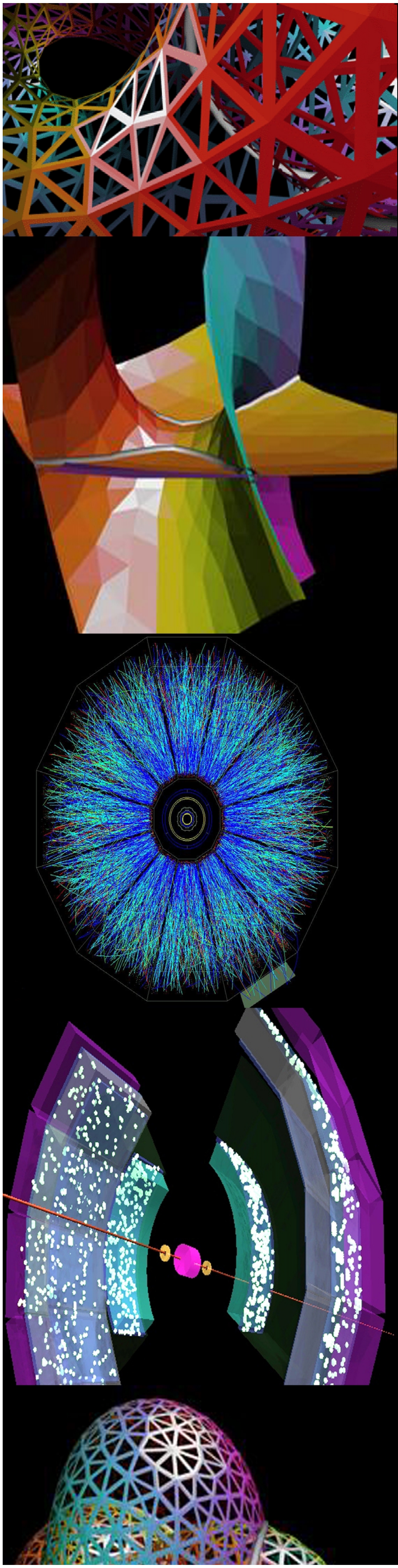

Approaches to Combat Terrorism (ACT):

Opportunities for Basic Research

A Joint Workshop by

The Directorate for Mathematical and Physical Sciences, NSF

and

The Intelligence Community

19-21 November 2002

Approaches to Combat Terrorism (ACT):
Opportunities for Basic Research

Report of a Joint Workshop Exploring the Role of the Mathematical and Physical Sciences in Support of Basic Research Needs of the U.S. Intelligence Community

Submitted to the National Science Foundation
August 2003

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DISCLAIMER

The workshop described in this report was supported by the National Science Foundation under Grant No. MPS-0301254 and the Intelligence Technology Innovation Center of the United States Intelligence Community. Any opinions, findings, or conclusions are those of the authors and do not necessarily reflect the views of the National Science Foundation or the United States Intelligence Community.

Table of Contents

1. Introduction

Terrorism of international reach has forced new approaches to ensuring national security. The threat did not suddenly materialize with the tragic events of September 11, 2001, but those events did precipitate the new national focus on combating terrorism that in turn brought together the intelligence community (IC) and the National Science Foundation Directorate for Mathematical and Physical Sciences (NSF/MPS) as joint sponsors of this workshop on basic research opportunities.

The MPS academic community and the broader basic research community have a significant history of providing the scientific and technological underpinnings of our national security posture. Indeed, the partnership between the research community and the national security establishment during World War II, which generated and applied basic research from cryptography to radar to nuclear weapons, in many ways led to the establishment of the current United States basic research enterprise.

- A strong focus on conducting basic research at universities, where research and education are intimately linked
- Pluralistic support for basic research across Federal departments and agencies that depend heavily upon scientific and technical advances and upon a talented mathematics, science, and engineering workforce
- Development of a substantial national and federal laboratory system specifically emphasizing the link between research and Federal agency missions.

This unparalleled system of research support continues to serve the nation well, not only for national security, but also for economic development, health, and other public goods.

Over the last half century, military capabilities have provided support for basic research by national security agencies. The asymmetric threat of international terrorism now places a considerable premium on strengthening our technological capabilities for homeland defense and for intelligence collection.

This workshop aims to start the process of familiarizing the NSF/MPS and IC communities with their respective objectives, capabilities, and needs and identifying basic research areas and opportunities that can provide the technological base for:

- Early recognition and tracking of terrorist threats
- Disruption of terrorist operations
- Early warning of imminent and emerging threats from weapons of mass destruction, including use, significant testing milestones, and technological “surprises,”
- Accurate information and assessments of weapons of mass destruction development programs, including identification and tracking of critical technologies and materials

The academic and intelligence communities will almost certainly meet challenges as they seek out areas of aligned interest. The former works in an open environment that encourages maximum exchange of ideas, finds progress by building on the shared results of earlier research, and generally embraces international collaboration and participation. The latter inherently deals with high levels of secrecy and compartmentalization of information. Success will require:

- Recognition and respect of the other’s norms (such as openness and international student engagement in academic basic research)
- A focus on open basic research that can enable technology development that, when integrated with other technologies, will provide future IC capability in combating terrorism
- Development of appropriate mechanisms by NSF/MPS and the IC for recognizing basic research results of interest to the IC, along with tailored mechanisms for carrying that research through succeeding stages of technology development to deployment in appropriate settings.

The technology that can serve the needs of the intelligence community can be quite different from that addressed to other elements of national security, such as military capability or homeland defense. Energy sources provide an example: those used in homeland defense applications will generally have full access to the energy supply infrastructure, such as electricity; a battlefield application may require mobile high power energy sources with associated logistical support for fuel and maintenance; and an intelligence application may require a very low power source that can be inserted covertly in remote hostile environments by unskilled people, be left unattended, and operate without external signature. Clearly, the enabling research for such disparate applications can be quite varied, with novel research opportunities opened up by the IC needs. One goal of the workshop was to focus on special requirements driven by the terrorist threat and presented by the various basic intelligence sources or collection disciplines:

- Signals intelligence (SIGINT): this is derived from signal intercepts, however transmitted.
- Measurement and signature intelligence (MASINT): this is technically derived intelligence data (other than SIGINT and IMINT) that provide distinctive characteristics of targets emphasizing disciplines such as nuclear, optical, RF, acoustics, seismic, and materials sciences.
- Human source intelligence (HUMINT): this is derived from human sources, whether clandestine or overt.
- Open source intelligence (OSINT): this is publicly available information appearing in print or electronic form.
- Geospatial intelligence: this is the analysis and visual representation of security-related activities on earth produced by integration of imagery, imaging intelligence, and geospatial information.

These collection disciplines applied against international terrorism clearly have demanding requirements, such as:

- Extracting key information from massive unstructured heterogeneous databases, often in the face of deception
- Sensing the signatures of biological and chemical weapons or their precursors, perhaps through environmental measurements
- Powering collection equipment remotely without detection, and transmitting key data in a timely fashion.

With this background, five MPS areas were chosen for discussion at this workshop:

1. **Sensors and detectors**. New materials tailored to recognize very small amounts of target substances, miniaturization to the micro- and nano-scales, networks of communicating sensors, and biological sensing systems are examples of important research directions of interest to the IC.
2. **Optical spectroscopies**. Remote identification of small concentrations of specific chemicals and biological agents in complex environments is a major challenge requiring new spectroscopic methods and instrumentation advances. Understanding the fate and transport of such chemicals or biological agents is a key part of an effective detection system.
3. **Energy sources**. Advances in energy sources – higher energy density, longer life, more durable, lowered signatures – are key enabling technologies that cut across collection disciplines. Nanoscience and nanotechnology will be especially critical for meeting the energy needs of many IC collection requirements. Transformation of "ambient" energy into useful energy sources is a very challenging high-payoff research direction.
4. **Image reconstruction and analysis**. Imagery is clearly a very powerful tool for the intelligence analyst. Major benefits would be derived from advanced data integration from multiple sources and times, recognition of occluded shapes, dimensionality reduction, quality assurance, and data presentation.
5. **Mathematical Techniques**. This is again a major enabling discipline for the IC. Perhaps the greatest challenge is that of creating sense out of enormous quantities of unstructured data, including data mining and analysis across disparate multi-media information sources, often using different

languages, perhaps with encryption and active attempts at deception.

Each of these five areas is covered in a chapter of this report that summarizes the thoughts and discussions of the expert groups. These groups of leading researchers have produced a wealth of suggestions for basic research opportunities that may serve long term IC needs, and each chapter ends with a compilation of some of these opportunities. In addition, they collectively identify important crosscutting themes such as the key role of nanotechnology and computational modeling in materials development, the importance of cross-disciplinary research and of a peer-review process that can handle meritorious but "risky" proposals, and the overarching need to educate new generations of researchers. Our hope is that this report has captured the discussions adequately enough to bring these opportunities to the attention of a broader research community that may then heed the call for proposals from the NSF/MPS. In doing so, the opportunity for excellent—possibly breakthrough—basic science and engineering research will be aligned with service to the nation's national security needs.

Finally, we note that some of the areas covered are applicable in the homeland defense context, rather than in the intelligence context, and thus will not be included in a joint NSF/IC request for proposals. Clearly support can be pursued in other channels, since the problems are important in the overall national security picture.

2. Sensors and Detectors

2.1 Introduction

Analysis usually requires three distinct steps—sampling, pre-processing, and measurement. Sensors combine all three steps into a single, fully functional system. For sensors, sampling is performed simply by placing the sensor where the measurement is desired; no pre-processing of the sample is required and the measurement is an integral part of the sensor.

