Nanotechnology, Biotechnology, and Information Technology: Implications for Future Science at EPA

A Workshop of the EPA Science Advisory Board
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1.0 WORKSHOP BACKGROUND AND OBJECTIVES

The U. S. Environmental Protection Agency (EPA or the Agency) science programs have primarily focused on characterizing and managing risk from environmental exposure to chemical and biological, and physical stressors. Much of the Agency’s ongoing work is based on managing historical sources of pollution. The Agency will continue working on these legacy problems, but it also faces opportunities and challenges from emerging technologies, products and services. EPA research programs currently look toward emerging environmental issues. However, science and technology continues to expand at unprecedented rates. This expansion has been referred to as a new industrial and economic revolution. It offers new opportunities, but also brings unanswered questions about their potential environmental risks and benefits. The present science and technology expansion coincides with flat to declining EPA science budgets for the foreseeable future. Accordingly, the Agency is faced with resolving existing environmental problems and developing new strategies for emerging concerns.

The EPA Science Advisory Board (SAB or the Board) has urged the Agency to develop a new science vision for human health and environmental protection that incorporates the latest scientific and technological advancements. Developments and emerging applications in Nanotechnology, Biotechnology and Information Technology over the past decade have been dramatic, and will continue into the foreseeable future. Advancements within and between these and other technologies will revolutionize industrial production and economic expansion, as well as the environmental sciences.

The SAB anticipates that as the Agency mission becomes more involved with Nanotechnology, Biotechnology and Information Technology products and services, the Board will be asked to provide advice to the Administrator on EPA science and research needs in these area. The primary objective of this workshop was to educate and inform the SAB, and to initiate a dialogue on the implications of these technologies for science and research advice to the EPA.

2.0 WORKSHOP OVERVIEW

Workshop participants included members of the SAB, the Clean Air Scientific Advisory Committee (CASAC), the Advisory Council on Clean Air Compliance Analysis (COUNCIL), and their committees. The workshop (Agenda in Appendix A) included invited presentations on Industrial Ecology, Nanotechnology; Bioproduction; Genomics; Sensor Networks; Large Scale Computing Applications; and Converging Technologies. Industrial Ecology was selected as a potential unifying theme for the six subsequent technology subjects.
Following the invited presentations, the speakers, invited subject matter experts (Biosketches in Appendix B), and workshop participants met in six breakout groups (Breakout Group Assignments in Appendix C) corresponding to the six technology areas. Following breakout group discussions (Breakout Group Questions in Appendix D) the workshop participants discussed the break out group results in plenary session.

This document summarizes: key findings and cross-cutting recommendations of the workshop (Section 3.0); the Industrial Ecology keynote address (Section 4.0 and Appendix E); and invited presentations and breakout group reports for Nanotechnology (Section 5.0 and Appendix F), Biotechnology – Bioprocessing (Section 6.0 and Appendix G), Biotechnology - Genomics (Section 7.0 and Appendix H), Information Technology – Sensor Networks (Section 8.0 and Appendix I), Information Technology – Large Scale Computing (Section 9.0 and Appendix J), and Converging Technologies (Section 10 and Appendix K).

3.0 KEY WORKSHOP FINDINGS & CROSS CUTTING RECOMMENDATIONS

The workshop demonstrated that advances and applications within and between Nanotechnology, Bioproduction, Genomics, Sensor Networks, Large Scale Computing, and Converging Technologies are occurring at an unprecedented rate. Such advancements offer substantial opportunities and challenges for EPA science and research planning and implementation and are provided in subsequent sections of this report. Further, they will undoubtedly impact the work of the Agency now and into the future. Key workshop findings and cross-cutting issues raised during the workshop are provided first, followed by the findings and recommendations for the specific technologies.

- Industrial ecology can be used as an evaluation framework for the development, application, commercialization, dispersal and potential environmental opportunities and challenges of materials and products resulting from new technologies.

- Industrial ecology can assist a shift from simple control and engineering solutions for product artifact manufacture and disposal; to evaluation of complex adaptive systems that incorporate real time adjustment and dialogue to address broader cultural impact of services.

- A strategic examination of how industrial ecology might integrate new technologies to assist the Agency in setting priorities for its most pressing problems may be warranted.

- Possible applications of nanotechnology and nanomaterials include their use in batteries and fuel cells, smart packaging and labeling, catalysts and separation membranes, paints and coatings,
lubricants, composites, medical diagnosis and drug delivery systems, and self-replicating robots and assemblers.

- Aspects of nanotechnology and nanomaterials that require additional investigations include quantifiable estimates of their benefits, and their environmental, health and social impacts.

- Bioprocessing and the biorefinery concept can be used to produce a broad spectrum of products from engineered plants (e.g., starches, sugars, proteins, fibers, fuels, oils, antibodies and drugs) using economical, and environmentally friendly processes.

- Bioprocessing challenges include determining the environmental impact of biorefineries; bioprocess design; limited knowledge of metabolism and control mechanisms; and health and environmental effects of new classes of products.

- As an emerging science, -omics technologies (genomics, proteomics, metabolomics, etc.) offers significant potential to improve and refine EPA’s mission of protecting human health and the environment.

- Obstacles to –omics based health and environmental applications include:
  
  o The lack of quantitative methods, full genomic sequences, reference and technical standards, and notation datasets for at-risk populations; and

  o Limited knowledge of cross-species generalizations; environmental generalizations, genes that confer environmental agent sensitivity, normal states, and damage indices.

- Embedded sensor networks include micro sensors, onboard processing, and wireless interfaces at very small scale that enable spatially and temporally dense environmental monitoring of previously unobservable phenomena

- Important challenges for sensor network applications include the development of sensors, platforms, software protocols, energy
awareness and conservation, scaling and adaptation to variable resources and stimuli.

- Large-scale Computer applications can reduce the time for applying science in environmental decision-making, and have the potential to revolutionize how EPA might manage environmental decisions in diverse areas including:

- Computational chemistry and toxicology, modeling, monitoring, real time emergency response, econometrics; decision analysis; optimized economic growth; urban system management; and scenario analysis for economic, social and environmentally sustainable solutions under uncertainty.

- Potential environmental applications for converging technologies range from wearable sensors and computers to enhance awareness of health, environment, potential hazards, natural resources; to environmental networks of cheap, smart sensors that constantly monitor the condition of the environment.

- Advancements in new technology are occurring at unprecedented rates, making it difficult for government agencies to keep abreast of:
  - emerging developments;
  - science and technology skill mix needs;
  - priorities of new technologies against existing research strategies and multi year plans;
  - collaboration and interaction with other governments, federal agencies, science advisory committees, industry, academia, and the public.

- Emerging technologies can resolve complex environmental and energy problems with multiple and conflicting objectives, asymmetric information, short decision cycles, long analysis times, and few technically qualified people.

- Emerging technology development and applications require consideration and integration of social sciences (economics,
decision sciences, etc.) to determine potential environmental benefits and impacts.

- The range of applications offered by new technologies that would benefit EPA’s science and research activities is vast, and priorities should be strategically targeted to address the Agency most pressing priorities.

- Conventional toxicological and risk assessment approaches have largely been developed for chemicals and require modification for nanotechnology, biotechnology, and sensor deployment.

- The SAB might consider workshops that focus on strategic issues associated with the development and deployment of new technologies, as well as targeted workshops on novel applications of specific technologies for specific problems.

- The SAB might consider additional committees to address the development of new technologies.

In the closing discussion, participants noted that technology appears to be on the verge of altering the entire context of environmental protection and social welfare. Some questioned whether conventional risk assessment and regulatory structures are appropriate for the potential environmental challenges of emerging technologies. Others asked whether consideration needed to be given to altering our institutional structures to meet these challenges. Still others thought that the SAB might provide deeper thinking about where the EPA needs to be in ten years, and what it needs to do to get there.

In closing remarks Dr. Granger Morgan, Chair of the SAB, noted that the topics and recommendations emerging from the workshop were diverse. He observed that specific recommendations were valuable, but that real impact of the workshop was a diffusion process. That is, workshop participants take what they have learned back to their offices, and incorporate new thinking into their work. For the SAB, this means new ideas in reviewing EPA projects, programs, planning documents, and the science budget. He stated that the ideas discussed at this workshop will set the stage for additional SAB deliberations regarding how to best advise the Agency on the use of new technologies in its science enterprise.

4.0 KEYNOTE ADDRESS SUMMARY

4.1 Industrial Ecology Principles: A Unifying Theme for Environmental Applications of New Technologies -- Dr. Braden Allenby, School of Engineering, Arizona State University (See Slides Appendix E)
Industrial Ecology is a systems approach to environmental analysis. It addresses industrial emissions, specific products, and the complex network of services, products and activities that make up the economy. Industrial ecology can guide holistic thinking about environmental problems. The need for guiding principles is illustrated by the rapid societal changes being brought about by advancements in technology. Technology causes fundamental changes, and the rate of change currently exceeds the ability of governments to react in a timely manner. Therefore, timely decisions and specific courses of action are preempted by rapid societal change, which often lacks systematic consideration of holistic environmental consequences. Dr. Allenby discussed two case studies that demonstrated the need to shift environmental analysis and problem-solving away from simple command and control of product manufacture and emissions, and towards complex adaptive systems. Several key points follow, and Dr. Allenby’s complete slide presentation is shown in Appendix E.

- Traditional environmental science and engineering has been directed toward controlling physical environmental impacts associated with energy consumption and toxic products related to artifact manufacture and disposal.

- Although less intuitive and much less studied, cultural environmental impacts from such services may be potentially large. Critical thinking is required to resolve ethics, fundamental changes in human cognition and perception through computers and information technology.

- Industrial ecology principles (earth systems engineering and management related to design engineering, governance and theory) provide a unifying theme for environmental applications of new technologies.

- Bothersome Questions for the SAB to consider

  - Should EPA have a Technology and Science Advisory Board, and should an Industry Advisory Board be added?

  - Should EPA become a competency that diffuses itself throughout government?

  - How will EPA and government generally, develop the ability to engage dialogue with, rather than regulate, complex human/natural systems?
- How will EPA develop the ability to operate on a time cycle that aligns with the phenomenon for which it is responsible?

- How will EPA function as its core conceptual foundations (environment, wilderness, nature) become increasingly contingent, and change substantively over shorter time periods?

- What is EPA’s role as the world increasingly becomes a product of human design?

- How does EPA avoid becoming more and more effective, at less and less important tasks, as environmental impacts increasingly become a function of strategic and non-environmental technological and business decisions?

5.0 NANOTECHNOLOGY

5.1 Invited Presentation: Nanotechnology – Dr. Roland Clift, Centre for Environmental Strategy, University of Surrey (See Slides Appendix F).

Nanotechnology is an emerging technology based on solid particles in the size range of 1-100 nm (a nanometer is 1X 10^-9 meter and comparable in size to viruses) where properties are determined by size and surface area rather than bulk properties. A member of the Royal Society/Royal Academy of Engineering Working Group on Nanoscience and Nanotechnologies, Dr. Clift provided a European perspective based the Working Group report Nanoscience and Nanotechnologies: Opportunities and Uncertainties (2004). He discussed possible applications including the use of nanomaterials in batteries and fuel cells, smart packaging and labeling, catalysts and separation membranes, paints and coatings, lubricants, composites, and medical diagnosis and drug delivery systems, and self-replicating robots and assemblers. He focused his remarks on three areas of concern: quantifiable benefit estimates; health and environmental impacts; and social impacts of new and emerging technologies. Several key points follow, and Dr. Clift’s complete slide presentation is shown in Appendix F.

- Systematic life cycle assessments of the benefits and risks of nanotechnology have not yet been conducted, the potential health and environmental impacts are uncertain, and social impacts are unknown.
• Conventional hazard and risk endpoints may provide a basis for regulation, but standard tests (e.g., toxicity, persistence, bioaccumulation) may not be applicable for nanomaterials due to surface property alterations at the nanoscale.

• Toxicity information is lacking, and regulation must be based on likely nanoparticle exposure scenarios (e.g., vehicle emissions, sunscreens, cosmetics, and combustion).

• The precautionary approach suggests a moratorium on certain nanotechnology applications (e.g., fuel additives, bioremediation of groundwater, and end-of-life product disposal). However, nanoparticles are likely to be made at point of use, making arguments for a production moratorium irrelevant.

• The Royal Society/Royal Academy of Engineering Working Group recommended that Europe conduct horizon scanning of emerging technologies by asking what impacts and regulatory issues might arise.

5.2 Nanotechnology Breakout Group Report

The breakout group participants (Appendix C) discussed current government and industrial initiatives and projects, applications, and possible risk assessment and risk management issues regarding nanomaterials. The following points were prepared for the plenary presentation and discussion.

Basics

• Nano-size and nano-materials have to be considered together.

• Life cycle assessments should consider what is being made, where it goes, and where it ends up?

• Presently, over 200 companies worldwide are involved in making nanoproducts.

• Nanotechnology development may be going the way of uncritical praise and optimism, and there may be lessons to be learned from earlier controversies (e.g., genetically modified organisms and nuclear power).
Opportunities

• Nanotechnology application holds great promise for electricity transmission, solar conversion, catalysis, sensors, treatment and purification technologies, and the remediation of hazardous wastes.

Challenges

• Public discussion on nanotechnology should be encouraged and amplified.

• Life cycle assessment should be applied to nanomanufacturing and nanoproduct footprints.

• Standards and measurements (testing protocols) need to be developed for nanotechnology research.

Future Role of SAB

• SAB can help identify the most urgent environmental problems (SAB nanotechnology review, need for environmental nanotechnology science plan, etc).

• Should SAB help EPA reconsider its relationship to industry (Being informed enough to know what will be happening; doing collaborative research)?

6.0 BIOTECHNOLOGY – BIOPROCESSING

6.1 Invited Presentation: Bioprocessing: Opportunities and Challenges – Dr. Harold Monbouquette, University of California – Los Angeles (See Slides Appendix G)

Bioprocessing exploits a broad universe of metabolic processes and enzyme activities to synthesize specialty and commodity chemicals. The biorefinery concept is closely associated with bioprocessing, but provides a commodities development perspective. Presently, there is a diverse enzyme toolkit available to industry. Of approximately 30,000 known enzymes, about 3000 have been well characterized, and about 300 are commercially available. Accordingly, available techniques allow engineering of plants, microbes and enzyme systems for production of chemicals using economical, and environmentally friendly processes. Bioprocessing can be used to produce a broad spectrum of products from engineered organisms, including starches, sugars, proteins, fibers, fuels, oils, antibodies and drugs. Dr. Monbouquette
focused on several applications in his area of expertise. Several key points follow, and his complete slide presentation is shown in Appendix G.

- Bioprocessing and the biorefinery concept exploit metabolic processes and enzyme activities for the production of specialty and commodity chemicals.

- Examples include: production of carotenoid pigments from genes cloned into *E. coli*; biosynthesis pathways for aspartame, melanin, and indigo; and the integration of enzymes into chemical synthesis processes to reduce environmental impacts.

- Bioprocessing has the potential to provide new products including chiral drugs, flavorings, aromas, herbicides and pesticides, hyperthermophilic glycoside hydrolases for oil and gas well fracturing. New systems may be needed to assess environmental impact of these processes and products including, for example, methods for detecting potential endocrine disrupting chemicals (EDCs).

- Bioprocessing presents several opportunities beneficial for the environment including: genetically modified organisms to synthesize chemicals from renewable resources; and enzymes to improve selectivity and yield of industrial chemical synthesis steps thereby reducing environmental impact.

- Challenges presented by bioprocessing include determining the environmental impact of biorefineries; bioprocess design; limited knowledge of metabolism and metabolic control mechanisms; and health and environmental effects of new classes of products and processes.

6.2 Bioprocessing Breakout Group Report

The breakout group participants (Appendix C) discussed potential bioprocessing applications, as well as risk assessment, risk management, and policy needs. The following points were prepared for the plenary presentation and discussion.

**Opportunities**

- Switching from a petroleum-based economy to bioproduction provides opportunities to reduce the toxicity of industrial waste and byproducts.

- Bioproduction offers opportunities to use agricultural products and waste materials (e.g., agricultural waste) in fermentation processes.
• Small community-based systems are important to allow innovations in bioproduction at the local scale.

• Metabolic engineering using recombinant DNA technology has the potential to improve production of chemicals by host organisms, and allow production of new chemicals.

• Currently, some biomass (e.g., cellulose) cannot be effectively used in conventional bioproduction. Gasification, followed by biosynthesis provides a near term opportunity for effective use of cellulitic biomass as raw materials in production processes.

• Technology is being developed to use biomass such as grass, wood and waste material in bioproduction processes.

• Bioproduction offers opportunities for animal waste reduction and more efficient use of nutrients (e.g., phosphorus fed to chickens).

• In the near term, advancements in viable, environmentally safe technology should be a priority (e.g., use of systems in landfills to remove methane).

