediction
  - Large-scale environmental modeling
  - Adaptive coordination of results of predictive models with experimental observations
  - Earthquake ground motion modeling in large basins
  - High-performance computing for land cover dynamics
  - Massively parallel simulation of large-scale, high-resolution ecosystem

- Molecular Biology and Biomedical Imaging
  - Biomolecular design
  - Imaging in biological research
  - Advanced computational approaches to biomolecular modeling and structure determination
  - Understanding human joint mechanics through advanced computational models

- Product Design and Process Optimization
  - High-capacity atomic-level simulations for the design of materials

- Space Science
  - Black hole binaries: coalescence and gravitational radiation
  - Formation of galaxies and large-scale structure
  - Radio synthesis imaging

DOE/SC

- Energy
  - Mathematical combustion modeling
  - Quantum chromodynamics calculations
  - Oil reservoir modeling
  - Numeral Tokamak project

- Environmental Monitoring and Prediction
  - Computational chemistry
  - Global climate modeling
  - Groundwater transport and remediation

- Molecular Biology and Biomedical Imaging
  - Computational structural biology

- Product Design and Process Optimization
  - First-principles simulation of materials properties

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NASA
- Large-scale structure and galaxy formation
- Cosmology and accretion astrophysics
- Convective turbulence and mixing in astrophysics
- Solar activity and heliospheric dynamics

NIH
- Molecular biology
- Biomedical imaging

NIST
- Product design and process optimization

EPA
- Linked air and water quality modeling

NOAA
- Climate change prediction and weather forecasting
APPENDIX 3: NITRD GRAND CHALLENGES AUTHORS

Knowledge Environments for Science and Engineering—C.S. Iacono (NSF), W. Bainbridge (NSF)

Clean Energy Production Through Improved Combustion—C. Romine (DOE/SC)

High Confidence Security Systems—G. Koob (DARPA), H. Gill (NSF)

Improved Patient Safety and Health Quality—J.M. Fitzmaurice (AHRQ)

Informed Strategic Planning for Long-Term Regional Climate Change—W. Turnbull (NOAA)

Nanoscale Science and Technology: Explore and Exploit the Behavior of Ensembles of Molecules and Atoms—C. Romine (DOE/SC)

Predicting Pathways and Health Effects of Pollutants—S. Fine (EPA)

Real-Time Threat Detection, Assessment, and Response to Natural and Man-made Threats—C. Romine (DOE/SC)

Safer, More Secure, More Efficient, Higher Capacity Multi-Modal Transportation System—E. Lucier (FAA)

Anticipate the Consequences of Universal Participation in a Digital Society—C.S. Iacono (NSF), W. Bainbridge (NSF)

Collaborative Intelligence: Integrating Humans with Intelligent Technologies—C.S. Iacono (NSF), W. Bainbridge (NSF)

Generating Insights From Information at Your Fingertips—M. Pazzani (NSF)

Managing Knowledge Intensive Dynamic Systems—C.S. Iacono (NSF), W. Bainbridge (NSF)

Rapidly Acquiring Proficiency In Natural Languages—L. Reeker (NIST)

SimUniverse: Learning by Exploring—J. Scholtz (NIST)

Virtual Lifetime Tutor for All—J. Scholtz (NIST)
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<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AHRQ</td>
<td>Agency for Healthcare Research and Quality</td>
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<tr>
<td>BIRN</td>
<td>Biomedical Informatics Research Network</td>
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<tr>
<td>CAFE</td>
<td>Corporate Average Fuel Economy</td>
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<tr>
<td>DARPA</td>
<td>Defense Advanced Research Projects Agency</td>
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<td>DoD</td>
<td>Department of Defense</td>
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<tr>
<td>DOE/SC</td>
<td>Department of Energy/Office of Science</td>
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<tr>
<td>EPA</td>
<td>Environmental Protection Agency</td>
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<td>FAA</td>
<td>Federal Aviation Administration</td>
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<tr>
<td>FACMI</td>
<td>Fellow of the American College of Medical Informatics</td>
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<tr>
<td>Gigabits</td>
<td>billions of bits</td>
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<tr>
<td>HCI&amp;IM</td>
<td>Human-Computer Interaction and Information Management</td>
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<tr>
<td>HEC</td>
<td>High End Computing</td>
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<tr>
<td>HPCC</td>
<td>High Performance Computing and Communications</td>
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<tr>
<td>HVAC</td>
<td>heating, ventilation, and air conditioning</td>
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<tr>
<td>IT</td>
<td>Information Technology</td>
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<tr>
<td>ITR</td>
<td>Information Technology Research</td>
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<td>IWG/IT R&amp;D</td>
<td>Interagency Working Group on Information Technology Research and Development</td>
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<td>LSN</td>
<td>Large Scale Networking</td>
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<tr>
<td>Moore’s Law</td>
<td>computing performance roughly doubles every 18 months while chip size, power, etc., remain constant</td>
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<tr>
<td>MTTR</td>
<td>mean time to recovery</td>
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<tr>
<td>NCO/IT R&amp;D</td>
<td>National Coordination Office for Information Technology Research and Development</td>
</tr>
<tr>
<td>NEES</td>
<td>Network for Earthquake Engineering Simulation</td>
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</tbody>
</table>
NIH  National Institutes of Health
NIST  National Institute of Standards and Technology
NITRD  Networking and Information Technology Research and Development
NOAA  National Oceanic and Atmospheric Administration
$\text{NO}_x$  Ozone
NSA  National Security Agency
NSF  National Science Foundation
NSTC  National Science and Technology Council
NVO  National Virtual Observatory
ODDR&E  DoD’s Office of the Director, Defense Research and Engineering
OSTP  White House Office of Science and Technology Policy
PARS  people, agents, robots, and sensors
R&D  Research and Development
SCADA  Supervisory Control and Data Acquisition
SDP  Software Design and Productivity
SPARC  Space Physics and Aeronomy Research Collaboratory
Teraops  trillions of operations per second
UARC  Upper Atmospheric Research Collaboratory
UAV  Unmanned Air Vehicle
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