Before a sensor can be designed, the information required from it must be defined. The simplest type of sensor is an alarm type sensor in which presence/ absence of the analyte is detected. At the next level, sensors may be required that can determine what is present in the sample. In addition, sensors may be required to quantify the substances being detected. Each level of measurement requires additional sophistication in both the sensor and the data processing. The ideal sensor should be continuous, cheap, manufacturable, stable (chemical, drift, calibration), simple, universal, networked, and self-powered.

For bio-agents, today's technology targets either a DNA sequence or a particular protein present in the organism. For DNA, the polymerase chain reaction is often employed to specifically amplify the DNA from the target agent; the amplified DNA is then detected. If multiple DNA sequences are to be analyzed, DNA microarrays are employed. Proteins are typically measured using immunoassays. An alternative approach is to use mass spectrometry for both nucleic acids and proteins. The mass spectral patterns can be correlated to the agent of interest. For chemicals, such as nerve agents and explosives, ion mobility spectroscopy is used most frequently for point detection measurements. In addition, a wide variety of promising technologies are on the horizon and could be implemented for applications to the IC.

2.2 Research Opportunities

2.2.1 New Materials

Materials for all aspects of sensors, including recognition, transduction, and detection are essential to the advancement of the field.

2.2.1.1 Recognition materials

One of the most critical needs in the sensing field is in the area of new materials for recognition. Such materials could be used as simple affinity-capture binders in order to bind, concentrate, and collect samples from the environment that would be subsequently analyzed at a central laboratory. The design of molecular recognition compounds to specifically bind analytes of interest is a critical component of new sensors. In addition to their binding functionality, these materials should also have a means for converting the binding event into a signal (transduction). Opportunities for designing and synthesizing such materials are in the fields of organic, polymer, and inorganic chemistry.

2.2.1.2 Smart material: Signal processing at the materials level

Raman spectroscopy is referred to as a fingerprint technique because it can identify compounds based on their unique pattern of molecular vibrations. Because the phenomenon is not particularly sensitive, collection of a Raman spectrum requires high-powered lasers and large, sensitive, high-resolution spectrometers. The discovery of surface enhanced Raman spectroscopy (SERS) changed these requirements significantly. SERS involves measurement of the Raman spectrum on nanostructured silver or gold clusters, and it is an example of how an advance in nanotechnology revolutionized the implementation of a technique. This discovery, in combination with the development of compact CCD-based spectrometers and efficient diode lasers, now allows the acquisition of Raman spectra in the field, using spectrometers that sit in the palm of your hand.

The SERS technique also provides an example of how a new material or the discovery of a new physical phenomenon can eliminate the need for power-hungry and time-consuming signal averaging computation in a chemical analysis. The more signal conditioning and processing that can be done at the materials level, the better.

Fundamental investigations into nanoscale optical and electronic phenomena should lead to many new applications of use for the intelligence community. These types of studies are also suited to the long-term research goals of the NSF.

The challenges in detection of biological agents are similar to those facing chemical agent detection. However, biological toxins can be much more toxic on a per-molecule basis than chemical agents, and in some cases they can be transmitted and amplified from one individual to the next. In addition, it is very difficult to distinguish toxic biological agents from the harmless biological compounds ubiquitous in our environment, or to distinguish toxic, naturally occurring agents from toxic, man-made agents. Chemical agents are generally easier to identify using spectroscopic techniques. As with chemical agent detection, significant challenges involve improving sensitivity, specificity, and power requirements of devices. Eliminating the need for reagents with finite shelf life is an issue that is more relevant for the biological agents, and of particular importance to the intelligence application. Development of the capability to identify pathogenicity by class or function, as opposed to specific gene sequence, will improve our ability to respond to unknown or emerging threats. For example, materials that trigger as a result of a molecule transporting across a membrane may be able to detect a range of toxins or pathogens whose mode of operation involves membrane transport.

2.2.1.3 Taggants: Development of new methods for tagging and tracking precursors for nuclear, chemical, or biological weapons and explosives

Stable isotope enrichment of a chemical that may be used as a precursor in the manufacture of chemical agents, biological agents, or explosives can be useful in source attribution. New, inexpensive approaches to devices that can tag and track materials in a clandestine manner could be useful to the intelligence community.

2.2.1.4 New materials for advanced sensors/electronics

The development of shipboard phased-array radar systems over the last few decades has provided the military with a key advantage in the battlefield. This advance is grounded in the basic research that has gone into the manufacture and properties of wide bandgap semiconductors over the past 20 years. Such fundamental, paradigm-changing discoveries in the materials chemistry and physics areas cannot be predicted, although a robust basic research program is effective in promoting such discoveries. Materials that can lead to faster computers, higher density storage, and more efficient telecommunications will enable the development of low-power sensor devices of use to the intelligence community.

2.2.2 Miniature/Microscale Systems

A major trend in the analytical field is toward miniaturization. Entire analytical measurement systems, such as mass spectrometers and DNA analysis systems, are shrinking such that shoebox or handheld devices are being fabricated. There is a genuine opportunity to create small but powerful sensing devices. The progress seen in shrinking computer memory could also be realized in the sensor field. Miniaturization presents a major opportunity for sensor system design and integration.

2.2.2.1 Microfluidics

The revolution in “lab on a chip” technologies is exemplified by the field of microfluidics. Microfluidics employs chip-based manufacturing methods to provide functional systems with samplers, valves, separations, thermal cyclers, mixers, and detectors integrated onto a chip. The resulting systems can manipulate and analyze nano to picoliter volumes. The ability to convert tremendous functionality into a microscale device offers significant promise to the IC in terms of systems integration into a small sensor/ analysis package. Microfluidics may be applicable to either fully integrated sensing devices or they could serve to perform the front end processing for presentation of the sample to the back end sensor/detector. Microfluidics is one of the most promising areas for exploitation in the sensor area.

The need to monitor multiple types of analytical information is driving the need for sensor arrays (both specific and broadband). The requirement for deploying potentially hundreds to thousands of sensors will require additional advances in micro and nanofabrication to ensure that the overall device size remains small.

There are many other areas in which miniaturization will benefit sensors, including microphones and microspectrometers.

Shrinking Mass Spectrometers

Mass spectrometry is one of the most rapid, broadly applicable means we have to detect chemical and biological warfare agents. Extensive work is underway to miniaturize and ruggedize these devices. The vacuum requirements and the needs to minimize field effects from stray surface charges on the walls of the ion analysis channels of these devices present a core challenge as the size is reduced. Even so, we may be able to do much better in reducing the size and power demands. NSF should be receptive to any new ideas along these lines.

2.2.3 Nanotechnology

2.2.3.1 Single walled carbon nanotubes

Carbon nanotubes made of a single layer of hexagonally bonded carbon have emerged to be one of the most interesting new materials in nanotechnology. Depending on the exact way the hexagons wrap around the circumference of the tube, these molecules are either metallic, or direct band-gap semiconductors. Recently the semiconducting tubes have been shown to display direct band-gap photoemission, with each tube showing a specific, narrow emission line. The tubes have been used to make the first single molecule transistors, and have recently been formed into the first integrated nanotube circuits. Since every atom of the tube is on the surface, the conductance of the tubes has been shown to be highly sensitive to the presence of molecules adsorbed to their surface. The single walled nanotubes are expected to form the basis for a wide range of new electronic, electromechanical, and/or electrochemical devices, and almost certainly will be at the core of much of the nanoelectronics of the future.

Critical challenges that must be addressed in this area include sorting the nanotubes by electrical type, and learning how to "clone" individual specific nanotubes to produce large numbers of identical copies. Means must be developed to control the length of the tubes, and derivitize them selectively at each end. Techniques must be developed to arrange selected tubes into predetermined patterns, and connect them to each other and other structures with precision.

2.2.3.2 Nanophotonics

Complementary to nanoelectronics, tiny nanoscale structures can be used to modify the interaction of light with matter, a new area termed "nanophotonics." For example, triangular structures of Ag, Au, or Al with sides on the scale of 100 nm and points with 10 nm radius of curvature show localized enhancements of the incident light of up to several hundred or more in intensity, due partly to antenna effects and partly to plasmon resonances. These shapes can be formed into bowtie pairs, or into arrays. With such localized field enhancements, a variety of optical processes may be enhanced, such as fluorescence, Raman scattering, two-photon absorption, and so on, with higher enhancements for the higher-order processes. Such nanoscale structures provide the possibility for high sensitivity detection by producing extremely large local light intensities with very low power light sources. Moreover, since the region illuminated effectively is so small, the background signals can be minimized, and detection limits down to the single-molecule level are possible. Similar effects should be expected from other metallic structures such as fractal aggregates and from photonic crystals with high-Q resonances. The details of the coupled optical interaction between molecules and electromagnetically enhanced structures are not fully understood and must be explored. Thus, research in the general area of nanophotonics could lead to major advances in ultrasensitive detection and miniaturization.

2.2.4. Biologically-Inspired Systems

Biological sensing systems, such as olfaction, vision, and taste are fertile areas for sensor design. Biologically-inspired systems use different sensing principles than traditional sensor designs. One notable example is the mammalian olfactory system. In this system, an array of non-specific receptor cells generates response patterns upon exposure to different odorants. These patterns are recognized by the brain and can be learned such that they are associated with a descriptor that can be either specific (acetone, benzene) or more general ("explosive," floral). The training and learned response is then committed to memory and lasts a lifetime even though the receptors are replaced every few months. Recognition is not dependent on the typical ligand-receptor interaction but is distributed over an array of sensors.