• How EPA might regulate the use of new technologies is a key issue. Science needs and regulatory impediments should be addressed for regulating genetically modified organisms used in and products from bioproduction.

• EPA should consider incentives to advance the state of the science through innovative approaches like credit trading programs for waste generators.

• EPA needs to catalyze formation of university/industry/other federal agency partnerships to conduct innovative research and development and more effective integration of bio-based green chemistry work.

• EPA should articulate research needs and provide more external support for research and training of graduate students in emerging areas.

• EPA should develop multidisciplinary approaches for life cycle analysis. To encourage innovation, a framework not a standard protocol is needed.
Challenges

- Environmental problems associated with more intensive agricultural production in different crops must be considered.
- Energy and fertilizer demands in agriculture are high.
- Degradation of soil, displacement of wildlife, and water quality problems (hypoxia caused by nitrogen and phosphorus runoff from farm fields) must be considered.
- Tradeoffs between environmental benefits of bioproduction and benefits of reducing the intensity of agriculture (e.g., taking marginal land out of production, converting land to wetlands) should be evaluated.
- Research is needed to understand ripple effects of bioproduction through land use and social and economic systems (these may be very large).
- Potential environmental effects of accidental releases of recombinant DNA must be considered.
- Biosafety guidelines are needed for bioproduction technologies.
- Studies of genetically modified organisms used in more open processes such as biorefineries should be conducted to quantify environmental benefits and evaluate benefits versus risks.
- Regulatory authority for genetically modified organisms between agencies should be clarified.
- New toxicology tools should be developed to examine bioproduction.
- EPA should develop good management practices for testing new technologies to determine whether they may cause environmental problems.
- Good sensors are needed to conduct assessments of new technologies.

Future Role of the SAB

- SAB should continue to hold technical workshops like this one in order to anticipate emerging issues.
• SAB should encourage EPA to work closely with the science advisory committees of other government agencies, particularly DOE, USDA, and Commerce on bioproduction issues.

7.0 BIOTECHNOLOGY – GENOMICS

7.1 Invited Presentation: Towards genomics-based analyses of environmental agent impacts on biological systems – Dr. Bruce Aronow, Cincinnati Childrens Hospital (See Slides Appendix H)

The term genomics specifically refers to the study of the structure, activity and functions of genes. It includes gene regulation, mRNA expression, and cell-type specificity. Genomics is often imprecisely used to cover other “-omics” sciences such as physiomics (tissue dynamics, systems biology, and the outcome in clinical populations) and proteomics (protein expression, structure, interactions, localizations and pathways). Dr. Aronow focused his presentation on using genomics to assess environmental effects on biological systems, with emphasis on mouse and human models for colon cancer. Several key points follow, and his complete slide presentation is shown in Appendix H.

• Genomics can provide new tools to assess the impact of environmental agents.

• Systems biology approaches will assist the integration of genomics data and analyses into human health and environmental assessment scenarios.

• Technical barriers currently present obstacles to genomics-based health and environmental monitoring. These include:
  - Lack of quantitative methods, full genomic sequences, reference and technical standards, and notation datasets for at-risk populations;
  - Limited knowledge of cross-species and environmental generalization, genes that confer environmental agent sensitivity, normal states, and damage indices.

• Two case studies were presented using human and mouse central nervous system genes; and comparative transcriptional profiling for mouse and human colon cancers.
The case studies demonstrated the classification of human tumors based on behavior of developmentally regulated mouse gene orthologs that have implications for outcomes to individuals.

7.2  **-Omic Sciences Breakout Group Report**

The breakout group participants (Appendix C) discussed potential genomic applications, as well as risk assessment, risk management, and policy needs. The following points were prepared for the plenary discussion.

**Opportunities**

- *-Omic* technology is not limited to genomics, but includes proteomics, metabolomics, etc.

- As an emerging science, *-omics* technology offers significant potential to improve and refine EPA’s mission of protecting human health and the environment.

- Complexity, costs, and effective implementation of *-omic* technology demands new models of research partnerships, both within and across federal agencies, and with external research communities and sectors.

- Engage ongoing efforts in NAS, OECD and others developing application plans for biotechnology.

- *-Omic* technology has value for EPA’s mission (e.g., identifying susceptible populations, surveillance analysis, prioritization, reduced use of animals for testing).

**Challenges**

- EPA should develop a Framework (Multi-Year Plan) focused on implementation of *-omic* technology that covers: partnerships; attraction, retention, and training of human resources; bioinformatic needs and integration with other databases; systems biology and integrated modeling capacity; development of performance standards; commonality of methods; consistency of performance/baseline measurements; external data submission; and training sets for interpretation.

- The Multi-Year Plan research plan should be developed in keeping with OMBs Program Assessment Review Tool (PART).
Future Role of SAB

- Consider interactions with other agency Science Advisory Boards, and examine new models of cross-agency funding and resource sharing, funding needs, ethics, and the value of -omics technology to key customers.

- Consider priorities of -omics technologies relative to other multi-year plans.

8.0 INFORMATION TECHNOLOGY – SENSOR NETWORKS

8.1 Invited Presentation: Wireless Sensor Networks for Environmental Monitoring – Dr. Deborah Estrin, University of California – Los Angeles (See Slides Appendix I)

Embedded sensor networks include micro sensors, onboard processing, and wireless interfaces at very small scale to monitor phenomena up-close; enable spatially and temporally dense environmental monitoring; and reveal previously unobservable phenomena. Dr. Estrin focused her presentation on ecological and contaminant transport applications, as well as regional and global possibilities for sensor network development. Several key points follow, and her complete slide presentation is shown in Appendix I.

- The emerging technologies discussed in this workshop offer opportunities for development of new sensor networks to observe, monitor and model various functions.

- The specific embedded sensor networks applications discussed included contaminant transport in soils, plankton dynamics in marine environments, and ecosystem processes.

- In situ Sensing will transform observations of spatially variable processes in heterogeneous and obstructed environments. Example applications include a locally dense surface and subsurface sensor network to observe soil nitrate transport; spatial and temporal distributions of algal blooms in coastal ecosystems; ecosystem processes such as microclimate monitoring, image and acoustic sensing, and infrastructure mobility.

- Important challenges for sensor network applications include sensors, platforms, software protocols, energy awareness and conservation, scaling and adaptation to variable resources and stimuli.
• Heterogeneous sensor networks of small linked robotic sensors that host higher-end sensors are needed to enable adaptive, fidelity-driven, three-dimensional sampling.

• The development of embeddable sensor networks and multi-scale observation and fusion networks have broad relevance to global issues.

8.2 Sensor Networks Breakout Group Report

The breakout group participants (Appendix C) discussed the rapid advancement of sensor network technology, and possibilities for cheap, small sensors capable of multi-factor analysis, data-relay, and network integration. Future applications might well include laboratories on a chip, and mass spectrometers the size of sugar cubes. The breakout group focused their attention on new technologies, demonstration projects, and prepared a set of network development technology principles, challenges and future role of the SAB for presentation and discussion at the plenary session.

Principles for Sensor Network Development

• Affordability (The National Ambient Air Monitoring Strategy is one approach for redesign within existing annual total costs (http://www.epa.gov/ttn/amtic/files/ambient/monitorstrat/allstrat.pdf).

• Problem-oriented applications focused on solving environmental problems of critical importance to EPA’s mission and regulatory mandate.

• Technologies that are realistically and demonstrable in the near-term

• Partnerships should be developed to:

  - Ensure commercial viability of new technologies to capitalize on corporate investments made by industry;

  - Utilize existing data networks in the federal, state, tribal, and local sectors;

  - Partner with other government agencies engaged in basic and applied sensor-network research to leverage research funding and capabilities.
• Focus on multi-use, multi-pollutant sensors and applications that include sensors for ecological, biological and human health applications.

• Specify interoperability and comparability of data by design and select data networks and embedded sensors that are interoperable with analytical data equivalence.

• Employ multi-layer, large to small scale sensor networks (e.g., satellite imagery and smaller-scale remote-sensing to local on-site sensors).

• Ensure data are easily interpretable and include data visualization techniques (i.e., visual display of dense, complex quantitative and qualitative information from embedded sensor networks), leading to clear unambiguous interpretation.

• Demand high performance and reliability over time (i.e., consistent and accurate data transmission without need for recalibration); robustness (i.e., imperviousness to adverse in situ conditions); value and affordability; adaptability; sustainability (both technical and institutional); real-time data transmission; and portability.

• Pursue a “systems” approach for sensor networks in complex ecosystems.

• Deploy “early-warning” systems throughout the country that are relatively inexpensive, widespread networks that direct attention to deeper problems as they develop.

Challenges

• Network design is perhaps more challenging than actual sensor development, and highly dependent on the specific objective and network scale.

• Wide ranging potential applications were discussed including: mercury in air and water in the Eastern U.S.; Mississippi River watersheds and Gulf of Mexico dead zone; the Great Lakes; Chesapeake Bay; TMDLs in Northwest redwood region; and CAFOs in the San Joaquin Valley.
Future Role of the SAB

- A workshop on the use of new sensor network technology in the context of two or three Agency problems (e.g., Great Lakes). The developers as well as EPA problem identifiers are necessary to formulate templates and networks in the context of the Agency strategic and multi-year plans. Such activities should be directed toward developing a clear conceptual model that delineates what the system looks like and how it works, to appropriately use sensors in hypothesis testing. Adaptive management would then allow continued use of the network.

9.0 INFORMATION TECHNOLOGY – LARGE SCALE COMPUTING

9.1 Invited Presentation: Information Technology (IT): Implications for Future Science at EPA – Dr. Gregory McRae, Massachusetts Institute of Technology (See Slides Appendix J)

Information Technology (IT) includes a spectrum of computers, databases, communications, sensors, visualizations, algorithms, and their management. Information technology can also reduce the time for applying science in environmental decision-making. Therefore, advances in information technology have the potential to revolutionize how EPA might manage environmental decisions. Dr. McRae focused his presentation on driving forces for change, new dimensions of working in teams, routine visualization of complex phenomena, and global environmental problems. Several key points follow, and his complete slide presentation is shown in Appendix J.

- Real and perceived environmental risks exist, and IT can help develop proper science and policy responses and revolutionize how EPA manages environmental risks.

- Computers, databases, communications, sensors, visualization, algorithms, and their management can reduce the time for applying science in environmental decision-making.

- Forces driving information technology development include bandwidth, optical networks, remote access, and routine visualization of complex environmental problems.

- IT can resolve complex environmental and energy problems which often involve multiple and conflicting objectives, asymmetric information, short decision cycles, long analysis times, and few technically qualified people.
• Air Quality, Genomics, and Bioinformatics are areas where IT has been used with varying degrees of success in environmental problem solving.

• Data for environmental problem solving are not often integrated, may lack useful uncertainty estimates, are variously documented, and of variable quality. Solving these data problems would enhance the pragmatic use of IT in environmental decision-making.

• Moving away from conventional compliance assessment to inverse modeling and deterministic control strategy designs would minimize control costs and maximize air quality, minimize exposure to pollution, and minimize risk of exceedances.

• Solving these problems requires cost-effective monitoring systems using advanced technology.

• The development of novel inexpensive sensors and innovative deployment would assist the detection and resolution of environmental problems before they become acute.

• Greater use of life cycle assessment models like MIT’s Environmental Evaluation Model would assist the development of optimized design and control strategies for new industrial products and processes.

• Dr. McRae posed several needs and questions for the SAB’s consideration.

  - There is a critical need for multimedia integration of databases and models to prevent problems such as MTBE contamination.

  - A most critical issue is how to find and employ people with appropriate training and expertise in information technology

  - Information technology is a critical enabling resource and asked if EPA needs a Chief Technical Officer or Chief Information Officer?

  - How can database access be improved for use in decision-making?
- How can more science be integrated into control strategy design processes?

9.2 Large Scale Computing Breakout Group Report

The breakout group participants (Appendix C) discussed possible applications of information technology with an emphasis on supercomputing applications, and prepared the following points for presentation and discussion at the plenary session.

Opportunities

- Information technology is crucial to advancement of computational chemistry, computational toxicology, air quality modeling, biochemical modeling, groundwater transport and remediation, watershed management, surface water quality and hydrodynamics.

- Additional opportunities include the use of information technology in real time emergency response; multimedia, ecological, and respiratory airway modeling

- Similarly, information technology can be used to enhance the applications in: econometrics; decision analysis; optimized economic growth; urban system management; and scenario analysis for economic, social and environmentally sustainable solutions under uncertainty

Challenges

- Support and educate a diverse generation of scientists and engineers capable of using innovative and state-of-the-art large scale computing applications.

- Data availability, access, and quality

- Model evaluation

- Computing capability

- Practical methods for large-scale optimization

- Prioritize resources to resolve uncertainties

- Collaboration between Agencies
Future Role of the SAB

- Create an advisory panel to prioritize opportunities and identify challenges and outline necessary resources
- Organize a “supercomputing workshop”
- Put together a “supercomputing road map” of needs to be considered for EPA
- Inclusion of other Agencies with supercomputing capabilities/interest
- Engage industry in the mission so they can share experiences and EPA can learn new technologies

10.0 CONVERGING TECHNOLOGIES

10.1 Invited Presentation Summary: Converging Technologies (NBIC) – Dr. William Bainbridge, National Science Foundation (See Slides Appendix K)

Converging technologies represents a movement focused on the unification of science and technology, and is defined by interactions between Nanotechnology, Biotechnology, Information Technology, and Cognitive Sciences (often referred to as NBIC or convergence). Dr. Bainbridge focused his presentation on general principles and applications of convergence. Several key points follow, and his complete slide presentation is shown in Appendix K.

- Opportunities for science and technology convergence are based on shared methodologies which provide opportunities for developing transformative tools
- One-way convergence is taking an idea, tool or discovery from one field and applying it to another.
- Mutual convergence is when scientific theories and models are applied across different fields facilitating exchange.
- The principles of convergence include:
  - Material unity of nature at the nanoscale;
  - Technology integration from the nanoscale;
- Key transforming tools for NBIC;
- The concept of reality as a closely coupled complex hierarchical systems;
- Goals to improve human performance.

• Application areas for improving human performance using converging technologies have emerged including:
  - The expansion of human cognition and communication;
  - Improving human health and physical capabilities;
  - Enhancing group and societal outcomes;
  - Strengthening national security and competiveness, and
  - Unifying science and education

• Several converging technologies application areas were presented.
  - Spatial cognition through wearable sensors and computers to enhance awareness of health, environment, potential hazards, natural resources, etc.
  - National security applications including information rich fighter systems, intelligence gathering systems, and effective counter measures for biological, chemical, radiological and nuclear attacks
  - Agriculture and food industry applications to increase yields through networks of cheap, smart sensors that constantly monitor the condition of plant, animal and farm products.
  - New categories of materials, devices and systems for use in manufacture, construction, transportation, medicine, emerging technologies and scientific research.
  - Processes of the living cell, which is the most complex known form of matter with nanoscale components.
  - Principles of advanced sensory, computational and communications systems integrating diverse components into a ubiquitous, global network
10.2 Converging Technologies Breakout Group Report

The breakout group participants (Appendix C) discussed actions the SAB might take with respect to converging technologies. The breakout group focused their attention on priorities and prepared the following points for presentation and discussion at the plenary session.

Highest priority SAB Actions

- New Reducing Risk/Over the Horizon-type report focusing on where existing regulatory science and policy lags behind new technology issues.
- Address Administrator’s priorities by identifying opportunities for converging technologies (e.g., mercury).
- Review EPA’s Science Inventory for activities related to converging technologies and identify gaps and opportunities.
- Develop low-cost exploratory steps to increase fluency in converging technologies and influence exchange within and between EPA, other Agencies, and stakeholders.
- Develop joint proposals with other Federal Agencies

Other Possible SAB Actions to Highlight Opportunities and Address Challenges

- White paper on challenges and opportunities-- addressing national and global dimensions
- Advise on EPA’s plans to expand its skill set
- Catalyze multi-disciplinary collaboration -- “Synthesis U,” rotational assignments, fellowships
- Data issues -- meta data needs
- Address EPA’s gap in cognitive and behavioral science
- Address environmental education, risk perception, risk communication issues
APPENDIX A

WORKSHOP AGENDA
Nanotechnology, Biotechnology, and Information Technology:
Implications for Future Science at EPA
Agenda

Day 1 -- Wednesday, December 1, 2004

8:30  Welcoming Remarks - Dr. Granger Morgan, Chair, SAB
      Workshop Introduction - Dr. Anthony Maciorowski, SAB Staff
      Office

8:45  Industrial Ecology Principles: A Unifying Theme For
      Environmental Applications of New Technologies - Dr. Braden
      Allenby, School of Engineering, Arizona State University

9:15  Nanotechnology - Dr. Roland Clift, Centre for Environmental
      Strategy, University of Surrey

9:45  Biotechnology – Bioproduction - Dr. Harold G. Monbouquette,
      Department of Chemical Engineering, University of California –
      Los Angeles

10:15 Biotechnology – Genomics - Dr. Bruce Aronow, Cincinnati
      Children's Hospital Medical Center

10:45 Break

11:00 Information Technology – Sensor Networks - Dr. Deborah
      Estrin, Department of Computer Science, University of California
      – Los Angeles

11:30 Information Technology – Large Scale Computing/Modeling
      Applications - Dr. Gregory McRae, Massachusetts Institute of
      Technology

12:00 Lunch

1:30  Converging Technologies - Dr. William Bainbridge, National
      Science Foundation

2:00  General Discussion
Nanotechnology, Biotechnology, and Information Technology: Implications for Future Science at EPA Agenda (Continued)

Day 1 -- Wednesday, December 1, 2004

2:30 Breakout Groups
  Nanotechnology
  Biotechnology – Bioproduction
  Biotechnology – Genomic
  Information Technology – Sensor Network
  Information Technology – Large Scale Computing/Modeling
  Converging Technologies

5:30 Adjourn for the Day

Day 2 -- Thursday, December 2, 2004

8:30 Breakout Groups (Continued)

  Nanotechnology
  Biotechnology – Bioproduction
  Biotechnology – Genomics
  Information Technology – Sensor Networks
  Information Technology – Large Scale Computing/Modeling
  Converging Technologies

9:45 Breakout Group Reports

10:45 Break

11:00 Wrap up and discussion of next steps

12:30 Adjourn
APPENDIX B

BIOSKETCHES OF INVITED SPEAKERS AND SUBJECT MATTER EXPERTS
BIOSKETCHES OF INVITED SPEAKERS AND SUBJECT MATTER EXPERTS

Industrial Ecology

Invited Keynote Speaker

Professor Braden Allenby is a Professor at Arizona State University’s Ira A. Fulton School of Engineering in the Department of Civil and Environmental Engineering. Prior to that he was Vice President, Environment, Health and Safety at AT&T, an adjunct professor at The University of Virginia’s School of Engineering and at Princeton Theological Seminary, and the inaugural Batten Fellow at Darden Graduate School of Business at the University of Virginia. He is well known for his work in industrial ecology, and works with information systems and technology from an earth systems engineering and management perspective, studying the economic, environmental and social implications of technological systems, communications, infrastructure, and services. Dr. Allenby as co-edited, authored and coauthored numerous textbooks in industrial ecology and systems engineering. He received his B.A. cum laude from Yale University, J.D. and Masters in Economics from the University of Virginia, and Masters and Ph.D. in Environmental Sciences from Rutgers.

Nanotechnology

Invited Speaker

Professor Roland Clift is Distinguished Professor of Environmental Technology, and founding Director of the Centre for Environmental Strategy at the University of Surrey. He was previously Head of the Department of Chemical and Process Engineering at the University of Surrey, and is a visiting Professor in Environmental System Analysis at Chalmers University, Göteborg, Sweden. He is a member of the: Royal Commission on Environmental Pollution; International Expert Group on Application of Life Cycle Assessment to Waste Management; and the Rolls-Royce Environmental Advisory Board. He is a past member of the UK Eco-labeling Board, and currently serves as an Expert Adviser to a House of Lords enquiry into energy efficiency. In 2003, Professor Clift was awarded the Sir Frank Whittle Medal of the Royal Academy of Engineering for outstanding and sustained engineering achievement contributing to the well being of the nation.

Invited Experts

Dr. Catherine Alexander has a broad background in communications that combines study in social trends, public attitudes and communications methodology with work experience in the media, public affairs and scientific communications. Upon graduation from the University of Michigan (Ann Arbor), Ms. Alexander moved to
Washington, DC where she became a television news producer and writer for the local ABC affiliate. After five years in that position, she worked in corporate communications at a local energy company, serving as corporate spokesperson and news media manager. Later, as an independent writer and producer, Ms. Alexander specialized in news media relations consulting and writing on alternative energy and environmental issues. She has worked for the American Association for the Advancement of Science as Senior Communications Officer and as Vice President of Americans for Medical Progress, a group that advocates for biomedical research. Ms. Alexander became Communications Director for the National Nanotechnology Coordination Office, the secretariat of the U.S. National Nanotechnology Initiative, in February 2003. She has completed graduate work at Johns Hopkins University and George Mason University.

**Dr. Matteo Pasquali** (Invited Subject Matter Expert) is an Assistant Professor of Chemical and Biomolecular Engineering at Rice University, where he also serves as co-director of the Nanomaterials Production Facility of the NSF-Rice Center for Biological and Environmental Nanotechnology. He is an active member of the: Center for Nanoscale Science and Technology; the Carbon Nanotechnology Laboratory; and the Computer and Information Technology Institute. Before joining Rice University, he earned a Ph.D. and conducted post-doctoral work at the University of Minnesota. Dr. Pasquali's research interests involve the interactions of flow and liquid micro- and nano-structure in complex fluids, with application to the processing of engineered materials, with a particular focus on DNA solutions and carbon nanotube dispersions.

**EPA Experts**

**Dr. Michael Gill** is currently the ORD Hazardous Waste Technical Liaison (HSTL) for EPA Region 9. This position is one of technical support and information brokering. He helps make the connection between hazardous waste technical needs and ORD Lab expertise. His customers are for the most part project managers in the Superfund Program, but may include RCRA and other Regional EPA staff, State environmental staff, industry and the public. Mike also participates in research planning, environmental technology demonstrations, and workshop planning. Mike has been in his present position as HSTL since 1998 and has been at EPA since July of 1992, when he was hired as a Remedial Project Manager in Region 9's Superfund Program.

**Ms. Marti Otto** is an environmental engineer in the Technology Assessment Branch of the Technology Innovation and Field Services Division of the Office of Superfund Remediation and Technology Innovation of the U.S. Environmental Protection Agency. Ms. Otto has almost 20 years of experience in hazardous waste site evaluation and remediation and environmental regulation and policy development. She earned a Bachelor of Science degree in Biology and a Master of Science degree in Environmental Science and Engineering from Virginia Tech.
Dr. Dennis Utterback is a senior policy analyst in the Office of Science Policy in EPA's Office of Research and Development. He represents ORD science policy positions in the development of Agency decisions on toxic substances and pesticides. Specific areas of expertise include flame retardants, PFOA, nanotechnology, human studies and cumulative risk assessment. He has also designed and presented a half-day course on risk assessment basics for a non-technical audience. Prior to ORD, Dr. Utterback led various workgroups in EPA's Office of Pesticide Programs, in managing risks for high risk chemicals and development of an import tolerance policy. He has a B.A. in political science from Augustana College and a Ph.D. in public administration from Syracuse University.

Biotechnology – Bioproduction

Invited Speaker

Dr. Harold G. Monbouquette is a tenured professor in the UCLA Chemical Engineering Department. Professor Monbouquette received an AB in Biochemical Sciences from Harvard College and a Ph.D. in Chemical Engineering from North Carolina State University. He conducts research on biosensors, the biotechnological applications of extremely thermophilic microorganisms, and on the molecular engineering of surfaces for materials and nanoelectronics applications. He joined the faculty at UCLA in 1987 as assistant professor. He was a recipient of a Department of Energy Young Faculty Award and was presented a TRW Excellence in Teaching Award.

Invited Experts

Dr. Robert M. Kelly is a Professor in the Department of Chemical Engineering at North Carolina State University. He holds a Ph.D. in Chemical Engineering from North Carolina State University. His research interests include biochemical engineering; biocatalysis; microorganisms from extreme environments; microbial physiology and bioenergetics; functional genomics. He has served as Director, NCSU NIH Graduate Student Biotechnology Training Program, and as the Associate Vice-Chancellor for Research Development, Research and Graduate Studies.

Dr. Robert Mark Worden is a Professor in the Chemical Engineering and Materials Science Department of Michigan State University. He received a Ph.D. in Chemical Engineering from the University of Tennessee. His research program integrates recombinant-protein production, biocatalysis, and nanotechnology to develop new systems for bioproduction, biosensing, and bioremediation. He holds patents on microbiosensors for in situ use and cell-growth methods. He established and directs the MSU Center on Nanostructured Biomimetic Interfaces, a graduate training program on Technologies for a Biobased Economy, the MSU Protein Expression Laboratory, and the Multidisciplinary Bioprocessing Laboratory.
EPA Experts

Ms. April Richards is the Deputy Director of the Small Business Innovation Research (SBIR) program for the U.S. Environmental Protection Agency (EPA). The SBIR program links new, cutting-edge, high-risk innovations with EPA programs in water and air pollution control, solid and hazardous waste management, pollution prevention and environmental monitoring. April is an environmental engineer with EPA’s National Center for Environmental Research in the Office of Research and Development (ORD) where she works on several extramural research programs aimed at developing environmentally friendly technologies. She worked for 5 years in private industry with an environmental engineering consulting firm in Florida primarily in the area of drinking water treatment. She has a Master’s degree in Civil/Environmental Engineering and is a licensed, professional engineer.

Biotechnology – Genomics

Invited Speaker

Dr. Bruce Aronow is an Associate Professor of Pediatrics and Co-director of the Computational Medicine Center at the Cincinnati Children’s Hospital Medical Center. He received a Ph.D. degree from the University of Kentucky. His research group works to identify similar and/or cis-element clusters in genes, and has developed a Web-based tool called TraFac (Transcription Factor Comparison). TraFac identifies the cis-elements in phylogenetic footprints. They are also working to identify compositionally similar cis-regulatory element clusters in groups of co-regulated genes, which may serve as valuable probes for genome-wide identification of regulatory regions. His group is also building an integrated gene annotation tool with the capability of user-added annotations.

Invited Experts

Dr. Mark Pershouse is an Assistant Professor in the Department of Biomedical and Pharmaceutical Sciences at the University of Montana. He earned a Ph.D. in Biomedical Sciences from the University of Texas at Houston, and was a Postdoctoral Fellow at the M.D. Andersen Cancer Center, and a Postdoctoral Research Associate at Baylor College of Medicine. His major research focuses on the genetic events, which lead to human mesothelioma formation following asbestos exposure. Through his role as the University of Montana Microarray core director he also focuses on the molecular response to toxicants such as asbestos, silicates, organophosphates, or metals, providing new insight into response mechanisms of, and avenues for, therapeutic intervention. The characteristic cohort of genes responding to a stimulus can provides a toxic signature, and offer tools for monitoring exposures and finding genes responsible for our individual risk of disease following exposure. He is also collaborating through the core facility on such diverse issues as biomarkers of exposure to biological and chemical warfare agents, the molecular and cellular response to high altitude, and the search for molecules which direct innervation of skeletal muscle during development.
Dr. Parke Rublee is a Professor of Biological Sciences at the University of North Carolina – Greensboro. His interests are in aquatic microbial ecology and a current research focus is the development of microarrays for use in water quality assessments. He has developed gene probes for the determination of the geographic distribution of Pfiesteria piscicida, a toxic dinoflagellate, which has been linked to fish kills in North Carolina coastal waters. He has also addressed the structure and function of aquatic microbial food webs in Alaskan arctic lakes, and how genetic variability in Alaskan fish populations relates to landscape features.

EPA Experts

Dearfield, Kerry L., b. Washington, DC, September 21, 1952, m. '78, c.2; Education: BS ’74 (Biology) College of William & Mary, Williamsburg, VA; MS ’78 (Cell Biology) University of Pittsburgh, Pittsburgh, PA; Ph.D. ’84 (Pharmacology) George Washington University Medical Center, Washington, DC. Predoctoral fellowship: ’75-’78 graduate teaching fellowship. Current Position: ‘03-present U.S. Environmental Protection Agency, Senior Scientist for Science Policy, Office of the Science Advisor, Washington, DC (help develop policies, guidance, and directions to address cross-cutting, high level EPA science priorities). Previous work experiences: ’95-’03 U.S. Environmental Protection Agency, Biologist/Pharmacologist, Office of Science Policy, Washington, DC; other U.S. Environmental Protection Agency positions starting in ‘84 include: ’84-’87 Pharmacologist, Office of Toxic Substances and ’87-’95 Geneticist/Supervisory Pharmacologist, Office of Pesticide Programs; ’79-’84 Research Associate, Laboratory of Environmental and Radiological Hazard Research, Department of Radiology, George Washington University Medical Center, Washington, DC. Society memberships: Environmental Mutagen Society (EMS; Board of Councilors ’98-’01; Executive Board ‘98-’00; Editorial Board; Public Relations and Communications Committee, ’91-’00, Chair ’97-’99; Program Committee, ‘91, ‘03), Genetic Toxicology Association (GTA; Board of Directors ’88-’91, ‘98-’01; Chairman ’89-’91), Society of Toxicology (SOT), AAAS, Association of Government Toxicologists (AGT; President-elect ’04). Scientific interests: development of genetic toxicology assays with endogenous metabolic activation; modes of action for toxicity (including mutational, physiological and pharmacological mechanisms); use of genotoxicity data in regulatory decisions (heritable risk, carcinogenicity, general toxicity); mutagenicity testing guidelines; development of science policy; development and use of peer review; risk assessment and risk management issues. Publications: numerous peer-reviewed publications on: genetic toxicology of chemicals; genotoxicity in regulatory decisions and guidelines; peer review and risk assessment practices. Address: U.S. Environmental Protection Agency, Office of the Science Advisor (8105R), 1200 Pennsylvania Ave., NW, Washington, DC 20460.

Dr. Robert Frederick is currently a Senior Scientist in the Environmental Protection Agency’s Office of Research and Development at the National Center for
Environmental Assessment (NCEA). With the Agency since 1984, his responsibilities have included coordination of the Biotechnology Risk Assessment Research Program and the risk assessment of genetically modified products. He has served as an EPA representative to the National Institutes of Health Recombinant DNA Advisory Committee; a Federal Coordinating Biotechnology Research Subcommittee; the United States-European Community Task Force on Biotechnology Research; and as EPA coordinator of Office of Science and Technology Policy’s crosscut on biotechnology research. He is currently a member of the Evaluation and Advisory Board for the USAID sponsored Program on Biosafety Systems administered through the International Food Policy Research Institute. Dr. Frederick has extensive international experience in the development of biotechnology regulatory frameworks and biosafety training programs. From 10/93 to 9/96, he was Executive Secretary of the Biotechnology Advisory Commission (BAC) at the Stockholm Environment Institute, Stockholm, Sweden. While with BAC, he organized and taught in six international workshops on biosafety and biodiversity in Nigeria, Argentina, Zimbabwe, Kenya, and Sweden. He has lectured and instructed on biosafety issues in many countries including Argentina, Chile, China, Cameroon, Colombia, Denmark, Germany, Hungary, India, Kenya, Malawi, Mexico, Namibia, Serbia, South Africa, Sweden, Syria, Zambia, and Zimbabwe. In 2002, he spent six weeks with the US Embassy in Lithuania evaluating the status and potential for biotechnology development in that country. Dr. Frederick has published more than 25 articles on biotechnology regulatory development and implementation and is a principal author of a training manual for Biosafety and Risk Assessment in Agricultural Biotechnology available in English, French, Portuguese and Spanish. He earned a PhD at Michigan State University and did his postdoctoral work at Tufts University School of Medicine.

Information Technology – Sensor Networks

Invited Speaker

Dr. Deborah Estrin is a Professor of Computer Science at UCLA and Director of the Center for Embedded Networked Sensing (CENS). Estrin has been instrumental in defining the research agenda for wireless sensor networks, first chairing a 1998 DARPA study and then a 2001 National Research Council study. Estrin's research has focused on the technical challenges posed by these long-lived, autonomous, massively distributed and physically coupled systems, with a particular focus on environmental monitoring. In 2002 she founded the NSF Science and Technology Center for Embedded Networked Sensing. During the earlier parts of her career Professor Estrin focused on the design of network and routing protocols for very large, global networks. Estrin received her Ph.D. in Computer Science from MIT (1985), her BS in EECS from UC Berkeley (1980), and was on the faculty of Computer Science at USC from 1986 through mid-2000. Estrin is a Fellow of the ACM, IEEE, and AAAS and serves on the NSF Advisory Committees for CISE and ERE Directorates, and on the National Research Council Computer Science and Telecommunications Board (CSTB).
Invited Experts

Dr. David A. Caron is the Bayer Professor and Chair, Department of Biological Sciences, at the University of Southern California. He received the Ph.D. in Biological Oceanography from the Massachusetts Institute of Technology and Woods Hole Oceanographic Institute. His research interests focus on marine and freshwater microbial ecology, with emphasis on trophic relationships among single celled microorganisms, and the development of molecular biological approaches for studying the ecology of free-living microorganisms. He has received the Mary Sears Chair for Excellence in Biological Oceanography, WHOI Seymour Hutner Prize (Society of Protozoologists), and is the President-Elect of the Society of Protozoologists.