Limited selectivity of individual chemical sensors can be efficiently overcome by use of chemical sensing arrays. This approach is particularly effective in cases where a group of chemicals that constitute a chemical *signature* characteristic of a certain object or activity needs to be detected. For example, because of the unknown dilution factor, the acquisition of information about ratios of individual components in a mixture is more important than determination of their absolute concentrations. Such arrays are used to detect signature patterns. These artificial or electronic noses have been used for broadband detection and are not limited to specific compounds. Thus, they are more anticipatory in that they can recognize a wide range of analytes. The resulting arrays are able to detect as many different substances as the number of different patterns they can generate. Training is required for these sensing systems to learn to recognize a pattern.

Processing is an important aspect of such systems. Training is task specific—i.e., one can train these systems to recognize specific compounds, specific components of mixtures, or classes of compounds. The deployment of chemical sensing arrays is predicated by our ability to microfabricate individual sensors and by the availability of algorithms for extraction of multivariate information from such arrays. Both prerequisites are the focus of current research in many groups active in the chemical sensing area. There is a genuine opportunity to begin to develop tiny, inexpensive, lightweight low power chemical nose type arrays and sensor networks based on bio-inspired systems.

Biological systems often look for signal bursts to correlate them with the stimulus. Such bursts can be on the millisecond time regime, offering extraordinary detection speeds. Biological systems often have the capacity to determine not only the identity of the analyte but also the direction of the plume. For example, the dog uses wind direction, determined by its wet nose, coupled with gradient tracking. The insect uses differential temporal responses of its antennae to determine the location of the plume.

On the receptor/transducer side, the principles of olfactory systems as well as insect antenna arrays should be investigated. One of the traditional approaches to biosensors is to employ components of biological systems such as tissue based, whole insect antennas, and living cells.

These systems have intrinsic shelf life problems and efforts should be focused instead on applying their operating principles to the design of artificial systems.

Bio-inspired systems offer a rich area for exploration. The principles used in the recognition, amplification, signal processing, and system maintenance and regeneration should be investigated and exploited for sensor system design Miniaturization presents a major opportunity for system design and integration.

2.2.4.1 Microfluidics

The revolution in "lab on a chip" technologies is exemplified by the area of microfluidics. Microfluidics employs chip-based manufacturing methods to provide functional sytems with samplers, valves, separations, thermal cyclers, mixers, and detectors integrated onto a chip. The resulting systems can manipulate and analyze nano-picoliter volumes. The ability to convert tremendous functionality in a microscale device, Microfluidics, may be applicable to either full sensing devices or it could serve to perform the front end processing for presentation of the sample to the back end sensor/detector.

2.2.4.2 Microspectrometers

Integrated systems containing a light source, filters, dispersion elements, and a detector that can be fully integrated into a micro-spectrometer.

- Systems Integration
- Amplification
- Recognition

2.2.5 Amplification

A signature of biological systems is their built-in signal amplification. This amplification results from cascade pathways in which a single receptor binding can result in an ion channel opening, Ca^{++} release, catalytic cycle activation, or other signal amplification mechanism. The end result is an amplification of the initial binding event leading to a tremendous signal gain.

Signal amplification schemes are an intrinsic aspect of many sensing systems. For example, a fluorescent molecule can produce up to a million photons before it photobleaches. Photomultipliers, intensified CCD cameras, and avalanche detectors have built in signal amplification. Additional methods for coupling binding with amplification are needed for solving the high sensitivity requirements of the IC.

Amplification can also be part of the sample processing. The polymerase chain reaction (PCR) is an amplification technique in which a single DNA sequence is replicated exponentially with each reaction cycle. In this way, the initial analyte concentration is selectively amplified. Methods for amplifying other target analytes using a PCR-type analog should be developed to enable high sensitivity detection.

Other methods for amplifying signals include the use of time integration, including the strategy of observing coherence/coincidence between many sensors, as well as acquiring the signals from many sensors to achieve a $\sqrt{N}$ enhancement in S/N.

2.2.6 Systems Integration

Advances in microelectronics have enabled the fabrication of compact, portable, low-power devices such as cellular phones and computers, and advances in power sources, miniaturization techniques, nanofabrication tools, and fundamental materials chemistry should allow this trend to continue. Of particular importance to the intelligence community, miniature devices such as concealable analytical laboratories the size of a cigarette pack or smaller will dramatically improve the effectiveness of agents in the field. The challenges in this field rest on integrating sensitive, specific sensors into low-power palmtop, wristwatch-size, or smaller devices that can communicate to the user or to a network. The need for interdisciplinary effort in this area is great. These efforts will involve chemists, materials scientists, physicists, biologists, computer scientists and engineers. Integration of power, computation, communication, and sensors into miniature, low-power devices is limited by the compatibility of materials and their processing steps. The crosscutting issues in this area include:

- Packaging and interfacing sensory materials at the device and at the network level
- Harnessing biomimetic systems without the need for conventional biological reagents that can have very limited shelf life
- Incorporation of intelligent sensor and self-regenerating sensor concepts into conventional remote sensing methodologies
- Development of materials that can operate in harsh/extreme environments and the incorporation of failure analysis and failure prediction models
- Miniaturization
- Sensor data fusion
- Rapidly reconfigurable, readily addressable, or self-organizing system

2.2.7 Sensor Integration and Sensor Networks

Wireless sensor networks, in which tens to thousands of individual sensors communicate over a large area is a robust field of research with significant current commercial interest. Examples of applications are industrial process monitoring and control; detection and tracking of pollutants in soil, air, and water; and domestic emergency response. Developments in this field are important to the IC. There are several problems that are somewhat unique to the IC. Sensors may be in place for months or even years before they are queried. The mode of communication of the sensor must be minimally detectable to unintended recipients. The sensor may need to be concealed or camouflaged such that its purpose is not revealed but that its functionality is not impaired. Sensors for chemical or biological warfare agents or their precursors, nuclear materials, or explosives are important to this community, but the time scale in which the data are needed is not as short as in a domestic security application. For example, an anthrax detector array deployed domestically in a subway station needs to respond in near real time, whereas an anthrax detector array deployed around a site suspected of producing the agent can respond in less than one week and still be of use to the intelligence worker.

Sensors operating in a trigger mode, where a sensor with a relatively low fidelity of information triggers the capture of a sample that is later subjected to a more thorough analysis, may also be important to the intelligence community, where a definite answer is needed within a few days or weeks rather than minutes.

Future developments are expected in the introduction of "arrays of arrays" (or "superarrays." In such hierarchical structures, clusters of individual sensors are arranged in arrays in order to achieve the selectivity and these arrays are then distributed in space to form a spatially distributed network of arrays. Such an arrangement enhances the possibility of obtaining spatial/temporal information about, e.g., spreading of a fugitive plume of signature gases through an urban landscape. If the individual arrays are located in fixed positions they are referred to as a static superarray. An example is a network of smoke detectors in a large commercial building interconnected into one central control point. There is a possibility for making the sensing arrays mobile by placing them, e.g., in cell phones or other portable electronics. Such arrays would be called dynamic arrays or stochastically dynamic arrays. Both types are again predicated on microfabrication, data reduction algorithms, and, in case of the stochastically dynamic array, on means of triangulation. This area of research is fertile for further exploration. Chemical information can be further supplemented by measurement of various physical parameters, such as wind (or liquid flow) velocity, temperature, pressure, sound, and EM inputs, etc. The integration of information obtained from these new data acquisition structures into models (e.g., threat situations) is imperative.

Other aspects of system integration include the strategy of coupling molecular recognition directly to the electronics or logic functions of the sensor. In addition, the idea of performing as much local processing of data at the sensor prior to transmission of the signal will enable data compression and allow for more efficient system designs with lower power and communications demands.

The possibility of a complete integration of sensors, data processing, and communications functions into low cost flexible electronic textiles, sheets, etc., for use in fabrics offers significant potential for many IC needs.

2.3 Concluding Comments

2.3.1 Education / Societal Outreach

Countering terrorism in the U.S. will be a high priority for decades to come. It is one of those issues, like clean energy and environment that resonates deeply in the hearts of young students and the general public. The challenge of developing sensors and detectors of the sort described here can only be met by bright, highly trained and motivated people in the physical sciences and engineering. This need is precisely the area of greatest concern in the U.S. workforce. The NSF should consider this aspect of the War on Terrorism in its education outreach programs. With careful nurturing, we may be able to spark a sense of mission in a cadre of bright young people who will then go into these extremely difficult professions, and help the general public realize the importance of sustained high level support.

2.3.2 General Remarks

One of the most critical aspects of sensors is their manufacturability. Sensors must be manufacturable in sufficient quantities to meet the market demand. Ideally, there would be a low variation from sensor to sensor and they would be able to be calibrated at the factory.

Another major need for low-level detection is in the area of samplers/collectors. For low levels of analytes, particularly for bio-agents, there is a need to collect large volumes of air, concentrate the collected particles/contaminants, and present the concentrated material in a small volume to the sensor. Such samplers could be simple passive affinity capture materials that bind and concentrate the targets, or they could be active collectors that draw through many volumes of sample and either filter or bind the analyte and concentrate it into a small volume. Both air and liquid-based collection systems will be required.

The ideal sensors for the IC would be universal and ubiquitous. Universal sensors suggest the need for arrays in which hundreds or thousands of sensing elements are present to detect all the analytes of interest as well as being anticipatory for new agents. In order to make such arrays ubiquitous, it will be necessary to shrink the dimensions of the entire sensor system to microscale dimensions. Assuming the entire sensing system is microscale, it is likely that some components of the system will be at the nanoscale.