Dr. Yu-Chong Tai is a Professor of Electrical Engineering and Bioengineering at the California Institute of Technology (Caltech). His main research interest has been MEMS (including micro sensors and actuators) since his graduate school in 1983. He graduated from UC Berkeley working on polysilicon micromechanisms and micromotors, and he joined Caltech in 1989. At Caltech, he built the Caltech MEMS Lab, which is a facility with 7,000 square feet of laboratory (including 3,000 square feet of class-100 clean room). His research interest is to build integrated systems on a chip using MEMS and nano technologies. Currently, he leads a group of about 20 researchers working on various MEMS projects such as integrated micropackaging, microfluidics, bio MEMS, smart MEMS skins, lab-on-a-chip and micro power generator. For the last few years, his research has expanded significantly into polymer MEMS, especially on Parylene material. Examples of his Parylene MEMS works include retinal implants and HPLC-on-a-chip. He has more than 200 technical articles in the field of MEMS. He was involved in many MEMS Conferences and, for example, he was the General Chairman of the 2002 IEEE MEMS Conference. He is also a Subject Editor of the IEEE/ASME J. of MEMS. He is a fellow of the Institute of Physics.

EPA Experts

Dr. John A. Glaser is a research leader for a team of scientists and engineers investigating sustainable technology and biotechnology. As research scientist with the U.S. Environmental Protection Agency in the Office of Research & Development at the National Risk Management Research Laboratory in Cincinnati, Ohio he leads the NRMRL biotechnology research program that is investigating risk management issues related to the pesticide incorporated protectant crops. This research program involves the investigation of remote sensing for monitoring the new crops, new computing capabilities to model the development of resistance in pest populations, toxin assay standardization, and testing of existing simulation models for the evaluation of pest resistance development. He was awarded an EPA Gold Medal for his research on the EXXON Valdez oil spill in Prince William Sound, Alaska. As research leader in fungal technology for treatment of soils and solids contaminated with hazardous waste, he received the joint recognition of USDA and US EPA for the development of a field-scale technology using lignin-degrading fungi. He led two research teams to develop unique bench-scale testing facilities to evaluate bioslurry and compost treatment of hazardous waste contaminated
soils to permit evaluation of the two technologies using contaminated field materials. He has organized a NATO advanced research workshop on "The Utilization of Bioremediation to Reduce Soil Contamination: Problems and Solutions" that was held in Prague, Czech Republic. At this workshop fifty participants in attendance represented 26 nations. NATO has designed the workshop format to enhance the scientific and technical exchange between the Eastern European republics and the West with the desire of improving understanding of our different cultures and societies. Dr. Glaser’s current work focuses on the evaluation of technology and products to meet the criteria of sustainability, e.g. transgenic crops and biobased production. Dr. Glaser has provided technical evaluation of current treaty activities to ensure that they support environmental laws and objectives. He has also been tapped to provide input to US EPA and USDA contributions to the 2002 World Summit in Johannesburg South Africa.

Information Technology – Large Scale Computing/Modeling Applications

Invited Speaker

Dr. Gregory McRae is the Professor of Chemical Engineering in the Department of Chemical Engineering at the Massachusetts Institute of Technology. He received the Ph.D. from the California Institute of Technology. His research interests include atmospheric processes responsible for oxidant formation, acid deposition and global climate change, particulate dynamics, and chemical transport and transformations in multimedia environments. He is also interested in molecular design and computational chemistry, applications of very high performance computing, high-level language compilers and data visualization, and the design of cost-effective public policies for environmental problems. He has received numerous honors and awards for computer graphics and visualization, and has served on various Government technical committees (U.S. EPA, National Research Council, National Academy of Sciences, Sandia National Laboratory, U.S. DOE).

Invited Experts

Mr. James Kasdorf is the Director of Special Projects, Pittsburgh Supercomputing Center, Carnegie-Mellon University and the University of Pittsburgh. Mr. Kasdorf works to influence the computing industry and technology futures, especially processor and system architectures, system effectiveness and efficiency for high-end applications and large-scale storage servers. Mr. Kasdorf was instrumental in establishing the supercomputing centers at the University of Nevada - Las Vegas and the University of Alaska-Fairbanks. His work with university-based supercomputing centers gained international recognition for Westinghouse in 1992 through a Computerworld Smithsonian Award in the Science category. In 1993, the Pittsburgh Supercomputing Center won the Computerworld -Smithsonian Award in the Science category for its simulations of protein interaction with DNA. He has served on various panels regarding high-performance computing for DOE, NSF, NOAA and NIH. He is currently on the

**Dr. Robert Romanosky** is a Technology Manager for Power Systems Advanced Research at the U.S. Department of Energy, National Energy Technology Center in Morgantown West Virginia. He received the Ph.D. from West Virginia University in analytical chemistry/instrumentation. His responsibilities include research activities in Materials, Coal Utilization Science, Bioprocessing, University Research, and Computational Energy Sciences. The Materials Program fosters exploratory research to generate new materials, ideas and concepts to improve the performance or cost of existing fossil systems or to enable development of new systems. The Coal Utilization Program develops advanced sensors, controls, and models for power generation. The modeling development effort works with the Computation Energy Science Program to speed development and reduces costs of new power generation technologies. The Computational Energy Science work entails the development of science-based models of fossil fuel conversion phenomenon, simulation capabilities that couple unit processes in advanced power generation technologies, and virtual power plant simulations.

**Dr. Christine A. Shoemaker** is the Joseph P. Ripley Professor of Engineering, School of Civil and Environmental Engineering, at Cornell University. She is also the past Chairman of the Department of Environmental Engineering, and an elected Fellow of the American Geophysical Union. She is the recipient of the Humboldt Research Prize, as well as the Julian Hinds Award of the American Society of Civil Engineers (ASCE) for her leadership and research in ecosystems management, water resources systems analysis, and groundwater modeling and protection. She has encouraged women in engineering for which she received the "Distinguished Educator Award" from the National Society of Women Engineers. Prof. Shoemaker Co-Chaired an international project on Groundwater Contamination sponsored by SCOPE and the UNEP. She has participated in National Academy of Sciences panels on groundwater contamination and pest management, on the Scientific Advisory Board of the ATSDR.

**Converging Technologies**

**Invited Speaker**

**Dr. William Bainbridge** is Deputy Director, Division of Information and Intelligent Systems, of the National Science Foundation. He holds a Ph.D. in Sociology from Harvard University. He has held NSF positions as the Director of the Knowledge and Cognitive Systems Program, the Human-Computer Interaction Program, and the Innovation and Organizational Change Program, as well as academic positions in Sociology and Anthropology (Towson University, Illinois State University, Harvard University, and University of Washington. He has edited and co-edited several books including the Encyclopedia of Human-Computer Interaction, Converging Technologies
for Improving Human Performance, and Societal Implications of Nanoscience and and Nanotechnology. His research interests have focused on the sociology of religion, family, utopian communities, and science fiction. He has received numerous NSF awards for Collaborative Integration, Above and Beyond the Call of Duty, Collaborative Excellence, and Program Management.

Invited Experts

**Dr. Robert St. Amant** is an Associate Professor in the Department of Computer Science at North Carolina State University. He earned a Ph.D. from the University of Massachusetts. His research interests include a blend of human-computer interaction and artificial intelligence, with an emphasis on planning concepts. He is interested in building intelligent tools to help users with complex tasks. Examples include interface softbots, affordances and tool use, cognitive modeling, and visualization assistance.

**Dr. Nathan Swami** is the Associate Director of University of Virginia’s Institute for Nanoscale & Quantum Engineering Science & Technology (http://www.nanoquest.virginia.edu) and a Steering Committee member of Virginia’s statewide nanotechnology initiative. His research interests are in the surface science of nanoparticles for sensing applications, and in the study of environmental risks from nanoparticles using scenario analysis within a regulatory structure. He received his Ph.D. in Materials Science, at the University of Southern California in Los Angeles, conducting research on novel fullerene and carbon nanotube materials. His prior work as a Principal Scientist at Clinical Micro Sensors, Inc. (a Caltech start-up) and Motorola Labs was in the area of developing microelectronic interfaces to molecular biology for eventual application as DNA sensors and lab-on-chip devices. He served as Director of Virginia’s statewide nanotechnology initiative (http://www.INanoVA.org/), from 2000-2002, and he joined the faculty at UVA’s Electrical & Computer Engineering Department in 2004. For more information: [http://www.ee.virginia.edu/profile.php?ID=90](http://www.ee.virginia.edu/profile.php?ID=90).

EPA Experts

**Dr. Michael Brody** is a senior environmental scientist with EPA’s Office of the Chief Financial Officer. His major responsibilities involve building Agency capacity in environmental futures analysis to support long-term strategic planning. He recently led an international futures project at the North American Commission for Environmental Cooperation. At the Organization for Economic Cooperation and Development he served as EPA’s senior technical lead to the development of the OECD Environmental Strategy for the First Decade of the 21st Century. He also currently manages an environmental capacity building assistance project with the Ministry of Environment of Ukraine. In earlier work at EPA, he was a co-author of EPA’s Framework for Ecological Risk Assessment and other reports on ecological risk assessment and management. He also managed projects in ecosystem valuation and edited a special issue of the Journal of Ecological Economics. He also led EPA training courses in environmental policy and risk assessment, in Eastern Europe. He held previous positions with the US Fish and
Wildlife Service, and with the National Oceanic and Atmospheric Administration through a Sea Grant Fellowship, and earned his Ph.D. in Zoology from the University of Texas at Austin.

**Dr. Nora Savage** obtained a bachelors degree in Chemical Engineering in May 1992 from Prairie View A&M University, in Prairie View, Texas. She received two Masters degrees - one in Environmental Engineering and one in Environmental Science - from the University of Wisconsin-Madison, in Madison, Wisconsin in May 1995, and a doctoral degree in Environmental Science from the same institution in August 2000. She has had summer internships at the Ernest Orlando Lawrence Berkeley and Lawrence Livermore National Laboratories, and at the Eastman Kodak Company as an undergraduate student. She worked for seven years at the Wisconsin Department of Natural Resources in the Air Monitoring Division in Madison while attending graduate school. In addition, she worked as a mentor/counselor for both high school and undergraduate students through involvement in various educational programs at UW-Madison, including serving as a Counselor for the Ronald E. McNair Program. Upon completion of her doctorate, she obtained a one-year post-doctoral research associate position at Howard University, where she taught a senior-level Civil Engineering class and worked on various educational initiatives at the graduate school. She is currently working as an environmental engineer at the Environmental Protection Agency in Washington, DC in the Office of Research and Development. Her focus areas include nanotechnology and environmental justice. She is also involved in various civic and scientific organizations, both as a volunteer and as a member.
APPENDIX C

BREAK OUT GROUP PARTICIPANTS
NANOTECHNOLOGY BREAK OUT GROUP

Invited Speaker: Dr. Roland Clift

Invited Experts: Dr. Catherine Alexander
Dr. Matteo Pasquali

EPA Experts: Dr. Michael Gill
Dr. Martha Otto
Dr. Dennis Utterback

SAB Breakout Chair: Dr. Thomas Theis

SAB Breakout Members: Dr. Viney Aneja
Dr. Brian Dodd
Dr. Wayne Gray
Dr. Roger E. Kasperson
Dr. Reid Lifset
Dr. Randy Maddalena
Dr. Genevieve Matanoski
Dr. Armistead (Ted) Russell
Dr. Gary Sayler
Dr. David Sedlak
Dr. Deborah Swackhamer
Dr. Lauren Zeise
Dr. Yousheng Zeng

Designated Federal Officer: Ms. Kathleen White
BIOTECHNOLOGY – BIOPRODUCTION BREAK OUT GROUP

Invited Speaker: Dr. Harold Monboquette

Invited Experts: Dr. Robert M. Kelly
Dr. Robert Mark Worden

EPA Experts: Ms. April Richards

SAB Break Out Chair: Dr. Michael McFarland

SAB Breakout Members: Dr. Kenneth Dickson
Dr. Ivan J. Fernandez
Dr. Catherine Kling
Dr. Guy Lanza
Dr. Mark Miller
Dr. James Oris
Dr. John R. Smith
Dr. William Smith

Designated Federal Official: Dr. Thomas Armitage
BIOTECHNOLOGY – GENOMICS BREAK OUT GROUP

Invited Speaker: Dr. Bruce Aronow

Invited Experts: Dr. Mark Pershouse
Dr. Parke Rublee

EPA Experts: Dr. Kerry Dearfield
Dr. Robert Frederick,

SAB Breakout Chair: Dr. James Bus

SAB Breakout Members: Dr. George Corcoran
Dr. Mary Davis
Mr. Keith Harrison
Dr. Katherine Kiel
Dr. James E. Klaunig
Dr. Michael Kleinman
Dr. George Lambert
Dr. Ulrike Luderer
Dr. Melanie Marty
Dr. Gina Solomon

Designated Federal Officer: Dr. Suhair Shallal
INFORMATION TECHNOLOGY- SENSOR NETWORKS BREAKOUT GROUP

Invited Speaker: Dr. Deborah Estrin

Invited Experts: Dr. David A. Caron
Dr. Yu-Chong Tai

EPA Experts: Dr. John A. Glaser

SAB Breakout Chair: Dr. Bob Twiss

SAB Breakout Members: Dr. Anna Alberini
Dr. Kenneth Cummins
Dr. T. Taylor Eighmy
Dr. William H. Glaze
Dr. Stanley B. Grant
Dr. Philip Hopke
Dr. Allan Legge
Dr. Joan B. Rose
Dr. Laura Steinberg

Designated Federal Officer: Mr. Fred Butterfield
Invited Speaker: Dr. Gregory McRae

Invited Experts: Mr. James Kasdorf
Dr. Robert Romanosky
Dr. Christine A. Shoemaker

SAB Breakout Chair: Dr. H. Barry Dellinger

SAB Breakout Members: Dr. Dallas Burtraw
Dr. John C. Crittenden
Dr. A. Myrick Freeman
Dr. William C. Griffith
Dr. Michael Kavanaugh
Dr. Charles Pittinger
Dr. Kathryn Saterson
Dr. Chris Walcek

Designated Federal Officer: Mr. Daniel Fort
## CONVERGING TECHNOLOGIES – BREAK OUT GROUP

**Invited Speaker:** Dr. William Bainbridge

**Invited Experts:**
- Dr. Robert St. Amant
- Dr. Nathan Swami

**EPA Experts:**
- Dr. Michael Brody
- Dr. Nora Savage.

**SAB Breakout Chair:** Dr. Dave Rejeski

**SAB Breakout Members:**
- Dr. Gilles Bussod
- Dr. Trudy Cameron
- Dr. Bart Croes
- Dr. Ted Gayer
- Dr. Meryl Karol
- Dr. Jill Lipoti
- Dr. Morton Lippmann
- Dr. M. Granger Morgan
- Mr. Ralph Morris
- Dr. William Pizer

**Designated Federal Officer:** Dr. Angela Nugent
APPENDIX D

BREAK OUT GROUP DISCUSSION QUESTIONS
BREAK OUT GROUP DISCUSSION QUESTIONS

Opportunities

1. Which technologies within the scope of this break-out session are likely to offer the greatest application potential for protecting the environment?

2. What opportunities may offer the greatest potential in the near term (3-5 years)?

3. What science and research issues need to be addressed to take effective advantage of those opportunities?

Challenges

4. What are likely to be the most significant challenges for environmental protection presented by these new technologies?

5. Which challenges would be most urgent to address in the near term (3-5 years)?

6. What science and research and environmental policy issues need to be addressed to confront these challenges effectively?

Future Role of the SAB

7. If the SAB is to prepare to help EPA meet those opportunities and challenges, how could it do so most successfully?
So long as we do not, through thinking, experience what is, we can never belong to what will be.

The flight into tradition, out of a combination of humility and presumption, can bring about nothing in itself other than self deception and blindness in relation to the historical moment.

**Information Infrastructure Boundary Issues**

<table>
<thead>
<tr>
<th>Level</th>
<th>Method of Study</th>
<th>Main Impact (Physical v. Cultural)</th>
<th>Typical IE Design Issues</th>
</tr>
</thead>
<tbody>
<tr>
<td>Artifact manufacture</td>
<td>Traditional environment and safety compliance (end-of-pipe)</td>
<td>Physical</td>
<td>Energy consumption in manufacture; toxics in product</td>
</tr>
<tr>
<td>Artifact over lifecycle</td>
<td>DfE, LCA</td>
<td>Physical</td>
<td>Understanding conditions of use; energy consumption in use; end-of-life management</td>
</tr>
<tr>
<td>Construction and maintenance of networks</td>
<td>Systems engineering</td>
<td>Physical</td>
<td>Evolution of technology (from telephony to internet protocol, wireless); interactions of systems components; efficiency per unit service; systems boundary</td>
</tr>
<tr>
<td>Services (e.g., broadband to home)</td>
<td>N/A</td>
<td>Physical/Cultural</td>
<td>Definition of “service”; relationship of service to physical network and social practices</td>
</tr>
<tr>
<td>Social practices based on services (e.g., teleworking)</td>
<td>N/A</td>
<td>Cultural</td>
<td>Both short and long term impacts important (and may not align); difficult to predict because of cultural component; triple bottom line implications, especially social (“digital divide”)</td>
</tr>
<tr>
<td>Knowledge economy/ infosphere</td>
<td>N/A</td>
<td>Cultural</td>
<td>Impact on social constructs (“wilderness”, “environment”). Enable postmodernist fragmenting of values? Enable world as artifact (real time comprehensive monitoring systems)? Substitution of information for energy/materials? End of “natural history” w/ human contingency built into natural system?</td>
</tr>
</tbody>
</table>

**Future Scan: What Do We Know**

1. The future will be technologically discontinuous as rates of technological evolution continue to accelerate - scenarios include:
   - NBIC (nano, bio, ICT, and cogsci convergence - from “monkey arm” to “brain in the plane”)
   - “Functional immortality” within 50 years (Netbased or wetware, your choice)
   - Multicellular organisms from molecules, 10 to 30 years (and scale ups - grow tables, chairs) - Viruses already done.
   - Increased biodiversity - but “built”, not “natural”
   - “Custom reality” - integrate virtual and physical
   - “Custom reality” - cogsci and ICT introduce “animal tourism”, where you can map your cognitive system into that of another species
   - Large “natural” systems integrated into human systems, and therefore their dynamics dominate - e.g., carbon cycle, hydrologic cycle, Everglades, biosystems at all scales become commoditized, and therefore “designed” by humans.
Future Scan: What Do We Know

- From the era of “simple systems” to the era of “complex adaptive systems”
  - Current policies, laws, and institutional structures assume “simple” systems – that is, systems are knowable, exhibit understandable causality, and are controllable
  - But emergent behavior of interest now arises from complex systems: unknowable, uncontrollable, with causal links that are indeterminate or at least not clear
  - CAS knowable only in real time, requiring policy, design, engineering, and management mental models shift from a priori control and definition to realtime adjustment and dialog
  - Examples of integrated human/natural CAS earth systems: Everglades, Baltic and Aral Sea; urban systems; major technology systems (e.g., transportation networks, Internet); carbon and nitrogen cycles

Future Scan: What Do We Know

- Ethical systems in age of CAS require serious augmentation
  - Traditional ethical judgments fundamentally based either on intent or outcome as compared to norm
  - With CAS, cannot judge intent because agent cannot predict system response; cannot judge based on outcome because agent cannot know that a priori
  - Need to move to process-based rather than outcome-based ethics: has one chosen right process to interact with CAS
  - Engineering ethics micro-based (individual practitioner); need macro-based (who or what is responsible for, e.g., Internet, biotech, or cogsci)
  - Ethical systems assume foundational truths; what happens when the underlying cultural constructs become contingent on rapid time cycle?
Future Scan: What Do We Know

- Fundamental structure of human cognition changing at accelerating pace
  - Internet becomes memory unit: facts stored in cyberspace, human brain increasingly provides questions and meaning
  - Technology as window through which humans perceive physical reality (Phoenix Zoo: kids raised on Nature Channel and Net time cycles can’t identify with “realtime” animals)
  - “Reality” as built structure of particular cultural constructs (“jungle” vs. “rain forest”; “swamp” vs. “wetlands”; “natural” vs. “supernatural” vs. “natural – human” dichotomy; “wilderness – evil” vs. “wilderness – Edenic”) – we used to be able to view constructs as fixed; now they are contingent
  - How to think when all concepts are contingent and changing

Future Scan: What Do We Know

- What is “Human”?
  - Is there any “normal”?
  - By what right do we impose our idea of current biological and cognitive limits on future generations?
  - Who or what decides what is “human”?
  - Is that question already obsolete?
  - What part of “human” is contingent, and what part is not – or is “human” all contingent?
  - Equity: who gets to evolve? Who decides?
  - Ethics and politics: what kind of conflict will occur if – when? - elements of “human” deeply held by powerful religions to be absolute are demonstrated to be contingent?
Bothersome Questions

- Should it be the Technology and Science Advisory Board, and shouldn’t an Industry Advisory Board be added?
- Should EPA become a competency that diffuses itself throughout government?
- How will EPA, and government generally, develop the ability to dialog with, rather than regulate, complex human/natural systems?
- How will EPA develop the ability to operate on a time cycle that aligns with the phenomenon for which it is responsible?
- How will EPA function as its core conceptual foundations – “environment,” “wilderness,” “nature” - become increasingly contingent, and change substantively over shorter time periods?
- What is EPA’s role as the world increasingly becomes a product of human design?
- How does EPA avoid becoming more and more effective at less and less important tasks as environmental impacts are increasingly a function of strategic and non-environmental technological and business systems (can the nano model be generalized)?

Global Economic History: 1500 - 1992

<table>
<thead>
<tr>
<th>Date</th>
<th>World GDP (indexed to 1500 = 100)</th>
<th>Per Capita World GDP (1990 dollars)</th>
<th>Per Capita (indexed to 1500 – 100)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1500</td>
<td>100</td>
<td>565</td>
<td>100</td>
</tr>
<tr>
<td>1820</td>
<td>290</td>
<td>651</td>
<td>117</td>
</tr>
<tr>
<td>1900</td>
<td>823</td>
<td>1,263</td>
<td>224</td>
</tr>
<tr>
<td>1950</td>
<td>2,238</td>
<td>2,138</td>
<td>378</td>
</tr>
<tr>
<td>1992</td>
<td>11,664</td>
<td>5,145</td>
<td>942</td>
</tr>
</tbody>
</table>

Source: Based on J. R. McNeill, 2000, Something New Under the Sun (New York: W. W. Norton & Company), Tables 1.1 and 1.2. (pp. 6-7, and sources cited therein.)
### Energy Production and Consumption 1800 - 1990

<table>
<thead>
<tr>
<th>Year</th>
<th>Biomass (in millions of metric tons)</th>
<th>Coal (in millions of metric tons)</th>
<th>Oil (in millions of metric tons)</th>
<th>Total Use (in millions of metric tons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1800</td>
<td>1,000</td>
<td>10</td>
<td>0</td>
<td>400</td>
</tr>
<tr>
<td>1900</td>
<td>1,900</td>
<td>1,000</td>
<td>20</td>
<td>1,900</td>
</tr>
<tr>
<td>1990</td>
<td>1,800</td>
<td>5,000</td>
<td>3,000</td>
<td>30,000</td>
</tr>
</tbody>
</table>

Total Use, Indexed to 1900

<table>
<thead>
<tr>
<th>Year</th>
<th>Total Use, Indexed to 1900 (in billions of metric tons of oil equivalent)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1800</td>
<td>21</td>
</tr>
<tr>
<td>1900</td>
<td>100</td>
</tr>
<tr>
<td>1990</td>
<td>1,580</td>
</tr>
</tbody>
</table>

1) in millions of metric tons
2) all forms, millions of metric tons of oil equivalent

Source: Based on J. R. McNeill, 2000, Something New Under the Sun (New York: W. W. Norton & Company), Table 1.4 and 1.5, pp. 14-15, and sources cited therein.

### Global Freshwater Use 1700 - 2000

<table>
<thead>
<tr>
<th>Year</th>
<th>Withdrawals (km³)</th>
<th>Withdrawals (per capita)</th>
<th>Irrigation</th>
<th>Industry</th>
<th>Municipal</th>
</tr>
</thead>
<tbody>
<tr>
<td>1700</td>
<td>110</td>
<td>0.17</td>
<td>90</td>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>1800</td>
<td>243</td>
<td>0.27</td>
<td>90</td>
<td>3</td>
<td>7</td>
</tr>
<tr>
<td>1900</td>
<td>580</td>
<td>0.36</td>
<td>90</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>1950</td>
<td>1,360</td>
<td>0.54</td>
<td>83</td>
<td>13</td>
<td>4</td>
</tr>
<tr>
<td>1970</td>
<td>2,590</td>
<td>0.70</td>
<td>72</td>
<td>22</td>
<td>5</td>
</tr>
<tr>
<td>1990</td>
<td>4,130</td>
<td>0.78</td>
<td>66</td>
<td>24</td>
<td>8</td>
</tr>
<tr>
<td>2000 (est.)</td>
<td>5,190</td>
<td>0.87³</td>
<td>64</td>
<td>25</td>
<td>9</td>
</tr>
</tbody>
</table>

1) In richer countries, water use stabilized after the 1970’s. In the U.S., total water use peaked around 1980 and had declined by a tenth as of 1995, despite simultaneous addition of some 40 million people.

Source: Based on J. R. McNeill, 2000, Something New Under the Sun (New York: W. W. Norton & Company), Table 5.1, pp. 121, and sources cited therein.
**Carbon Cycle Governance System**

- **Biomass**
  - CO₂ Emitted
  - Fossil Fuel Energy Production System
    - Fossil Fuel Power Plant
      - Electricity
        - Fixed Uses
        - Buildings
        - Mobile Uses (e.g., transportation)
      - CO₂ Sequestered
  - H₂

- **Fossil Fuel**
- **Municipal Waste**
  - CO₂ Sequestered

**Control Functions**
- Input: B + xMW
- Output: CO₂ Emitted, CO₂ Sequestered
- Target: CO₂ Concentration Metric: in Atmosphere

---

**Carbon Cycle: Earth Systems Engineering Schematic**

- **Water cycle**
- **Biodiversity and habitat systems**
- **Nitrogen cycle**
- **Carbon cycle**
- **Other cycles**
  - Other systems
  - Energy system
  - Ocean fertilization
  - Biomass agriculture
  - Fossil fuel industry, etc.
  - Fish farming, etc.
  - Organic chemical industry, etc.

- **Implementation at firm, facility, technology and process level**

**Engineering/Management of Earth system relationships**

- **Engineering/Management of carbon cycle**

- **Traditional engineering disciplines**

---

Dr. Braden Allenby
Earth Systems Engineering and Management Principles:  Design and Engineering

- Earth systems engineering and management (ESEM) initiatives should all be characterized by explicit and transparent objectives or desired performance criteria, with quantitative metrics which permit continuous evaluation of system evolution (and signal when problematic system states may be increasingly likely).

- Design, engineering, and implementation of ESEM initiatives must not be based on implicit or explicit models of centralized control in the traditional rigid sense. Rather than attempting to completely define or dominate a system, the ESEM professional will have to see themselves as an integral component of the system, coupled with its evolution and subject to many of its dynamics. This will require a completely different psychology of engineering.

- ESEM projects should be incremental and reversible to the extent possible.

- ESEM should aim for resiliency, not just redundancy, in systems design. A resilient system resists degradation and, when it must, degrades gracefully even under unanticipated assaults; a redundant system may have a backup mechanism for a particular subsystem, but still may be subject to unpredicted catastrophic failures.

- ESEM should aim for inherently safe, rather than engineered safe, design. An inherently safe system fails in a noncatastrophic way; an engineered safe system is designed to reduce the risk of a particular catastrophic failure mode, but there is still a finite probability that such a failure may occur.

Earth Systems Engineering and Management Principles: Governance

- Earth systems engineering and management (ESEM) projects and programs by definition raise important scientific, technical, economic, political, ethical, theological and cultural issues. The only appropriate governance model under these conditions is one which is democratic, transparent, and accountable.

- ESEM governance mechanisms should foster inclusive, multicultural dialog.

- ESEM governance models, which deal with complex, unpredictable systems, must accept high levels of uncertainty as endogenous to the discourse, and view ESEM policy development and implementation as a dialog with the relevant systems, rather than a definitive endpoint. ESEM governance systems should accordingly place a premium on flexibility and the ability to evolve in response to changes in system state, and recognize the policymaker as part of an evolving ESEM system, rather than an agent outside the system guiding it.

- The ESEM environment and the complexity of the systems at issue require explicit mechanisms for assuring continual learning, including ways in which assimilation of the learning by stakeholders can be facilitated.

- There must be adequate resources available to support both the immediate ESEM project and the science and technology research and development necessary to ensure that the responses of the relevant systems are understood.
Earth Systems Engineering and Management Principles: Theory

- Only intervene when required and to the extent required (humility in the face of complexity).
- At the level of earth systems engineering and management (ESEM), projects and programs are not just technical and scientific in nature, but unavoidably have powerful cultural, ethical, and religious dimensions.
- Unnecessary conflict surrounding ESEM projects and programs can be reduced by separating social engineering from technical engineering dimensions.
- ESEM requires a focus on systems as systems, rather than as just constituent artifacts; a dynamic, rather than static, mental model of underlying phenomenon.
- Boundaries around ESEM projects and programs should reflect real world couplings and linkages through time, rather than disciplinary or ideological simplicity.
- Major shifts in technologies and technological systems should be evaluated before, rather than after, implementation.
NANOTECHNOLOGY

Professor Roland Clift,
Centre for Environmental Strategy,
University of Surrey, GUILDFORD,
Surrey GU2 7XH, UK
and
Royal Society/Royal Academy of Engineering
Working Group on “Nanoscience and nanotechnologies: opportunities and uncertainties”

• An emerging technology based on solid particles in the size range where their properties are determined by size and surface condition rather than bulk properties:
  typically 1 – 100nm
  (nm = nanometer = 10^{-9}m)
  comparable in size to viruses
SOME POSSIBLE APPLICATIONS

Evolutionary:
- Batteries and fuel cells
- “Smart” packaging and labelling
- Electronics and displays
- Catalysts and separation membranes
- Paints and coatings

Longer Term:
- Lubricants
- Composites
- Components and prosthetics
- Diagnosis and targeted drug delivery

“Blue Sky”:
- Self-replicating robots and assemblers

THREE AREAS OF CONCERN

1. Are the quantifiable benefits real? eg. energy savings
2. Health and environmental impacts of substances and manufactured products
3. Social impacts of new and emerging technologies
LIFE CYCLE ASSESSMENT

PRIMARY RESOURCES

- Extraction
- Material purification
- Manufacturing

Energy conversion

Recovery

PRODUCT IN USE

Wastes and Emissions

HEALTH AND ENVIRONMENTAL IMPACTS

Hazard: human toxicity or ecotoxicity of material

Risk: includes probability that “receptor” is actually exposed to material
**SOURCE pathway RECEPTOR**

Direct:
- Inhalation
  - eg. workplace
  - Emissions from vehicles, combustion, etc
  - Natural sources; eg. volcanoes
- Dermal exposure; eg. sun-screens; cosmetics
- Ingestion; eg. In water

Indirect: primarily via food chain

---

**BASIS FOR REGULATION**

- Toxicity estimation or testing (hazard):
  - animal testing
  - “in vitro” tests
  - “in silico” tests (incl. QSAR’s)
  - epidemiology
- Persistence
- Bioaccumulation
CAN NEW MATERIALS BE REGULATED AS “NEW CHEMICALS”?

Probably, but there are unresolved questions:

- size matters…. (surface area?)
- surface properties matter….  
- How do these affect persistence and bioaccumulation?
- Many products with small quantities

How to define production thresholds?
- Are current risk assessment procedures appropriate and sufficient?
- Regulate as consumer products or as medicines?
- Labelling of products?
PRECAUTIONARY APPROACH IMPLIES

- Presumption against release of nanoparticles into the environment:
  - Fuel additives (e.g., cerium oxide)
  - Bioremediation (e.g., iron; other metals)
  - End-of-life products

- Nanoparticles likely to be made at point of use

- Makes arguments for a moratorium on production irrelevant….

- Unless and until nanoparticles become commodities, this is probably not a general issue anyway….

---

Health and environmental impacts are uncertain.