Finally, it is important to recognize that the design of a particular sensor is directly tied to the application. The better defined the application, the simpler the design.

2.4 Suggested Request-for-Proposal Topics

1. Design molecular recognition compounds that bind specific analytes of interest, such as CW compounds and CW precursors, with the means to attach such compounds to basic materials such as fabrics, and the means to convert the binding event into a signal.

2. Investigate fundamental nanoscale optical and electronic phenomena.

3. Develop a device to acquire Raman spectra in the field that weighs less than 1 kg (including power supply).

4. Develop the capability to identify pathogenicity by class or function, for example materials that trigger as a result of molecular transport across a membrane.

5. Develop new methods that can tag or trace materials in a clandestine manner.

6. Investigate fundamental microfluidic technology that will enable critical steps in front-end sample processing such as cell analysis and DNA extraction.

7. Develop microfluidic techniques that will enable specific analytical functions such as HPLC.

8. Develop a device to acquire mass spectra in the field that weighs less than 1 kg. (including power supply and vacuum system).

9. Develop methods to control the length and derivatize selectively the ends of carbon nanotubes produced in quantities greater than l g.

10. Carry out fundamental studies of mammalian olfactory systems.

11. Develop tiny, inexpensive, lightweight, low-power chemical sensing assays based on the principles of mammalian or insect olfactory systems.

12. Explore methods similar to PCR for amplifying target analytes other than nucleic acids.

13. Develop systems for collection and concentration of air- or water-borne samples.

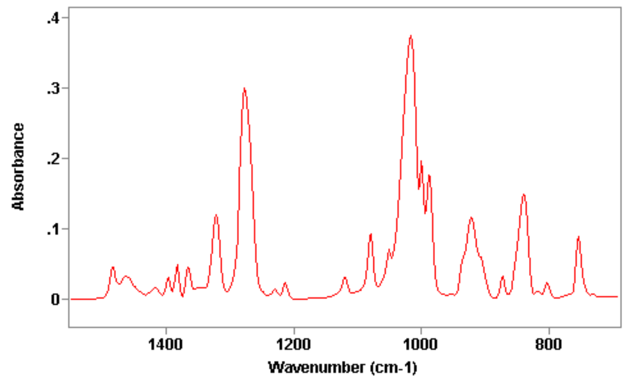
3. Optical Spectroscopies

3.1 Introduction

Optical spectroscopy is a key science for information gathering to combat terrorism because of its application to detecting materials and activities related to weapons of mass destruction (WMD). Spectroscopy techniques can be used to detect and evaluate all phases of the actions of a terrorist group or nation supporting terrorism: from the acquisition of WMD capability through production to use. Spectroscopy can also be used to support measures employed to counter terrorist activities: from inspection and verification through deployment of countermeasures to military action.

Detecting and quantifying WMD spectral signatures motivates the interest in spectroscopy for combating terrorism. Nerve agents for example are organo-phosphate compounds and have a distinctive spectral 'fingerprint' near 10μm the common presence of the P(=O) bond. Figure 1 is an example of the far infrared spectrum of the primitive nerve agent SOMAN [1]. The US Army's M21 chemical weapons detector [2] - a Fourier Transform Infrared Spectrometer – exploits this fact. This *does not* mean that the chemical or biological agent itself must be directly measured – only very small amounts of a nerve agent will be present in the environment before it is either tested or used. The amount of biowarfare agent – organism or toxin – is even smaller. The precursors and by-products of production are more likely to be present and will probably be present in more easily measurable quantities. In general, spectroscopy can be used on a variety of very difficult intelligence problems related to combating terrorism, many of which are beyond chemical and biowarfare. Spectroscopy may reveal clues about the presence of hidden facilities for WMD production and storage. It could give evidence for the reprocessing of nuclear fuel into weapons material by detecting the chemicals used in or by-products of this industrial process in the air or wastewater. It might determine the existence, location and capabilities of some delivery systems by spectral analysis of exhaust plumes and explosions. Finally, spectral techniques certainly can give assistance in the form of tip-offs and verification to many other collection techniques.

The intelligence community refers to using indirect measurements and signatures in this way as MASINT. Spectroscopy in particular and MASINT in general has added value to the intelligence community for two additional reasons: (1) it can give both qualitative and quantitative information about threats and, (2) it exploits the unavoidable results of physical processes. These characteristics mean that the conclusions from analysis of the information are difficult to disguise or alter. In the intelligence community lexicon, it is robust against Camouflage, Concealment, and Deception (CC&D). This characteristic may be better understood by contrasting two hypothetical intelligence reports: evidence of WMD storage at a foreign site from a spectroscopic measurement of leaked chemical-bioagent, versus a human report that the site is a conventional military facility. The spectral signature of a chemical-bioagent is both unmistakable proof of its presence and a plausible result of mass storage. Conversely, the human report could result from any of a number of factors including erroneous interpretation by an agent, deliberate disinformation, or excellent security. The only disadvantage of the spectroscopy finding is that it is non-literal information requiring sophisticated interpretation to understand its meaning and certainty.



A brief consideration of *possible spectroscopy applications* to combating terrorism is an aid to focusing on possible research opportunities. These will be broken out according to intelligence information gathering functions.

Indications that a terrorist organization or state is developing WMDs could come from the spectroscopic detection from an aircraft or satellite of precursor chemicals [3] of, for example, the manufacture of nerve agent. Although a definitive finding would be most desired, this information would more likely be a clue triggering further intelligence collection.

Technical intelligence regarding the nature of a terrorist threat might come from spectroscopic analysis originating from, for example, an unattended sensor, of the residue of a test or rehearsal using a particular toxin or agent. Alternately, a human agent in the country might employ field spectroscopic analysis to assess materials and decide which should be sent back to the U.S. for laboratory analysis. This information would allow the design of a specific countermeasure. Another type of technical intelligence might be the spectral analysis from a satellite or aircraft of a rocket exhaust showing the type, range, and capability of a delivery system [4]. The US Air Force's ARGUS program, for example, used airborne ultraviolet, visible, mid-wave and long-wave infrared imaging and spectroscopy for many years to collect data on rocket plume phenomena and re-entry vehicle signatures [5].

Warning of an imminent terrorist attack might come from spectroscopic detection of the fueling of a rocket. Alternately, detection of a significant quantity of a chemical-biowarfare agent in the air indicating a terrorist release or less than careful handling immediately preceding an attack, is a very specific warning. The Aum Shinrikyo cult employed a variety of ingenious and bizarre techniques to spread nerve agents that released spectroscopically detectable quantities of SARIN in the environment [6]. Obviously, the most desirable warning is both specific and timely enough to trigger defensive action.

A very sensitive spectroscopic sensor might be utilized by an inspector or in an automated portal monitor for *verification* of compliance by a country ordered to destroy its chemical weapons. This is an extension and generalization of current arms control regimes where γ-ray spectroscopy has an important role in nuclear weapons control verification. This particular function has both intrinsic advantages and special limitations.

Collection is not necessarily in as hostile an environment so that more laboratory-like sensors might be usable but, conversely, the type of sensor or technique may be limited by agreement. For example, inspectors might be limited to using only commercially available handheld spectrometers so that their capabilities are well known.

Spectral imaging from satellites, aircraft, and probably unmanned vehicles, would be used to *support military operations* against an organization or nation to preempt or retaliate for a terrorist act. This intelligence support could take the form of targeting of camouflaged assets [7], assessing post-air-strike damage to material, or determining whether a storage facility had been breeched by detecting chemical agent escape. Rapid environmental assessment to make up-to-date maps and charts from spectral imagery is another military support application. Figure 2 shows a terrain categorization map derived from hyperspectral imaging. Spectral imaging is particularly important in the intelligence preparation of the battlefield role when the environment changes rapidly as, for example, in coastal areas. See [8] for a review of remote sensing techniques for coastal areas and the role of satellite and aircraft spectral imaging.

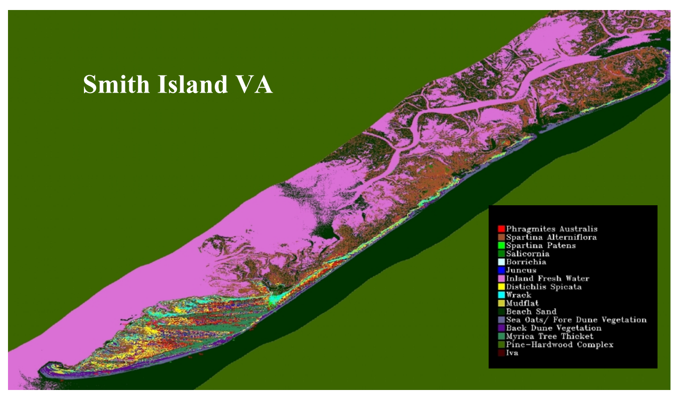


Figure 2

3.2 Research Opportunities

3.2.1 Challenges for Spectroscopy Research

Much of the utilization of spectroscopy for combating terrorism follows from research in environmental spectroscopy. Environmental spectroscopy developed for air and water quality measurement, atmospheric science, and weather forecasting has direct applications to the detection of gaseous and liquid effluents resulting from WMD activities. See [9] for a discussion of detection limits. Various active and passive spectrometers have been used in the laboratory and field to quantify aerosol properties and size distributions. Most WMDs use engineered aerosols as distribution vehicles. Hyperspectral imaging is used in mineral prospecting, agriculture and forestry, and estuarine and ocean research. It has a natural place for detecting hidden military activities and for collecting information to support military operations. However, most intelligence community applications do *not* have direct civil or scientific analogs and present special challenges. These differences or challenges may be used to define the broad research opportunities. Some of these broad opportunities are summarized below.

3.2.1.1 Increased sensitivity

Increased sensitivity for the detection and measurement of trace materials or processes is the most fundamental challenge. In practical applications, the useful limit for detection of optical spectroscopy techniques for trace species in the atmosphere (~1 ppmv) is actually quite poor. Real world terrorist organizations or states are unlikely to easily reveal themselves by exposing their weapons and means to collect intelligence so that the intelligence community has, at best, very small amounts of a material or agent with which to work. For similar reasons, standoff or remote sensing approaches are highly desirable. Satellite and aircraft sensors are both robust against area denial and broad in their area of regard increasing the probability of detection of occasional and accidental events. Spectroscopy is the scientific basis for almost all standoff sensors. Generally, the farther the standoff distance, the more sensitive the detection system must be.

3.2.1.2 Enhancing detectability

Enhancing detectability of terrorist activities has the highest payoff. This challenge might be rephrased as 'finding ways to detect the undetectable.' The best approach to an intelligence problem would be to find the 'smoking gun,' which in the case of a spectroscopic technique is to find a distinctive spectral fingerprint of a WMD. As noted, this is not usually possible. Instead, the intelligence community must exploit signatures of feedstock materials, precursors, by-products of testing or production, and other inadvertent or unavoidable signatures. These signatures are often hard to utilize: some are common materials or the result of both innocent and terrorist activities. Biowarfare agents are an excellent example of this problem. Organisms and biological processes do not generally produce very different signatures unless they attack an organism – their effect is their most distinctive signature. Even the processes involved in developing, manufacturing and deploying a biowarfare agent are only subtly different from innocent activities. Another difficulty results from the ambiguity and general lack of fundamental knowledge about some of the secondary signatures from terrorist activities. Terrorism is outside of the mainstream of activities normally studied or encountered. For example, Chemical-biowarfare agents are almost always carried on artificially produced or tailored aerosols to enhance their lifetime or effectives. The fundamental spectroscopy of materials on and in such aerosol states are both little studied and a potentially distinctive signature.

3.2.1.3 Using unusual platforms

Using unsusual platforms to carry spectroscopic detectors will require new approaches. Although there is a place for satellite and aircraft remote sensing type sensors, intelligence sensors might be deployed on different types of aircraft, including unmanned aerial vehicles. Unmanned ground or underwater vehicles or other robots are also possible platforms. Figure 3 shows an example of how compact these vehicles already are. Future vehicles may be even smaller. Unattended ground sensors either operated clandestinely or as part of a verification system have even different requirements. Perhaps the most important characteristic of a clandestine sensor is that it not be discovered or compromised. This aspect of the design of a spectroscopic sensor, like many of its intended targets is outside of normal scientific and technical practice.

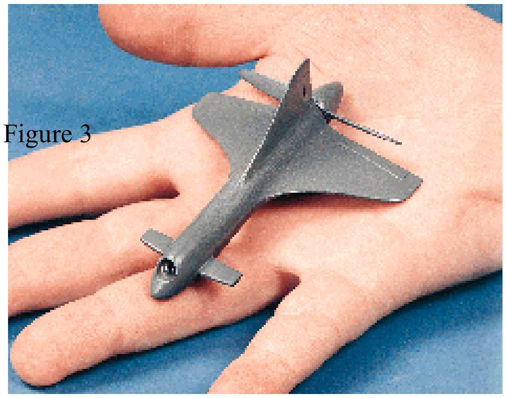


Figure 3

3.2.1.4 Rejecting confusion and backgrounds

Rejecting confusion and backgrounds is a challenge related to, but different from, enhancing detectability. This problem is particularly acute for any signature related to biowarfare activities. The natural background almost always makes the signal-to-confusion or signal-to-clutter ratio more important than the signal-to-noise ratio.

3.2.1.5 More efficient data handling

More efficient data handling is a final and very important challenge. Spectral imaging increases the dimensionality of data to be considered yet is vital to some of the possible spectroscopy applications. Unfortunately, the very nature of intelligence collection means that any data set, whether it is spectroscopic or not, is very information-sparse.

3.2.2 Areas of Priority

3.2.2.1 Fate and transport

The raw materials, processing chemicals, precursors, active agents, and byproducts associated with the manufacture of WMD are known and are generally well characterized. The mechanisms by which these compounds are transported in the environment are less well known. Successful downstream sampling of atmospheric plumes, groundwater, or surface water requires better understanding of both environmental transport mechanisms and the chemical transformations that may occur from source to point of measurement. Key areas requiring research include:

- Transport mechanisms (air, aerosol/particulate, water-borne)
- Distance/time-dependent transformation, including chemical, photochemical, surface chemical (aerosol/particulate)
- Adsorption of gaseous species by aerosols, particulates, or soils
- Biodegradation

3.2.2.2 Hyperspectral imaging

The ability to detect and quantify chemical compounds makes hyperspectral imaging from aircraft or satellite platforms an ideal tool for the detection of trace chemical constituents associated with WMD production. The ability to detect and quantify these compounds in the atmosphere, biosphere, and hydrosphere would be greatly improved by research in the following areas:

- True 3-D hyperspectral sensors
- Signature databases (both gas and solid phase)
- Improvements to atmospheric correction models including comprehensive cross-section tables over a broad range of temperature and pressure for atmospheric and anthropogenic gases
- On-board / real-time / automated processing

3.2.2.3 New/novel spectroscopic methods

The sensitivity of many current spectroscopic methods limits their usefulness for the detection of trace chemical constituents associated with WMD production. In addition, the requirement for the sensor to be in contact with the sampled medium also limits their usefulness. The needs of the IC call for spectroscopic techniques with lower limits of detection and methods that can be used in a standoff configuration. Key areas requiring research include: Novel light sources with unique capabilities that span broadband coherent femtosecond lasers and tunable, or multi-spectral compact sources.

Development of novel techniques such as spectral or temporal pulse shaping for selective excitation of relevant compounds and novel techniques with high sensitivity such as laser-trapped atom gravity gradiometers must be designed for field applications. Other novel spectroscopic techniques are BEC-based, gamma-ray, and THz techniques.

Example of a novel approach: Signal enhancement
Existing spectroscopic approaches to standoff detection, either passive or active, are limited by background clutter and sensitivity. For either approach it would be beneficial to develop means of signal enhancement. These could be either optical or chemical. Dispersal of binding agents, which exhibit enhanced cross-sections for absorption, emission or fluorescence, could be one method of improving detectability. Optical approaches could involve pump-probe or resonance methods such as Raman, fluorescence, or two-photon absorption. Synchronous perturbation of target molecule temperatures or absorptions offers the possibility of enhancing detectability by modulated detection. For example, could the vibrational temperature of target molecules be changed by pulsed laser irradiation into appropriate absorption bands? Utilizing a pair of beams with one as a reference and methods of sensing ultra-small phase shifts based on interferometry should be considered.

Example of a novel approach: Single Molecule Spectroscopy
The detection of single molecules represents the ultimate limit of detection. Currently such methods rely on strong fluorescence and ultra-small volumes. Possible methods include the measurement of polarization, lifetime, spectral shifts, and energy transfer.

3.2.2.4 Environmental Spectroscopy

The detection of the trace chemical constituents associated with WMD production in the natural environment poses unique challenges. Many of the techniques developed for air quality monitoring may be applied to the following:

- Spectroscopy of atmospheric and anthropogenic gases
- Spectroscopic techniques for characterization of atmospheric particulates (including compounds adsorbed on particulates)
- Other spectroscopic methods for determination/analysis of environmental condition
- Fundamental spectroscopy of target compounds

Example: DIAL with adaptive control and learning systems
Differential Absorption LIDAR is an established technique for air quality monitoring and atmospheric research. What are needed are enhanced specificity, sensor features and miniaturization. The use of this technique with femtosecond broadband excitation will provide new capabilities. DIAL is more specific and sensitive; clutter rejection and integration can enhance signal-to-noise ratio.

3.2.2.5 Miniaturization of Spectroscopic Instrumentation

While laboratory bench-sized instrumentation is suitable for many applications, the clandestine use of spectroscopic methods often requires the smallest, lowest power device possible. There are fundamental creative engineering and materials challenges related to miniaturization of spectroscopic instrumentation. In particular, there is a need for the development of micro-scale light sources, e.g. VCSELs.

3.3 Concluding Comments

A detailed understanding of the chemical signatures associated with the creation of WMD is key to the success of optical spectroscopic methods - not just the finished product, but precursors and methods of environmental transport and degradation. Advances in spectroscopic methods are required to lower detection limits, improve sampling efficiency and collection, and increase the standoff distance of the measurement. Advances in spectroscopic understanding of target compounds and their behavior in the environment is a current limitation for the application of spectroscopic methods. Techniques for processing and analysis of spectral data, in particular hyperspectral imagery, are also a critical need.

3.4 Suggested Request-for-Proposal Topics

1. Explore the fundamental spectroscopy of small molecules associated with weapons of mass destruction in and on aerosols, with emphasis on the discovery of systematic spectral changes and potentially distinctive signatures.

2. Determine the mechanisms of transport, adsorption and biodegredation in the environment of active agents as well as raw materials, processing chemicals, precursors, and byproducts.

3. Develop technology associated with hyperspectral imaging from aircraft or satellite platforms including true 3-D hyperspectral sensors, signature databases (both gas and solid phase), improvements to atmospheric correction models, and on-board real-time automated processing.