Social impacts are completely unknown…
Bioprocessing: Opportunities & Challenges

Harold G. Monbouquette, Chemical Engineering Department, University of California, Los Angeles, Box 951592, Los Angeles, CA 90095-1592, harold@seas.ucla.edu

- The broad universe of metabolic processes and enzyme activities for exploitation
- Specialty chemical bioprocessing: “Cheap stuff in, expensive stuff out”
- The promising biorefinery concept
- New bioproducts and bioprocesses

Diverse Lifeforms and Metabolic Pathways

- Hyperthermophiles in bold
- Hyperthermophiles appear to be the most primitive organisms

Diverse Enzyme Toolkit of Industrial Utility

<table>
<thead>
<tr>
<th>Enzyme class</th>
<th>Number classified available</th>
<th>Reaction type</th>
<th>Utility</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Oxidoreductases</td>
<td>650 90</td>
<td>Oxidation-reduction: oxygenation of C-H, C-C, C-O bonds, or overall removal or addition of hydrogen atom equivalents</td>
<td>+++ 25%</td>
</tr>
<tr>
<td>2. Transfereases</td>
<td>720 90</td>
<td>Transfer of groups: aldehydic, ketonic, acyl, sugar, phosphoryl or methyl</td>
<td>+ -5%</td>
</tr>
<tr>
<td>3. Hydrolases</td>
<td>636 125</td>
<td>Hydrolysis: formation of esters, amides, lactones, lactates, epoxides, nitriles, esters, glycosides</td>
<td>+++ 65%</td>
</tr>
<tr>
<td>4. Lyases</td>
<td>255 35</td>
<td>Addition-elimination of new molecules on C=C, C=N, C=O bonds</td>
<td>++</td>
</tr>
<tr>
<td>5. Isomerases</td>
<td>120 6</td>
<td>Isomerizations such as racemization, epimerization</td>
<td>± -1%</td>
</tr>
<tr>
<td>6. Ligases</td>
<td>80 5</td>
<td>Formation-cleavage of C-O, C-S, C-N, C-C bonds with concomitant triphosphate cleavage</td>
<td>± -1%</td>
</tr>
</tbody>
</table>

*The estimated ‘utility’ of an enzyme class for the transformation of non-natural substrates ranges from +++ (very useful) to ± (little use) [81]. The values (%) indicate the percentage of research performed with enzymes from a given class for the 1987-96 period.*

---

"Cheap stuff in, Expensive stuff out": The Penicillin Story

- 1939: Penicillin culture concentration ~0.001 g/L
- 1940: Unproven fermentation process chosen over chemical synthesis
- Microbiologists engage in mutation/selection; Engineers designed large-scale submerged culture process
- 1945: Sufficient penicillin produced for ~100,000 patients
- Current yields: ~50 g/L; Chemical synthesis approach still cannot compete!
Can we engineer life for the economical, environmentally friendly production of chemicals?

Metabolic Engineering: Genes from Three Microbes Cloned into *E. coli* for Production of the Carotenoid, Astaxanthin

Aromatic Biosynthesis Pathways Lead to Industrial Products

Advantages
- Aqueous solvent
- Moderate T, p
- Non-toxic intermediates
- Lower raw material cost

E4P, D-erythrose-4-phosphate; PEP, phosphoenolpyruvate; DAHP, 3-deoxy-D-arabino-heptulosonate-7-phosphate; DHQ, 3-dehydroquinate; DHS, 3-dehydroshikimate; PABA, p-aminobenzoic acid; PHB, p-hydroxybenzoic acid; Phe, phenylalanine; Tyr, tyrosine; Trp, tryptophan.


The Biorefinery Concept for Production of Chemicals (Cargill)

**Global Material & Energy Balances for Assessment of Environmental Impact**

- **PLA 1**: Current process
  - Corn starch
  - Dehise CWS
  - Lactic acid
  - PLA

- **PLA BWP**: 2002 target
  - Corn residue
  - Sugarcane Biorefinery
  - Lactic acid
  - PLA


**Slow Enzymatic Conversion of Cellulosics Avoided by Bioprocessing of Biomass-Derived Synthesis-Gas**

*Figure 5. Schematic diagram of a microbubble-sarged, synthesis-gas fermentation with a membrane-based cell-recycle system.*

Can enzymes be integrated into chemical synthesis processes to improve economics and to reduce environmental impact?

**Hyperthermophilic Enzymes for HFCS Production**

The A. fulgidus Alanine Dehydrogenase

- Alanine dehydrogenase catalyzes the reversible conversion of pyruvate to L-alanine:

\[
\text{O} \quad \text{CO}_2^- + \text{NH}_4^+ + \text{NADH} + \text{H}^+ \leftrightarrow \text{NH}_4^+ + \text{NAD}^+ + \text{H}_2\text{O} + \text{CO}_2
\]

- Specific activity in the aminating direction: 203 U/mg (Unit defined as 1 µmol NADH oxidized per minute at 86 °C)

- Biocatalytic applications include the synthesis of L-amino acids such as: L-alanine, 3-fluoroalanine, L-serine, and \textsuperscript{15}N-labelled L-alanine

\begin{table}
\centering
\begin{tabular}{|c|c|c|}
\hline
Temperature (°C) & Activity (%) & Activity (%) \\
\hline
20 & 203 U/mg & 203 U/mg \\
40 & 60 U/mg & 60 U/mg \\
60 & & \\
80 & & \\
100 & & \\
\hline
\end{tabular}
\end{table}

A. fulgidus alaDH shows extended stability in solution at 20 °C and retains 30% activity at 25 °C
**L-Alanine Reactor**

- Demonstrate AlaDH from *A. fulgidus* is an effective biocatalyst at room temperature
- 2nd enzyme (yeast formate dehydrogenase) for NADH regeneration
- Alanine dehydrogenase purified 3 months before reactor set-up and stored in solution at room temperature

**Initial Conditions**
- 50 mM pyruvate
- 500 mM NH₃, formate
- 100 mM Tricine pH 8.0
- 0.2 mM NAD
- 0.48 U/ml FDH
- 0.115 U/ml AlaDH
- Room Temperature

**Reaction Equations**

\[
\begin{align*}
\text{NH}_3 + \text{pyruvate} \rightarrow \text{L-alanine} \\
\text{AlaDH} + \text{NADH} + \text{H}^+ \rightarrow \text{CO}_2 + \text{formate}
\end{align*}
\]

**A. fulgidus AlaDH gives ~5 million turnovers in ~6 days at room T with no activity loss**

[Graph showing the remaining activity of AlaDH over time with and without AlaDH, indicating no significant loss of activity.]
Bioprocesses Provide New Products

- Chiral drugs, flavorings, aromas, herbicides, pesticides
- Polylactic acid
- Hyperthermophilic glycoside hydrolases for oil/gas well fracturing

Generalized EMAT for Detection of Endocrine Disrupting Agents

- APGP: p-aminophenyl β-D-galactopyranoside
- ONPG: o-nitrophenyl β-D-galactopyranoside

Detection Methods
- Optical
  - Color formation
- Electrochemical
  - Current flow
Detection of EDCs at < 10 ppb

- Bisphenol-A
- Genistein
- Nonylphenol

Opportunities

- Genomics enables design of life for environmentally friendly synthesis of chemicals from renewable resources
- Enzymes improve selectivity and yield of chemical synthesis processes at moderate conditions thereby reducing environmental impact
Challenges

- What is the true environmental impact of a biorefinery?
- Plant/microbe/bioprocess design for better cellulosics utilization
- Limited knowledge of metabolism, including control mechanisms
- Enzyme identification/design/evolution for synthetic reactions
- Health/environmental effects of new classes of products
Towards Genomics-based Analyses of Environmental Agent-Impact on Biological Systems

Bruce Aronow, Ph.D.
Associate Professor and Scientific Director
Center for Computational Medicine
Cincinnati Children's Hospital Medical Center
College of Medicine, University of Cincinnati

Environmental Agents Can Act at any Level of Genomic Information Flow

Genomics
- Gene-Regulation
- mRNA Expression
- cell type specificity
- Genetics
- QTL

Proteomics
- Protein Expression
- Structure
- Interaction
- Localization
- Pathways

Physiomics
- Tissue Dynamics
- Systems Biology
- Outcome: Clinical, Population

Structure -> Activity -> Function

Outcome: Clinical, Population
Environmental Agent Impact on Biological Systems

Environmental Agent Impact

- Biosphere
  - population loss
  - environment niche disruption
  - species sensitivity
  - loss of biodiversity

- Individual Organism
  - morbidity
  - mortality
  - risk

General Goals for Impact Assessment

Monitoring:
- environmental damage
- environmental agent-induced morbidity and mortality

Prediction:
- dangerous environmental agents
- at risk populations, species
- at risk environments
- sensitive individuals

Using Genomics to Aid in the Assessment of Environmental Agent-Impact on Biological Systems

<table>
<thead>
<tr>
<th>Environments</th>
<th>Organisms</th>
<th>Environmentally Damaging Agents</th>
<th>Biological Impacts</th>
<th>Genomics-based Assisted Monitoring of Biological Impact</th>
</tr>
</thead>
</table>

Dr. Bruce Aronow
APPENDIX H-SLIDE PRESENTATION
Biotechnology-Genomics

Nanotechnology, Biotechnology, and Information Technology Workshop

Systems Biology Approaches for the Integration of Genomics Data and Analysis into Assessment of Environmental Agent-Impact

Model Systems:
- Knowledge-Generation
- Reference Database Creation

Real-World Monitoring:
- Impacts
- Etiologies

Construction of Genomic/Proteomic Expression Databases
Toxic Agents/Altered Environments Impacting Organisms/Systems

Real-World Monitoring: Damage, Organisms, Tissues, Environments, Consequences

Creation of Systems Biology Integrated Databases:
Multi-Organismal, Tissue, Toxic Agent, Clinical, Phenotypic, Genetic, Gene Expression Databases

Analysis Goals
- Affected Samples
- Activated Pathways
- Cryptic Agents
- Therapeutic Opportunities
- Preventable/Critical Situations

Dr. Bruce Aronow
**Genomics-based Monitoring of Environmental Agent Impact: Obstacles**

### Technical Barriers
- Quantitative methods
- Lack of:
  - full genomic sequences
  - references and technical standards
  - annotation datasets of a range of “at-risk” populations
- Heterogeneity of descriptor data

### Immaturity of Scientific Knowledge
- Lack of knowledge of:
  - cross-species and -environment generalization
  - genes that confer environmental agent sensitivity
- Poor assessment of normal states and damage indices for environments
- Lack of reference data for model environmental agent-induced morbidity and mortality

---

**Optimizing Distributed, Synergistic Use of MicroArray Technology:**

Experimental design considerations for evaluation of platform performance and data reliability

<table>
<thead>
<tr>
<th>&quot;A-E“ dilution experiment</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
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</thead>
<tbody>
<tr>
<td>Day 1 whole mouse RNA (%)</td>
<td>100</td>
<td>75</td>
<td>50</td>
<td>25</td>
<td>0</td>
</tr>
<tr>
<td>Mouse adult colon RNA (%)</td>
<td>0</td>
<td>25</td>
<td>50</td>
<td>75</td>
<td>100</td>
</tr>
</tbody>
</table>

**Samples:**

Only 3 patterns should be observable

Dr. Bruce Aronow
Evaluating the use of a “Universal Reference” calibration standard in experimental design: data normalization

Cross-Institutional Reproducibility
Cross-Platform Reproducibility

Slope from linear least square regression approach to the comparison of reproducibility

Construction and Mining of a Generalized Mouse Gene Expression Database

8734 genes X 100 samples X 2 replicate arrays
Tissue and Organ-Specific Gene Expression

Mouse Genes Highly Expressed in CNS

Data description:
- Novartis U74A dataset
- 13 CNS tissues (2 replicates)
- 32 non-CNS tissues and cell lines

Filters:
- 1.3 fold change in average expression
- Welch t-test, p = 0.05, Benjamini and Hochberg false discovery rate
- 674 probesets were identified; 564 unique genes with symbol
Human Genes Highly Expressed in CNS

Data description:
- Novartis U133A dataset
- 22 CNS tissues (2 replicates)
- 57 non-CNS tissues and cell lines

Filters:
- 1.5 fold change in average expression
- Welch t-test, p = 0.05, Benjamini and Hochberg false discovery rate
- 1350 probesets were identified

Check Expression Pattern of Ortholog Gene Pairs Present in Both Genomes
Expression Pattern Similarity of Genes Highly Expressed in CNS of Humans and Mice

478 Human-Mouse ortholog pairs from 596 previously selected genes

Can Normal Colon Development Provide Insight Into Colon Cancer Gene Expression Programs?

Pooled twenty individual embryonic colon RNA samples from each time point using CD-1 outbred strain, and then repeated using C57BL/6 inbred strain

Pooled samples from each time point underwent two rounds of linear amplification

Cy5-labeled cDNA from linearly amplified product from each time point and from both strains hybridized with Cy3-labeled C57BL/6 E17.5 total pup cDNA as reference

Hybridizations repeated 3X each, dyes not switched

Cy5-labeled amplified embryonic colon cDNA

Cy3-labeled C57BL/6 E17.5 total pup cDNA reference

15K NIA staged mouse embryonic cDNAs and 5K Research Genetics mouse cDNAs
Normal Mouse Colon Development

GeneChip®
MOE430

Comparative Profiling of Mouse Models of Human Colon Cancer: Chemical & Genetic Tumor Models

<table>
<thead>
<tr>
<th>Model</th>
<th>Lab</th>
<th>RNA isolated</th>
<th>Intact RNA†</th>
<th>RNA Amplified</th>
<th>Microarray‡</th>
</tr>
</thead>
<tbody>
<tr>
<td>AOM_chemical</td>
<td>Threadgill</td>
<td>25</td>
<td>13/25</td>
<td>6/10</td>
<td>6/6</td>
</tr>
<tr>
<td>ApcMin_BR-SW_F1</td>
<td>Dove</td>
<td>47*</td>
<td>10/34</td>
<td>7/10</td>
<td>5/7</td>
</tr>
<tr>
<td>ApcMin_C57BL6</td>
<td>Groden</td>
<td>47*</td>
<td>10/34</td>
<td>7/10</td>
<td>5/7</td>
</tr>
<tr>
<td>Smad3 -/-</td>
<td>Graf</td>
<td>15</td>
<td>10/15</td>
<td>5/10</td>
<td>5/5</td>
</tr>
<tr>
<td></td>
<td>Coffey</td>
<td>6</td>
<td>6/6</td>
<td>5/6</td>
<td>5/5</td>
</tr>
<tr>
<td>Tgfb1-/-</td>
<td>Doetschman</td>
<td>9</td>
<td>3/9</td>
<td>3/3</td>
<td>3/3</td>
</tr>
</tbody>
</table>

† Intact RNA is defined by Bioanalyzer and photometry
‡ Vanderbilt 20k chips with amplified RNA
Comparative Transcriptional Profiling for Independent Genetic Mouse Models of Colon Cancer

Pool of 4991 genes identified by ANOVA X Fold-Rank for Model-Specific Colon Tumor Expression

Discovering a Gene Expression Signature for Chemical Exposure-Induced Colon Cancer

420 genes with AOM-Specific Colon Tumor Expression (BH-FDR p<0.001)

AOM tumor model: David Threadgill, PhD UNC Chapel Hill NIEHS Toxicogenomics Research Consortium

Dr. Bruce Aronow
Microarray Analysis of 288 Independent Human Colon Cancers: global approach to tumor sample subclassification and gene expression pattern discovery

HG-U133 plus 2.0
Filter: Genes Overexpressed in >12 of 288 human colon tumor samples

20,287 PS

Hierarchical clustering of genes and tumors

Sergio Kaiser-Cincinnati
Walter Jessen-Cincinnati
Tim Yeatman-Moffit Cancer Center

Classification of Human Tumors as “Mature” or “Immature” by the Behavior of Developmentally Regulated Mouse Gene Orthologs

1300 mouse mature genes
1455 mouse immature genes

20,000 human tumor genes

Top-1000 tumor correlated human gene orthologs of mouse genes up and down-regulated during normal mouse colon development

“subtypes”

“immature” (I)
“mature” (M)

“mature” probesets
“immature” probesets
**Expression profile-based Human Tumor Subtypes Show Strong Differences in Survival Outcomes**

- 116 primary colon Ca tumors with > 36 Mo F/U
- Strong gene expression pattern-based discrimination of differential survival groups

Tim Yeatman group
Moffitt Cancer Center

**The Human Interactome Powers Systems Biology Approaches to the Dissection of Disease**

- Johannes Freudenberg
- Ashima Gupta
- Anil Jegga
- Siva Gowrisankar
- Jing Chen
- Sue Kong
- Sarah Williams
- Theresa Setty
- Steve Connolly
- Sergio Kaiser
- Walter Jessen
- Jeremy Aronow
- Vivek Ramaswamy
- John Kleimeyer
- Michael Kleimeyer
- Pediatric Biomedical Informatics
- NIEHS Comparative Mouse Genome Consortium
- NCI Mouse Models of Human Cancer Consortium
- NCI Directors Challenge
- Digestive Disease Research Center
- Cathy Ebert
- Jennifer Marler
- Amy Moseley
- Jianhua Zhang
- David Witte
- Sue Thompson
- Bob Coffey
- Young Park
- Shawn Levy
- David Threadgill
- Bill Dove
- Rich Halberg
- Joanna Groden
- Tim Reichling
- Dan Carson
- Tom Doetschman
- Andy Lowy
- Greg Boivin
- Tim Yeatman
- Andrew Conway
- Jordan Stockton

Dr. Bruce Aronow
H-13
Wireless Sensor Networks for Environmental Monitoring

Deborah Estrin
(Dave Caron, Tom Harmon)
http://cens.ucla.edu/Estrin  destrin@cs.ucla.edu

Work summarized here is largely that of students, staff, and other faculty at CENS
We gratefully acknowledge the support of our sponsors, including the National Science Foundation, Intel Corporation, Sun Inc., Crossbow Technologies Inc., and the participating campuses.