4. Develop novel spectroscopic techniques with low limits of detection that can be used in standoff configurations.

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4. Energy Sources

4.1 Introduction

The fundamental equation of state for intelligence (or military) field operations is:

no power = *no mission* [Eq. 1]

The energy and power requirements of the intelligence community in pursuit of counterterrorist missions span a range of operational specifications, as summarized in Table 1. The energy and power source must harmonize with the specifics of the mission and the location of use. No single type or class of power source or energy-harvesting device will suffice for the range of operations necessary for current or anticipated counterterrorist missions. The overriding requirement remains performance, which translates to reliability of the power source over operational windows of time and temperature that are more demanding than those power sources developed for consumer or military use.

During the break-out session on research opportunities in the area of energy and power for the intelligence community, the panel restricted its discussion to electron-driven forms of power, as summarized in Table 2.

4.2 Research Opportunities

With performance as the preeminent criterion of future IC-relevant power sources, all the devices listed in Table 2 require improved materials to achieve the desired gains. The materials challenges are heightened because the power sources listed in Table 2 are all multifunctional in character and require some combination of electronic conductivity, ionic conductivity, thermal conductivity, separation of electron–hole pairs, mass transport of fuel and oxidant, catalytic selectivity, or mechanical transduction. The last decade has seen major advances in enabling control of the chemistry and arrangement of matter on nanometer-length scales. These advances offer unprecedented opportunities to dramatically change the way we store and convert energy because elementary and highly efficient energetic processes naturally occur at these small length scales.

Achieving independent control of the elementary processes that give rise to the various forms of energy-relevant functionality is difficult with bulk materials. One obvious research opportunity lies in determining how to assemble nanoscopic building blocks en route to multifunctional architectures that produce power. Architectures that self-organize would be especially desirable to facilitate manufacturability or to take advantage in the field of energy-harvesting strategies.

Using nature's development of cells and tissues for inspiration, it is now possible to imagine a scenario of “bottom up” design in order to build complex, hierarchical organizations whose properties and functions will reach far beyond those exhibited by the organic and inorganic building block components that are available to us today. We anticipate that pursuit of such bottom-up approaches will have a significant impact on the design of future compact and portable energy sources.

Researching advanced concepts of nanoscopically designed or molecularly tailored materials represents a sound investment for making major advances in energy and power sources. Specific research opportunities are described below for the classes of power sources listed in Table 2; emphasis is given to batteries, as this system is a workhorse power source with a minimal signature and compatibility with missions requiring portable or leave-behind power.

Table 1. Opportunities and constraints in the choice of power sources for IC counterterrorist missions.

Applications	Operational Bounds	Research Flexibility
Access (*e.g.*, robotics)	Power: microwatts to kilowatts	Cost is not (much of) an object • ultrapure materials or processing • one-of-a-kind manufacturing
Monitoring (*e.g.*, sensors)	Temperature: -40 °C to ≥100 °C	
	Time of reliability: 1–5 years	
		Less stringent environmental concerns • exotic fuels (e.g., radioisotopes)

Table 2. Types of electron-producing power sources.

Electrochemical	Thermal/Nuclear/Mechanical-to-Electric
batteries	thermoelectrics
fuel cells; semi-fuel cells; biofuel cells	pyroelectrics
supercapacitors; ultracapacitors	thermionics
photovoltaics	harvesting adventitious energy/work
harvesting adventitious energy/fuel	radioisotope thermoelectric generators, RTGs [α– or β–emitters]
	Beta cells (nuclear "solar" cells)

4.2.1 Electrochemical Power Sources

4.2.1.1 Batteries

In traditional rechargeable lithium batteries, a large amount of electrochemically active transition metal compound is necessary to achieve capacity (hours of current under load). The tradeoff between capacity and physicochemical stability of bulk insertion compounds has significantly hampered cathode development. A new materials paradigm is required in order to design transition metal compounds and architectures in which the metal cation can exchange multiple electrons in a narrow voltage range.

As an example of the contribution to be made by quantum chemistry in understanding charge storage, Figure 1 shows the calculated electron exchange in $Li(Ni_{0.5}Mn_{0.5})O_2$ when extracting all the Li ions. Virtually the complete electron exchange has occurred with 2 electrons per Ni (bright regions) [1]. This multiple electron exchange on Ni occurs with no discernable voltage step. The integration of the Ni^{2+}/Ni^{4+} couple into host structures that can accommodate more Ni could lead to electrodes with *four times the present-day capacity*. A key goal is to increase the number of

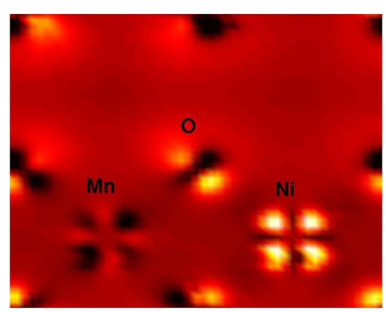


Figure 1. Quantum computation of electron exchange in delithiated $Li(Ni_{0.5}Mn_{0.5})O_2$.

electrons transferred per transition metal cation without causing deleterious structural or phase changes in the insertion material.

Mesoporous nanostructured materials comprising bicontinuous networks of electrochemically active nanoscopic solid and porosity have already demonstrated the importance of arranging nanoscale building blocks in space to create multifunctional power-source architectures [2]. Sol–gel-derived materials, such as aerogels, in which the porous network retains through-connectivity (by minimizing compressive forces during processing), provide a means to investigate how electrochemical processes are influenced by *(1)* minimal solid-state diffusion lengths; *(2)* effective mass transport of ions and solvent to the nanoscale, networked electrode material; and *(3)* amplification of the surface (and surface defect) character of the electrochemically active material.

Characterizing and exploiting the nature of defects in charge-storage materials is a key area of future research in the drive to improve the performance of batteries and ultracapacitors. The aerogel forms of disordered $V_2O_5 \bullet 0.5\,H_2O$ afford Li-to-V_2O_5 stoichiometries of 4–6 [3,4], while those for the bulk, crystalline material are 1–2. One clue to this impressive improvement in the Li-ion capacity of V_2O_5 can be found by inducing deliberate defects in polycrystalline V_2O_5 [5]: creation of proton-stabilized cation vacancies increases the capacity 23% relative to the ~170 mAh/g obtained with the as-received polycrystalline V_2O_5.

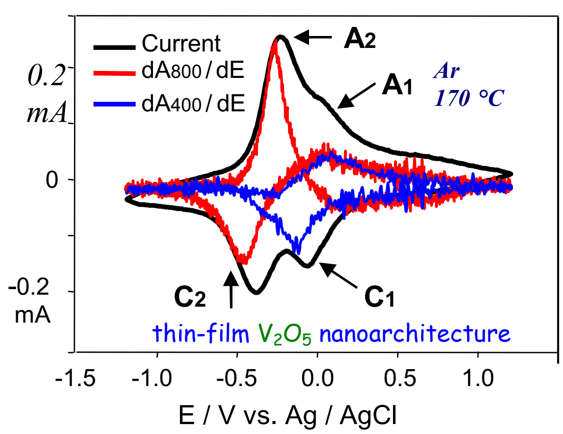


Figure 2. Correlation of electronic state (spectroscopic) and charge-insertion sites (electrochemical) in a thin-film hydrous V_2O_5 nanoarchitecture.

The charge-insertion oxides are also electrochromic materials, so the optical response tracks changes in the electronic state of the transition metal center as it undergoes reduction/oxidation and concomitant cation insertion/de-insertion. This approach has been especially effective with MnO_2 and V_2O_5 nanoarchitectures [6,7]; Figure 2 shows that the two energetic redox processes associated with reduction of V_2O_5 and insertion of Li^+ correlates with two previously identified [8] color centers: defect-free V_2O_5 (C1/A1; 400-nm absorption) and vanadium centers near anion-vacancies (C2/A2; 800-nm absorption).

The charge/discharge rates obtainable with meso- and macroporous nanostructured materials [2,9], including surfactant-templated architectures [10], are faster than those of standard electrochemically active transition metal compounds in traditional composite electrode structures, with discharge rates as high as 1000 C. It appears that these porous nanoarchitectures are natural hybrid materials that store charge in a manner that mimics that of a battery (slow rate, high energy density) and an ultracapacitor (high rate, high power density).

Other areas in which research investment will improve the performance of batteries include new electrolytes with stability at higher temperatures and EMFs; improved polymers as ultrathin (i.e., nanometers-thick) separators; and understanding packaging and sealing and interconnects with nanoscopic components. The latter two are areas in which self-organization should be explored.

4.2.1.2 Fuel cells

Performance of fuel cells directly scales with fuel and oxidant utilization—and fuel is oxidized and oxygen is reduced because of the activity of dispersed nanoscale or biomolecular electrocatalysts at the anode and cathode, respectively. All fuel cells require improved electrocatalysts and the route to improved electrocatalysts will require the best that nanoscale science can offer. The nature of alloys on the nanoscale—and the nature of their physicochemical stability under the temperature, pressure, and electrochemical potential of fuel-cell operation—is essentially unknown. Routes to low or no loadings of platinum-group metal electrocatalysts are necessary. Early results with

Pt-RuO_xH_y [11] and Pt-based intermetallics for methanol oxidation [12] and with oxide-dispersed Pt for oxygen reduction [13] offer new compositional phase space to explore—one that moves away from the reliance on metallic or alloy-based electrocatalysts for fuel-cell electroreactions. In general, as for any heterogeneous catalytic process, the transform function that converts the mechanistic information from model studies with single-crystal or bulk substrates needs to be reexamined when the chemical system is physically expressed on the nanoscale.

The mechanisms that lead to performance losses in fuel cells over long-duration operation are still not fully known and may arise from interactions between the electrocatalysts, the membrane, and the electron and ion conduction paths. Electrocatalysts that resist poisoning by less-than-pristine fuels or air are especially desirable for field or leave-behind operation—oxide-based catalysts are more resistant to sulfur and CO poisoning at low temperature than are metals. If solid and liquid sources of hydrogen are developed, the already-optimized Pt-catalyzed hydrogen-oxygen fuel cells are feasible.

The electrocatalyst is not the only functional structure of fuel cells that needs additional research. New proton-conducting membranes are desirable for fuel-cell operation at temperatures under which Nafion® loses effectiveness. The stability of polymer and solid-acid membranes catalyzed with Pt-based nanoparticles in the presence of organic fuels needs to be explored. For low power applications, membraneless fuel cells are viable options and can range from biofuel cells [14] to microfluidic-reactor-based systems, such as recently demonstrated with V(II)/V(IV) redox fuel cells [15]. Re-thinking the fuel cell as a multifunctional nanostructured architecture, rather than retaining the traditional masonry-like approach to building up functional planes of activity, should offer improvements simply by improving the ability of fuel and oxidant molecules to access electrocatalysts [16]. Ultimately, it may be possible to design fuel cells that integrate biomolecular catalysts and bio-organisms or that rely on nanowired inorganic catalysts in a carbon- and ionomer-free fashion.

4.2.1.3 Supercapacitors and ultracapacitors

Multifunction is also critical in electrochemical capacitors, which require high surface areas of a lightweight, solid-state material with high electronic conductivity and excellent chemical stability to get performance that maximizes energy density and minimizes resistive heat generating losses, with minimal degradation under potential in high-ionic-strength electrolytes. And the high performance charge-storing material must be arranged in space such that meso- to macroporous paths permit facile solvent–ion approach to the entire high-surface-area electrified interface. These architectures must be constructed such that the surface area contained within micropores (< 2 nm) is minimized, because electrolyte conductivity drops two orders of magnitude in pores sized at ~ 1 nm [17]. The surface area of the inner walls of carbon single-walled nanotubes can thus be unavailable for capacitive charge storage. Pseudocapacitive materials, which store >10-times the energy of carbon supercapacitors (typically at 50–100 F/g [18]) and are usually termed ultracapacitors, offer two means to store energy: as electrical double-layer capacitance, and as electron–ion insertion over a broad potential window.

The champion pseudocapacitive material to date is hydrous ruthenium oxide ($RuO_2 \; xH_2O$), which stores ~ 700 F/g of RuO_2 and exhibits excellent metallic conductivity [19]. Alternatives to scarce and costly ruthenium are necessary. Transition metal oxides need not be the only class of materials examined, although much can be learned from what is already understood, e.g., highly crystalline forms of ruthenium and cobalt oxides express low pseudocapacitance. Atomic pair density functional analyses of the x-rays scattered from $RuO_2 \; xH_2O$ (amorphous by XRD) show that it is an innate nanocomposite comprising a rutile, electron-conducting RuO_2 “wire” that is networked through hydrous, proton-conducting domains, where the volume fractions of the components track the mole fraction of structural water (x) [20]. In that this new model of the functional structure of $RuO_2 \; xH_2O$ shows it to be an inorganic mimic of organic block copolymers, new strategies to design pseudo-capacitive architectures should be explored. Some of these architectures may be inorganic–organic hybrids. Finally, photocapacitors should be re-investigated, particularly those that retain charge for long periods through temperature ranges relevant to counterterrorist missions.

4.2.1.4 Integration of electrochemical power sources with microfabrication and related processing

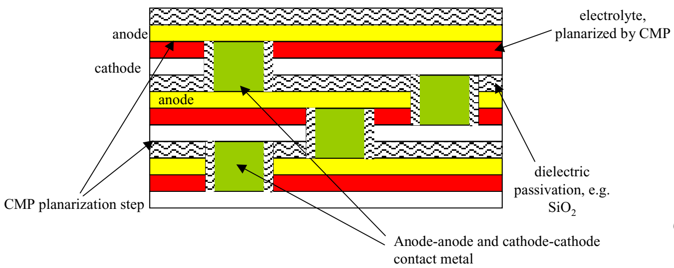


Figure 3. Proposed on-chip multicell construction [MIT]; CMP is chemical mechanical polishing.

An exciting new research direction is to integrate electrochemical power sources with microfabrication and other electronics processing. This approach offers two advantages: on-wafer integration can lead to independent (self-powered) microdevices; and cells with extremely thin (< 50 nm) electrolyte layers make extremely rapid charging possible. For example, Si systems integrated with 3-D, on-chip, battery stacks (Figure 3) could be used to make inexpensive and miniaturized devices for remote sensing or wireless communication. With integrated power sources based on photovoltaics or MEMS devices, fully autonomous devices that need never be connected to the outside world can be envisaged. Recharging could occur with even minimal motion or exposure to light.

The successful integration of power sources with Si technology may require the development of electrode and electrolyte materials that are clean-room "friendly," *i.e.*, do not contaminate Si circuits (*e.g.,* Cu, Fe). Such materials are being developed through a combined computational and experimental approach at MIT. An alternate approach being taken by a UCLA/Utah/Florida/NRL ONR–MURI team exploits microfabrication to design cubic-millimeter-sized power supplies based on three-dimensional (3-D) geometries for microbatteries that scale (through control of the depth of the etched features in Figure 4) according to the power requirements of the device [21]. The Si mold can be processed external to a clean room, so standard battery materials and processes can be used. Power-source integration with micromachined Si has also been extended at the University of Minnesota to direct methanol fuel cells. A power density of 42 mW/cm^2 was achieved at 90 °C [22].

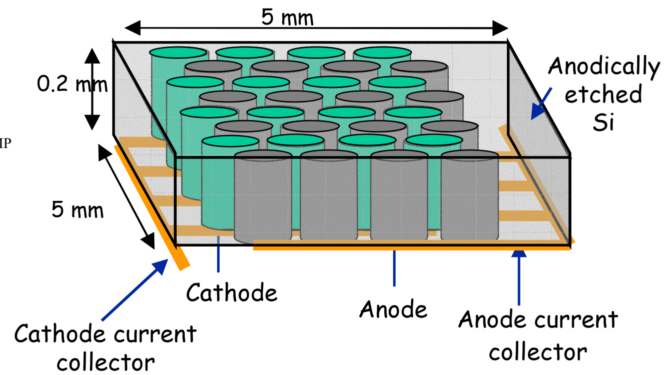
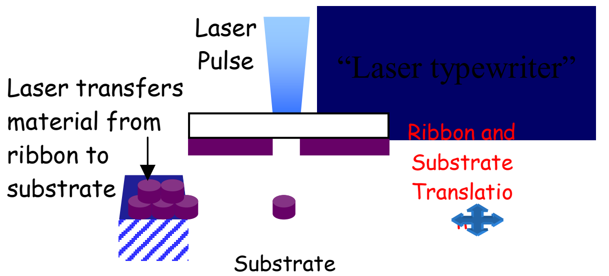


Figure 4. Three-dimensional microbattery created within a microfabricated Si mold [UCLA].

Another approach is to fabricate power sources using direct-write processes to tailor the properties and geometry of the power source to the specific power demands of each device, Figure 5 [23]. The focus is to decrease the weight and size of the total system (packaging, interconnects, etc.), which increases efficiency. The electronics substrate serves as part of the power-source packaging—the wires and rectifiers needed to distribute power from a central power source to multiple subsystems are no longer needed, which also lessens ohmic losses and electromagnetic interference. When combined with energy-harvesting devices (solar cells, RF antennae, etc.), rechargeable Li-ion batteries and ultracapacitors can serve as compact, low-maintenance, low-signature power sources for autonomous microsystems.

4.2.2 Thermal to Electric

A nanostructured materials/processing approach to thermoelectric-, pyroelectrics-, and thermionics-based power sources may break the historical limitations that exist with present-day



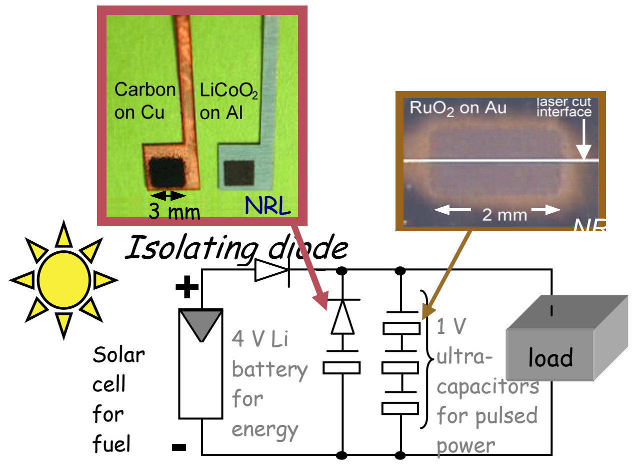


Figure 5. Fabricating on-board power sources via direct-write matrix-assisted pulsed laser evaporation (schematic, top); prototype hybrid power system (right) combines a solar cell, battery, and ultracapacitor. [NRL]

materials and which arise because of low-efficiency bulk materials or operational requirements of high temperature. Research over the past decade with systems composed of nanoscale constituents offers the possibility of independently controlling materials properties that are normally strongly coupled in conventional three-dimensional materials.