Embedded Networked Sensing

- Micro-sensors, on-board processing, wireless interfaces feasible at very small scale—can monitor phenomena “up close”
- Enables spatially and temporally dense environmental monitoring

Embedded Networked Sensing will reveal previously unobservable phenomena

Ecosystems, Biocomplexity

Marine Microorganisms

Contaminant Transport

Seismic Structure Response
Remote and In Situ Sensing

- Remote sensing has transformed observations of large scale phenomena
- In situ sensing will similarly transform observations of spatially variable processes in heterogeneous and obstructed environments

SPOT Vegetation
Daily Global Coverage
SWIR 3 Day Composite
San Joaquin River Basin
Courtesy of Susan Ustin-Center for Spatial Technologies and Remote Sensing

Predicting Soil Erosion Potential:
Weekly MODIS Data
Sheely Farm 2002
Crop map

Environmental Monitoring Applications Exhibit
High Spatial Variations and Heterogeneity

Overflow of embankment

Algal growth as a result of eutrophication
- Image courtesy of The J. for Surface Water Quality Professionals

Precision Agriculture, Water quality management
Environmental Application Drivers at CENS

- Contaminant Transport, Soils (Harmon, Allen)
  - Three dimensional soil monitoring
  - Error resiliency at node and system level
  - Data assimilation, model development

- Marine microorganisms (Caron, Requicha, Sukhatme)
  - Aquatic operation
  - Micro-organism identification
  - Sensor driven biological sample collection

- Biology/Ecosystem Processes (Hamilton, Rundel)
  - Robust, extensible microclimate monitoring
  - Image and acoustic sensing
  - Infrastructure based mobility

Wastewater reuse in the Mojave Desert

- Where does the County Sanitation District (CSD) of Los Angeles put 4 million gallons per day of treated wastewater in a landlocked region?

- Stakeholders:
  - County Sanitation District
  - Farmer
  - Water Quality Board
Locally dense surface and subsurface sensor networks

- Modular “clustered” sensing targeting specific questions
  - What is quantitative flux of nitrate past the plant’s root zone?
  - What are the spatiotemporal variations associated with nitrogen biogeochemical cycling in the soil?
  - How does the network optimally feedback toward sustainable fertilizer application?
- Spatial granularity: 10s of meters to cm...
- Remote sensing, stationary and mobile nodes (e.g., distributed soil pylons, autonomous tractor-mounted sensors, aerial NIMS devices)
- Data interpolation, network calibration, and forecasting using detailed computational models

Nitrate sensor mimicking plant root fibers

Geostatistical realization of soil properties

Courtesy of Tom Harmon

Plankton dynamics in marine environments

Spatial and temporal distributions of harmful alga blooms (red, green, brown tides) in marine coastal ecosystems

Experimental and observational studies of chemical, physical and biological features promoting bloom events
Important Challenges for EPA Applications

- Robust, portable, self-configuring systems
- Embeddable sensor devices for specific species, sensitivity, longevity
- Data Integrity, Calibration
- Multiscale Data Fusion

Systems Challenges

Key Constraints:
- Energy awareness and conservation
- Scaling and adaptation to variable resources and stimuli
- Autonomous, disconnected operation
- Data Integrity given sensing channel uncertainty
- Complexity of Distributed systems

Information Technology Research:
- Self configuring systems for autonomy in dynamic, irregular environments
- In Network Collaborative signal processing and Event Detection for Scaling in time and space
- Exploiting Heterogeneous Systems w/ Mobility
- Multi-mode, multi-scale data fusion for tasking, interpretation,
Information Technology – Sensor Networks

APPENDIX I – SLIDE PRESENTATION

Nanotechnology, Biotechnology, and Information Technology Workshop

Heterogeneous Sensor Systems Needed

- Spatially distributed static nodes
  - Allows simultaneous sampling across study volume (dense in time, but possibly sparse in space)
  - Limited energy and sampling rate
- Articulated Nodes
  - Provide greater functionality for sensors, communications
- Nodes with infrastructure-based mobility:
  Networked Info-Mechanical Systems (NIMS)
  - Sensor diversity: location, type, duration
  - Allows dense sampling across transect (dense spatially, but possibly sparse in time)
  - Adaptive provision of resources (sensors, energy, communication)
  - Enable adaptive, fidelity-driven, 3-D sampling and sample collection

Application-Driven (not Application-Specific)
Common System Software

Reusable, Modular, Flexible, Well-characterized Services/Tools:
- Routing and Reliable transport
- Time synchronization, Localization, Self-Test, Energy Harvesting
- In Network Processing: Triggering, Tasking, Fault detection, Sample Collection
- Programming abstractions, tools
- Development, simulation, testing, debugging

Dr. Deborah Estrin
Embeddable Sensor developments

- Environmentally robust sensors (stationary and mobile deployment)
- Initial emphasis on chemical species (ionic)
  - specifically nitrate
- Achievements and timeline
  - Nitrate Ion Selective Electrode, demonstrate scaleability
  - higher performance amperometric nitrate sensor (Silver working electrode sensitive for nitrate; Requires microfluidics)
  - general ion separation/identification capabilities (ion liquid chromatography-on-a-chip)
- Transitioning to gas/atmospheric project: CO2

(* Judy, Harmon, Ho, Tai)

Data Integrity:
How will we monitor the monitors?

...the river is receiving excessive nutrients from adjacent groundwater (not from surface runoff, not from atmospheric deposition)...
Data integrity in sensor networks: multilevel calibration

- Bench-top calibration
- Pilot deployment
  - develop in situ calibration protocol
  - characterize longevity, degradation
- Early in the deployment
  - Take advantage of the sensors’ integrity
  - Calibrate model (distributed parameters)
  - Integrate DAQ with simulator to accelerate process
- Later (as sensors become suspect)
  - Reverse the process
  - Let the network identity bad sensors: Self-Test
- Incorporate uncertainty into the process

Coupling simulations to sensor network calibration

- At the field scale:
  - rigorous conventional characterization sampling plans still required
  - for soils, geostatistical parameterization techniques may be needed
- Report network information and associated uncertainty
- Iteration between models and sensor
APPENDIX I – SLIDE PRESENTATION
Information Technology – Sensor Networks

Nanotechnology, Biotechnology, and Information Technology Workshop

Multiscale Observation and Fusion: Example, Regional (or greater) scale to local scale

- Satellite, airborne remote sensing data sets at regular time intervals
- coupled to regional-scale “backbone” sensor network for ground-based observations
- fusion, interpolation tools based on large-scale computational models

Example: identification of invasive riparian species using HyMap (airborne hyperspectral scanning)

Images from Susan Ustin, UC Davis

“NEON will transform ecological research by enabling studies on major environmental challenges at regional to continental scales. Scientists and engineers will use NEON to conduct real-time ecological studies spanning all levels of biological organization and temporal and geographical scales.”

- Biogeochemical cycles
- Biodiversity & ecosystem functioning
- Climate change
- Freshwater resources (especially linkage to land)
- Infectious diseases
- Land use change
- Land use change and
- Material flux or processing

Dr. Deborah Estrin
Embedded Sensor Networks for NEON

- A multiscale approach - San Joaquin River Basin: Water quality observation and forecasting—Sierra snowpack to San Francisco Bay
- Academics: UC Merced, UCLA, UCD, UCR, Caltech
-Govt Agencies: LLNL, LBNL, USBR, USGS, NPS, CA DWR
APPENDIX I – SLIDE PRESENTATION
Information Technology – Sensor Networks

Nanotechnology, Biotechnology, and Information Technology Workshop

Broad Relevance to Global Issues

- Theatre, Film, Television
- Global Climate Change
- Water Quality
- Early Warning, Crisis Response
- Security
- Precision Agriculture
- Public Health
- Coral Reef
- Global Seismic Grids/Facilities

For Further Investigation

- Center for Embedded Networked Sensing, http://cens.ucla.edu
- TinyOS and Mote platforms: UC Berkeley, Intel, Crossbow, Sensicast, Dust Networks, Ember

Dr. Deborah Estrin
Information Technology (IT) Implications for Future Science at EPA

Gregory J. McRae

MIT - Chemical Engineering

Information/Analysis/Knowledge/Outcomes!!
The “Problem”

Real Risks  Perceived Risks

How can IT help in the development of appropriate responses (science/policy) and in managing the complexity?

Outline of Presentation

- What is IT?
- How is EPA doing?
- What are new directions?
- Issues for workshop?

Key Message: Advances in IT have the potential to revolutionize how EPA might manage environmental risks.
What do we mean by “IT”?

- Computers (pc’s->sc’s)
- Data bases/management
- Communications
- Sensors
- Visualization
- Algorithms
- Audit for accountability
- PEOPLE

All are needed to reduce the elapsed time to solutions and to get relevant science into the decision making process before decisions are made.

What are the driving forces for change?

Driving Force For Change - *The Web*

Essential Utilities

Water  Gas  Electricity

The 4th Utility

Bandwidth

Source: Matt Spathas, SENTRE Partners
Driving Forces for Change - Optical Networks

<table>
<thead>
<tr>
<th>Performance per Dollar Spent</th>
<th>Number of Years</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optical Fiber</td>
<td>0</td>
</tr>
<tr>
<td>(bits per second)</td>
<td>1</td>
</tr>
<tr>
<td>(Doubling time 9 Months)</td>
<td>2</td>
</tr>
<tr>
<td>Silicon Computer Chips</td>
<td>3</td>
</tr>
<tr>
<td>(Number of Transistors)</td>
<td>4</td>
</tr>
<tr>
<td>(Doubling time 18 Months)</td>
<td>5</td>
</tr>
<tr>
<td>Data Storage</td>
<td></td>
</tr>
<tr>
<td>(bits per square inch)</td>
<td></td>
</tr>
<tr>
<td>(Doubling time 12 Months)</td>
<td></td>
</tr>
</tbody>
</table>

Driving Forces for Change - Remote Access

Two 6.5 Meter Telescopes at Las Campanas Observatory, Chile
Driving Forces for Change - The Movies

Routine Visualization of Complex Phenomena
New Dimensions of Working in Teams

Environmental Problems are Global inExtent

Los Angeles

London

Mexico City

Benzhi

Exposure to Environmental Health Risks (World Bank)
Characteristics of Energy/Environment Problems

- Complex
- Multiple (often conflicting) objectives
- Asymmetric information
- Short decision cycles
- Long analysis times
- Few technically qualified people
- ...

Can we “really” contribute to the policy process?
Three Questions - Air Quality Issues

1. What has been the hourly O₃ concentration over Washington for the last 10 years?

2. Can we detect the impact of emissions controls in a statistically meaningful manner?

3. What is the most cost-effective way to improve air quality in the North East?

Can we answer these questions and, even more importantly, in time scales compatible with needs of regulatory decision making processes?

Biological Data - Genetic Code

```
1  ggcacattct  ccttgtaggc  caggctatgc  tgaccacaat  gttgctgagc  tgtgccttac
61  tgtgctgact  gcccacactg  ctgagggccc  agataggtct  ggcacccctg  gaggtatagc
121  gaaagccttg  caaagcccttg  tccccagaca  tcocaagctga  gtcgagggcc  aagttgaggct
181  ggtgagggct  tggacatcctc  tggccacaaa  gtattctgct  tgtatgagcc  ctctctctcc
241  cttccccaccc  cccggcttgg  gaggtggttg  ttttctgcat  ggggtgtttc  gcccacctccat
301  cactctggcc  agatcagggc  ctgcagcccc  cactgaagag  caagctgcca  gaaaggccagc
361  aagggcctctc  gctgcgacac  gcgcagggca  aaggctttgc  aaggttacac  gttcagggca
421  gttgctaccct  gttgaccaac  gggattctgg  gttcctctgg  aagggctgagc  ggctaggtct
481  gtttcagctc  gttgctactc  gggattcctg  gttcctctgg  aagggctgagc  ggctaggtct
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661  tagaaaaa  aaactaaca  acacccctcc  ctgcaacctc  gacccccccc  aacccggcgcag
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841  gcaagcagct  cccccctctc  ggtcggtatc  ggtggaagag  cctgctggtctg  gacccccccc
901  taacctgtgc  cggccccctc  gtcacgtgct  actgcgcgctt  cttcagccgc  cttctctttc
961  ggggcagact  ggtggctgcc  ggctaccacc  cttccactcc  ctgctggtctg  gacccccccc
1021  gtcg

Sus scrofa agouti - related protein gene
```

Nucleotide Databases
- dbEST
- dbGSS
- dbSNP
- dbVar
- dbVar
- dbVar
- RefSeq
- UniGene
- Trace Archive
- UniSTS

Protein Databases
- GenPept
- RefSeq

Structure Databases
- Domains
- 3D Domains
- Structure dbMOL

Taxonomy Databases
- Taxonomy

Genome Databases
- Genomes
- COGs
- LocalLink

Expression Databases
- GEO
- SAGE

Growth of GenBank

There are approximately 28,507,990,166 bases in 22,318,883 sequence records as of January 2003

Why has Bioinformatics been so successful?

- An organized community with roadmaps
- Resources (NIH, NSF, DoE, ...)
- New people (Fellowships, ...)
- Multidisciplinary (Math, Eng, CS, Bio, Phys, Chem, ...)
- Focused on systems integration and leverage of community input
  - Databases (GenBank, ...)
  - Algorithms (Matching, ...)
  - Instrumentation (Microarrays, ...)
  - Linking of private/public data bases
  - Multi-scale integration (Genomes to life, ...)
- Standards for representation of chemistry (ATGC, proteins, ...)

IT has been a critical enabling element of success of genome project and has facilitated the emergence of new sciences
**PM$_{2.5}$ Controls – How is soot formed?**

**Challenges – Integration of Diverse Databases**

- **Thermophysical properties**
  - JANAF
  - NIST
  - CHEMKIN
  - DECHEMA
  - Group contribution, QM
  - ....

- **Kinetics**
  - NASA
  - Bielstein
  - DECHEMA
  - ....

- **Species and Mechanism**
  - LLNL
  - Literature, by-hand, GRI,....
  - Reaction path generation
  - ....

- **Etc.**

1. Not integrated
2. Do not give useful uncertainty estimates
3. Varying levels of documentation
4. Few links to the provenance of data
5. How to handle different data quality
6. Few organized experimental data bases for evaluation
What could we do with IT? - Some Examples

<table>
<thead>
<tr>
<th>SAB (Sciences)</th>
<th>Risk Reduction (Engineering)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physics</td>
<td>Emissions controls</td>
</tr>
<tr>
<td>Chemistry</td>
<td>Cost-effective design</td>
</tr>
<tr>
<td>Toxicology</td>
<td>Case studies</td>
</tr>
<tr>
<td></td>
<td>...</td>
</tr>
</tbody>
</table>

- Compliance assessment
- Avoiding problems in the first place
- Win-Win control strategies
- Prioritization of resources
- Etc.

Compliance Assessment:
How can we detect if environmental controls have been effective?
One Environmental Goal - *Meet Standards*

Control Policies ➔ Emissions ➔ Air Quality ➔ Exposure/Dose ➔ Health/Welfare ➔ Compliance Assessment

Deterministic Control Strategy Design

- Minimize cost of controls  
  - *Subject to meeting standards*
- Maximize air quality  
  - *Subject to budget constraint*
- Minimize exposure to pollution  
  - *Subject to limits*
- Minimize risk of exceedances  
  - *Subject to fluctuations*
- Etc.

\[ \min \quad f(E, x, t) \]  
\[ \text{subject to} \quad g(E, x, t) = 0 \]  
\[ h(E, x, t) \leq 0 \]
**Compliance Assessment - Inverse Modeling**

**Forward Modeling (M:{E,M,C}->AQ)**

- **Inputs**
  - Air Quality Model (M)
  - Air Quality

**Inverse Modeling (M⁻¹:AQ->{E,M,C})**

- **Bounds**
  - Inverse Model (M⁻¹)
  - Measurements

---

**Bayes Theorem - Inverse Probability**

\[
p(y, \theta) = p(y | \theta) p(\theta) = p(\theta | y) p(y)
\]

- Prior Knowledge \(p(\theta)\)
- Analysis System
- Posterior \(p(\theta | y)\)

\[
p(\theta | y) = \frac{p(y | \theta) p(\theta)}{p(y)} \propto p(y | \theta) p(\theta)
\]

- Posterior Distribution
- Likelihood Function
- Prior Distribution

\[
p(y) = \int p(\theta) p(y | \theta) d\theta
\]
Moving instrumentation to 21st Century

Cermet Sensor

$ 300,000  $ 10

Source: ANL and MIT

Schools as a Source for Data Intensive Science?

Students enrolled in grades K-12  6,000,000
Schools  9,000
Teachers  300,000
Classrooms with Internet access  200,000
Student per Internet-connected computer  7:1

Schools as sensor platforms for
- Air Pollution
- Water Quality and Quantity
- Seismic Activity
- Health of the Population
Potential for Dramatic Increase in Coverage

US EPA PAMS Sites

Schools in Los Angeles Unified School District

Avoiding Problems in the first place:

Can we use IT to anticipate potential impacts of products before they are introduced?
Choice of New Chemicals - Cleaning CVD Reactors

e.g. F₂ vs. NF₃ Cleaning Process in the Fab

Why are Technology Choices Complex?

Example: Choosing a chamber cleaning gas (NF₃ vs. F₂?)

<table>
<thead>
<tr>
<th>Decision Criteria</th>
<th>NF₃</th>
<th>F₂</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluorine usage rate at the same etch rate (mole/min)</td>
<td>0.15</td>
<td>0.17</td>
<td>Mechanism and properties</td>
</tr>
<tr>
<td>Cost/mole of Fluorine</td>
<td>$6</td>
<td>$0.8</td>
<td>Economics</td>
</tr>
<tr>
<td>LCA Global Warming Effect (kg CO₂ equivalent/kg)</td>
<td>3.3</td>
<td>2.4</td>
<td>Environment LCA</td>
</tr>
<tr>
<td>Toxicity LC₅₀ (ppm)</td>
<td>6700</td>
<td>180</td>
<td>Health OSHA</td>
</tr>
</tbody>
</table>

The Problem: How to choose between technologies
- When there are conflicting decision criteria
- Many uncertainties
Why we need to solve this problem!!

Industry recognition of need

“...There is a critical need for an integrated way to evaluate and qualify environmental impact of process, chemicals, and process equipment…”

-- ITRS, 2001 Edition, Environmental, Safety, and Health

Emerging Driving forces for Change

“...The European Commission Integrated Product Policy (IPP) will look at all stages of a product's life cycle from cradle to grave...we are calling on industry to bring IPP to life”

-- M. Wallström, EU Environment Commissioner

Press release 18th June 2003

MIT Environmental Evaluation Model

Design Decisions

Process Model

Upstream & Downstream Emissions, Material and Energy Usage

Flow Rates

Products

Byproducts

Chemical

Energy

Water

Waste

Yield

Process Time

... Environmental Properties

Chemical Properties

Exposure Properties

Fate, Transport, and Exposure Model

Human Toxicity

Global Warming

Effect

Ozone Depletion

Effect

Respiratory

Effect

Human Exposure

Environmental Concentration

Impact Indicator

Environmental Performance

Compliance with Regulations

Weighting Factors
Importance of Considering Multi-Boundaries

[Diagram showing various production processes and their relationships across different boundaries.]

Framework of Decision-Making Process

- Generate new alternatives
- Refine model, collect more data, increase data accuracy...
- Ranking and Sensitivity Analysis

Alternative Technologies:
- NF₃ vs. F₂
- Cu CVD vs. Cu plating

Uncertainty Analysis

- Economic Impact Model
- Process Model
- Environ. Impacts Model

Is info enough for decision?
- No
- Yes

- Do nothing, or change to alternative
Risk Management - Decision Uncertainty

Global warming potential (GWP)

There is an 85% likelihood that the F₂ has a lower global warming impact than the NF₃ cleaning.

Ethanol versus Methanol
Some Background

<table>
<thead>
<tr>
<th>Methanol</th>
<th>Ethanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil/Gas</td>
<td>Biomass</td>
</tr>
<tr>
<td>NO\textsubscript{x}, CO</td>
<td>NO\textsubscript{x}, CO</td>
</tr>
<tr>
<td>CH\textsubscript{3}OH,</td>
<td>C\textsubscript{2}H\textsubscript{5}OH,</td>
</tr>
<tr>
<td>HCHO,...</td>
<td>CH\textsubscript{3}CHO,...</td>
</tr>
</tbody>
</table>

Formaldehyde is a carcinogen!!

Atmospheric Chemistry of Methanol

\[
\text{CH}_3\text{OH} + \text{OH} \rightarrow \cdots \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{HO}_2
\]

\[
\text{HCHO} + h\nu \rightarrow \cdots \rightarrow \text{CO} + 2\text{HO}_2
\]

\[
[O_3] = \frac{k_1[NO_2]}{k_3[NO]} \quad 3\text{NO} \rightarrow 3\text{NO}_2
\]
Atmospheric Chemistry of Ethanol

\[ \text{CH}_3\text{CH}_2\text{OH} + \text{OH} \rightarrow \ldots \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CHO} + \text{HO}_2 \]
\[ \text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} \]

\[ \text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_4 + \text{CO} \]
\[ \rightarrow \text{CH}_3 + \text{HCO} \]
\[ \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O} \]

\[ \text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{O} \]
\[ \text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 \]
\[ \text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} \]

Atmospheric Chemistry of Ethanol (Cont.)

\[ \text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{CO} + \text{H}_2\text{O} \]
\[ \text{CH}_3\text{CO} + \text{O}_2 \rightarrow \text{CH}_3\text{C(O)O}_2 \]
\[ \text{CH}_3\text{C(O)O}_2 + \text{NO}_2 + \text{M} \rightarrow \text{CH}_3\text{C(O)O}_2\text{NO}_2 + \text{M} \]

PeroxyacetylNitrate (PAN)

- More NO to NO\(_2\) conversions than methanol (5)
- Formaldehyde is a photo-oxidation product
- Chemistry produces PAN, a phyto-toxicant
**Win-Win Control Strategies:**

How to view environment as an objective, not as a constraint, in design optimization?

### Motivating Problem – Improving old processes

- World capacity 22 billion lbs/year
- Very low margins
- > 50 year old process

\[ \text{C}_2\text{H}_4\text{O} \rightarrow \text{Ethylene Glycols} \quad \text{Coolants (29%)} \quad \text{Polyesters (32%)} \\
\rightarrow \text{Surfactants (13%)} \\
\rightarrow \text{Glycol ethers (7%)} \\
\rightarrow \text{Ethanolamines (6%)} \\
\rightarrow \text{Other (13%)} \]
**Win-Win Design - More product and less CO₂**

\[ C_2H_4 + \frac{1}{2}O_2 \rightarrow C_2H_4O \]

Product

\[ C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \]

Climate Problem

**Improving yield/ selectivity can improve both profit and reduce climatic impacts**

---

**Solution Strategy - Multiscale Engineering**

- **Catalyst Surface**
  - Many reactions / species
  - Surface thermodynamics

- **Reactor Tube**
  - Mass transfer resistances
  - Packing in homogeneity

- **Reactor**
  - Bundle of many tubes and
  - The need for shell flow details
Prioritization of Resources:

There are lots of uncertainties, the challenge is to identify those that contribute to uncertainties in outcomes?

A More Complicated (Realistic) Viewpoint

\[
\begin{align*}
\min & \quad f(E,x,t) \\
\text{s.t.} & \quad g(E,x,t) = 0 \\
& \quad h(E,x,t) \leq 0
\end{align*}
\]

\[
\begin{align*}
\min & \quad E[f(E,x,t)] \\
\text{s.t.} & \quad \Pr[g(E,x,t) = 0] > \alpha \\
& \quad \Pr[h(E,x,t) \leq 0] > \beta
\end{align*}
\]
**Valuing Decisions - NPV, Option Pricing,...**

- **Strategy A**
- **Strategy B**

Which control strategy(s) would you choose?

**Problem: Identifying Critical Parameters**

<table>
<thead>
<tr>
<th>Photochemical Reaction Mechanism</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ( \text{NO}_2 + \text{hv} \rightarrow \text{NO} + \text{O} )</td>
</tr>
<tr>
<td>2. ( \text{O} + \text{O}_2 + \text{M} \rightarrow \text{O}_3 + \text{M} )</td>
</tr>
<tr>
<td>3. ( \text{O}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{O}_2 )</td>
</tr>
<tr>
<td>4. ( \text{HCHO} + \text{hv} \rightarrow 2\text{HO}_2\cdot + \text{CO} )</td>
</tr>
<tr>
<td>5. ( \text{HCHO} + \text{hv} \rightarrow \text{H}_2 + \text{CO} )</td>
</tr>
<tr>
<td>6. ( \text{HCHO} + \text{OH} \cdot \rightarrow \text{HO}_2\cdot + \text{CO} + \text{H}_2\text{O} )</td>
</tr>
<tr>
<td>7. ( \text{HO}_2\cdot + \text{NO} \rightarrow \text{NO}_2 + \text{OH} \cdot )</td>
</tr>
<tr>
<td>8. ( \text{OH} \cdot + \text{NO}_2 \rightarrow \text{HNO}_3 )</td>
</tr>
</tbody>
</table>

Contributions from different parameters to uncertainty in predicted ozone levels
What is Driving Uncertainties in Outcomes?

**Parameters** (porosity, permeability, saturation, market economics,...)

**Performance Drivers**

- Permeability
- Porosity
- Water saturation

Effect of New Information on Risk

Reduced Risk and Increase in average NPV

NPV ($ Million)

Years

Reduced Risk and Increase in average NPV
Conclusions/ Workshop Questions

- IT is a critical enabling resource, does EPA need a CTO/CIO?
- How to improve access to data bases used for decision making?
- Critical need for multimedia integration of databases/models (MTBE!!)
- How to get more science into the control strategy design process?
- Most critical issue is where will the people come from?
Converging Technologies (NBIC)

William Sims Bainbridge, Ph.D.
National Science Foundation

NBIC =

- Nanotechnology
- Biotechnology
- Information Technology
- Cognitive Science - new technologies based on the convergence of computer science, psychology, neuroscience, philosophy, anthropology, economics, sociology, etc.
The Meaning of NBIC:

- Based on the unity of nature at the nanoscale
- A potential successor to the National Nanotechnology Initiative, and to the Information Technology Research Initiative
- Not an official government (or NSF) activity, but an exploratory movement of scientists and engineers
- Arising when the unification of science has become possible through the use of transforming tools
- A natural extension of work on the societal implications of nanotechnology

Unification of Technology

Manuel Castells writes, "Technological convergence increasingly extends to growing interdependence between the biological and micro-electronics revolutions, both materially and methodologically. ... Nanotechnology may allow sending tiny microprocessors into the systems of living organisms, including humans." (Castells, Manuel. 2000. The Rise of the Network Society. Oxford: Blackwell, p. 72.)
Unification of Science

In his influential book, *Consilience*, Edward O. Wilson wrote about the rapid unification of scientific knowledge that is taking place today, and he wondered whether the natural sciences would be able to unite with the humanities and religion that traditionally have claimed to understand humanity itself. (Wilson, Edward O. 1998. *Consilience: The Unity of Knowledge*. New York: Knopf.)

Hatching an Idea

Converging Technologies for Improving Human Performance: Nanotechnology, Biotechnology, Information Technology and Cognitive Science

*NSF/DOC-sponsored report*

*Conference at NSF, December 3-4, 2001*

http://www.wtec.org/ConvergingTechnologies/
Launching a Movement

First Publications


Next Steps


*Converging Technologies*
Kailua-Kona, Hawaii
February 23-25, 2005
http://www.biztechcomm.com/
(book expected, edited by Bainbridge, Montemagno & Roco)

The NBIC Tetrahedron

Nanotechnology
Biotechnology
Information Technology
Cognitive Science
Principles of Convergence

Convergence is based on:
1. material unity of nature at the nanoscale
2. technology integration from the nanoscale
3. key transforming tools for NBIC
4. concept of reality as closely coupled complex, hierarchical systems
5. goal to improve human performance

Application Areas

• Expand Human Cognition & Communication
• Improve Human Health & Physical Capabilities
• Enhance Group & Societal Outcomes
• Strengthen National Security & Competitiveness
• Unify Science & Education
One-way Convergence
Developments in one field are applied to another.

E.g.: Nanotechnology allows Moore’s Law to continue in production of ever smaller, faster, and cheaper microelectronic components – enabling continued progress in Information Technology.

An end to Moore’s Law could mean a shift to massive parallel computing, but cost and technical challenges have limited the use of parallel systems.

If IC chips become ordinary commodities, nations with low labor costs may mass produce them thereby destroying American (etc.) industries.

Mutual Convergence
Scientific theories and models are applied across many different fields, facilitating exchange.


Information Technology Grants

NSF Awards 0225656, 0225636, 0225609, 0225607: “Computational Learning and Discovery in Biological Sequence, Structure and Function Mapping” estimated total: $8,840,267; Carnegie-Mellon, U Pittsburgh, MIT, Boston U

Computer scientists, together with biological chemists will collaborate using statistical and computational tools and methods that the computer scientists have been developing for dealing with human language to better understand the function of proteins.

Evolution

Evolutionary biology to semantic evolution:

**Taxonomy:** Linnaean genus-species system, cladistics, numerical taxonomy

**Processes:** Gene, Sexuality, Transduction, Alleles, Natural Selection, Species, Stratigraphy, Catastrophism, Van Valen’s Law, Character Displacement, Allopatric Speciation, The Cope-Stanley Law, Exaptation
**Depth with Breadth**

“Combining depth with breadth in NBIC education and research of various groups.”

“Nanotechnology offers hope of depth plus breadth”

(W. M. Tolles: “Breadth, Depth, and Academic Nano-Niches” - 1st report)

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**Sustaining Progress**

Has progress stalled in aviation and spaceflight, energy production, artificial intelligence, social and behavioral science, health and longevity?

Succession of sigmoid (logistic) curves of progress (Newt Gingerich: “Age of Transitions”)
**Transforming Tools**

Opportunity for science & technology convergence based on shared methodologies (e.g. mathematics, computation, nanoscale observation and experimentation, etc.) & theories (e.g. hierarchical structures, complex systems, evolution, etc.)

Analogous structures in the different fields (James Canton: “Global Futures”)

**Illustrative Application**

Comfortable, wearable sensors and computers will enhance every person’s awareness of his or her health condition, environment, concerning potential hazards, local businesses, natural resources and chemical pollutants.

“Spatial Cognition and Converging Technologies”

(Reginald G. Golledge)
More Applications

National security will be greatly strengthened by light-weight information-rich war fighter systems, capable uninhabited combat vehicles, adaptable smart materials, invulnerable data networks, superior intelligence gathering systems, and effective measures against biological, chemical, radiological, and nuclear attacks.

Agriculture and the food industry will greatly increase yields and reduce spoilage through networks of cheap, smart sensors that constantly monitor the condition and needs of plants, animals, and farm products.

Becoming Renaissance People

Formal education will be transformed by a unified but diverse curriculum based on a comprehensive, hierarchical intellectual paradigm for understanding the architecture of the physical world from the nanoscale through the cosmic scale.

Engineers, artists, architects, and designers will experience tremendously expanded creative abilities, both with a variety of new tools and through improved understanding of the wellsprings of human creativity.
Discovering...

...new categories of materials, devices and systems for use in manufacture, construction, transportation, medicine, emerging technologies and scientific research.

...processes of the living cell, which is the most complex known form of matter - with nanoscale components.

...principles of advanced sensory, computational and communications systems integrating diverse components into a ubiquitous, global network.

...structure, function, and occasional dysfunction of intelligent systems, most importantly the human mind.

Social and Ethical Principles

....evolving socio-cultural context in which convergent research is funded

....societal needs that technology may satisfy

....popular misconceptions that science education will have to overcome

....infection of one field by issues from a different convergent field, e.g.: nano from bio
Oversight I

See:

“Societal Implications of Nanoscience and Nanotechnology”

at:

www.wtec.org/loyola/nano/societalimpact/nanosi.pdf

Oversight II

Second Report on Societal Implications to be Published Soon!
(Mihail C. Roco & William Sims Bainbridge, editors)
Improving Human Performance

…offering individuals and groups an increased range of attractive choices while preserving such fundamental values as privacy, safety, and moral responsibility

…substantially enhancing human mental, physical, and social abilities

Technological civilization faces the very real danger of stasis or decline unless something can rejuvenate progress.

Unification

Enhancement of human performance should serve the legitimate hopes of human beings, who in return will support the scientific and engineering work required to achieve technological convergence and the unification of science.

Convergence conferences have envisioned the next 20 years, but complete unification of science may require the entire 21st century.
Examples of NSF NBIC Grants

“Active Sensor Networks with Applications in Marine Microorganism Monitoring” (0121141, Requicha, USC). For monitoring microbes in the ocean or in water supplies: distributed network-coordinated nanorobots “to investigate the causal relationships between environmental conditions and microorganisms.”

“Pattern Recognition for Ecological Science and Environmental Monitoring” (0326052, Dietterich, Oregon State) Computer vision system designed to recognize and count insects - a new tool for studies of biodiversity & water quality monitoring.

More Examples of Grants

"Interactive Software Systems for Expert-Assisted Image Analysis and Classification of Aquatic Particles" (0325937, Sieracki, Bigelow Lab; 0325167, Riseman, U. Massachusetts; 0325018, Benfield, LSU). Computer vision, machine learning inspired by human cognition, to classify bacteria, plankton in ocean water.

“Sustainable and Generalizable Technologies to Support Collaboration in Science" (0085951, Olson, U Michigan). Studied online research collaboratories in: atmospheric science, behavioral neuroscience, biomedical informatics, computer science, earth science, engineering, genomics, and nanoscience.
Converging Technologies

W. S Bainbridge: wbainbri@nsf.gov