4.2.2.1. Thermoelectrics

Efficient thermoelectric conversion of thermal energy to electrical energy requires materials with high thermopower (or Seebeck coefficient), high electrical conductivity, and low thermal conductivity. These properties are strongly coupled in 3-D materials, but by introducing interfaces into nanosized isoelectronic structures, thermal conductivity is substantially reduced (to produce a phonon glass) without a corresponding reduction in electrical conductivity. The demonstration of enhancement in the Seebeck coefficient with decreasing size in quantum wells, quantum wires, and quantum dots is also significant, especially in terms of the further optimization that should be possible through controlled placement of the Fermi level at a maximum in the density of states [24]. The incorporation of these nanostructures into 3-D devices, either in self-assembled arrays or inside of crystalline materials (e.g., skutterudites, clathrates) presents a substantial research challenge for energy conversion. The development of low-cost processing technology for such systems represents a large materials challenge. Integrated systems that could benefit from the development of efficient thermoelectric conversion systems include small self-powered devices utilizing temperature gradients between body temperature and the ambient, in radioisotope thermoelectric generators, and for the conversion of harvested thermal energy to electrical energy.

4.2.2.2 Thermionics

Thermionic energy conversion arises from the work-function differential between a hot electron-emitting cathode and a cooler electron-collecting, lower work function anode. Thermionic sources can be highly efficient and operate without maintenance for years because electron emission and collection requires no mechanical motion. Efficiencies greater than 50% of the Carnot efficiency and power densities greater than 15 W/cm^2 are obtainable. Thermionic systems operated in space-based nuclear reactor cores used emitters with temperatures approaching 200° C (cooled via radiation to space), but such systems are not appropriate for most terrestrial applications. The three modes of thermionic emission (into vacuum; with space-charge neutralization; and

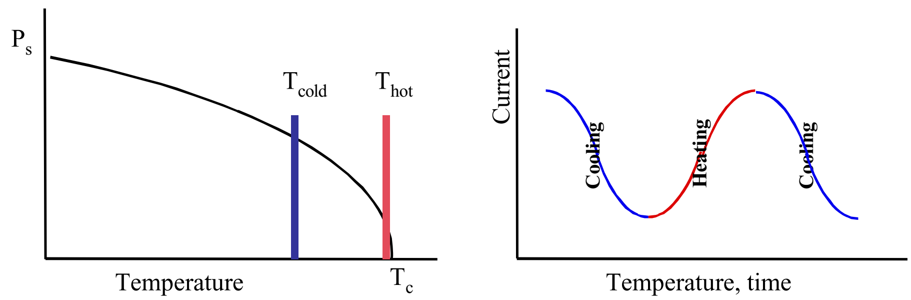


Figure 6: Spontaneous polarization P_s of a ferroelectric as a function of temperature (left). The pyroelectric coefficient, $p = \partial P_s / \partial T$, reaches extremely large values at the pyroelectric Curie transition temperature T_c. Cycling temperature between T_{cold} and T_{hot} produces an AC current (right).

via inter-electrode plasma) are well studied, and it is apparent that these approaches cannot be readily extended to lower temperature operation.

Lower-temperature operation of thermionic devices may be feasible with more efficient electron-emitting materials. As with thermoelectric materials, appropriate nanoengineering is key and could enable new approaches for electron emission in thermionic energy converters. These materials would have spatially varying electrical and morphological properties such that they could be engineered for electron emission at substantially lower operating temperatures, while also minimizing space-charge effects. Carbon nanotube and related nanotubular materials are examples of structures that could be employed for these applications.

4.2.2.3 Pyroelectrics

When pyroelectric materials are cycled between two temperatures, the change in spontaneous polarization induces electrical charge on the surface of the material, which generates an AC current. As indicated in Figure 6, charge flows in one direction on heating and in the opposite direction on cooling, with the amount of charge the same in both cases. For properly chosen and engineered materials, an efficiency close to that of an ideal Carnot cycle is possible. The optimum performance is obtained when the high temperature is near the pyroelectric Curie transition temperature. In ferroelectric-based pyroelectrics, the pyroelectric coefficients are significantly larger—typically on the order of 300 nC/m^{2}K. Perhaps the most notable use of these materials occurs in thermal imaging applications, in which incipient radiation increases the temperature by a small amount and the ensuing electrical signal is sensed. Ferroelectric materials, especially $Ba_{1-x}Sr_xTiO_3$ (BST), have been used with great success for this purpose.

Nanoengineered materials may offer all new approaches for application of pyroelectric energy conversion. Nanoelectromechanical systems (NEMS) approaches need to be developed to control the heating/cooling cycle. Nanoengineered ferroelectrics with a range of pyrolectric coefficients would allow tuned pyroelectrics to serve as thermal-to-electric converters over a broad range of operation temperatures.

4.2.3 Nuclear to Electric

4.2.3.1 Radioisotope Power Sources

Radioisotope power sources utilize the energy of radioisotope decays to produce electricity. With an energy release per decay of ≈10^4 to 10^6eV, the capacities (specific energies) of radioisotope fuels are enormous, ≈10^7 to 10^9Wh/kg. For comparison, the capacities of good chemical fuels are ≈10^4Wh/kg. Energy conversion devices that tap the huge capacities of radioisotope fuels can provide steady power for very long periods of time. For example, radioisotope thermoelectric generators (RTGs) are reliable, robust power sources that can produce milliwatts to hundreds of watts of power for tens of years [25]. The current RTGs are limited by the low efficiency of thermoelectric energy conversion. Novel thermoelectric materials with enhanced efficiencies, as discussed above, could allow smaller amounts of a radioisotope fuel to be utilized for a specified power output, which would minimize the thermal and radioactive emissions of a power source. Microfabricated charge-to-motion converters can also be used to power mechanical devices with radioisotopic fuels [26].

Non-thermal schemes of radioisotope energy conversion may also be proposed. In principal, these schemes would allow very small (µW to mW) power sources that would be difficult to detect. Beta cells are solid-state devices that accomplish such direct energy conversion. A beta particle (high energy electron) passing through a semiconductor can generate 104 to 105 electron–hole pairs. The internal field of a semiconductor junction device can separate and collect these generated charge carriers in a manner analogous to solar cells. However, the output of beta cells fabricated from conventional semiconductors rapidly degrades as a result of accumulating beta-induced damage. Radiation damage to certain unconventional semiconductors, icosahedral borides, appears to spontaneously self-heal [27], which is a property not predicted *a priori* to the observation. Research on unconventional semiconductors may thus yield useful power sources such as beta cells.

4.2.4 Energy Harvesting—Taking Advantage of Parasitic or Adventitious Energy or Fuel

The harvesting of thermal energy and its storage in phase-transition materials could provide a useful energy source for some applications. Molecularly designed organic or nanocomposite materials engineered to exhibit first-order solid–solid phase transitions offer opportunities for building thermal energy units into structures for subsequent energy harvesting. Here the challenge is to develop inexpensive materials systems that have high heat storage capacity over a tunable temperature range with minimal cycling expansion/contraction through the phase transition and with no special isolation requirements. The development of this concept is still at an early stage, and has so far been based on off-the-shelf items, such as paraffin. The use of advanced materials concepts and of selected nanostructures might offer dramatically improved opportunities for serious utilization of this energy storage/harvesting approach. Pulse-power would be possible by using thermal sources to charge electrochemical capacitors.

Manipulating biomolecular function offers other ways to use fuels present in the environment to generate power in biofuel cells, such as through the conversion of sediments [28] or decaying matter. A simple compartmentless miniature biofuel cell, in which glucose is electrooxidized and oxygen is electroreduced at two bioelectrocatalyst-coated 7-µm-diameter carbon fibers, operates in a physiological buffer solution 14]. The cell produces several microwatts of power for a week, enough to power a sensor transmitter system. This type of cell opens the way to autonomous sensor–amplifier–transmitter systems operating in animals, insects, and plants, exemplified by the grape in Figure 7. Another way to exploit biomolecular function for energy is through microorganisms that could be discovered or engineered to ferment biofuel to methanol in order to trickle charge the “fuel tank” of a leave-behind direct methanol fuel cell. An alternative would be to use the usual yeasts, but identify an effective electrocatalyst to break C–C bonds for use at the anode of a direct ethanol fuel cell.

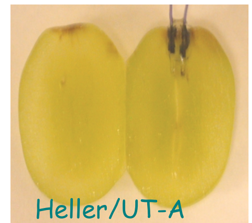


Figure 7. A biofuel cell that operates using the glucose fuel and water innate to a grape.

4.2.5 Computation and Modeling

First-principles computational modeling will play a crucial role in the design of novel materials concepts for materials generation and energy storage. Through computations it is possible to rapidly scan a large number of possible materials and evaluate their potential as an intercalation electrode, fuel-cell catalyst, or membrane. The impact of first-principles computation in understanding and improving materials for rechargeable Li batteries is well demonstrated [29]. Properties, such as voltage, stability, lithium diffusivity, and intercalation stresses, can now be routinely calculated for promising compounds well before efforts are expended to design them. The controlled environment offered by modeling makes it possible to rapidly isolate the key materials factors that influence a key property. Such knowledge can then be used in the design process.

When the dimensions between the active components of electrochemical power sources collapse to nanometer separations, systems modeling will be necessary to understand current and potential distributions and heat transfer of the power source under operation, especially at high rate and with non-standard geometries [30]. The intuition developed by scientists and engineers who work on the micrometer scale does not seamlessly translate to the nanoscale, where new scientific principles based on quantum mechanics become important. Fundamental data coupled with computational studies are necessary before the Handbook of Nanoscale Design and Engineering can be written.

4.2.6 Opportunities and Deficiencies When Periodicity and Order are Abandoned

In order to arrive at nanostructured, multifunctional architectures that provide premium performance, even when potentially disordered or porous, we need better theoretical, synthetic, and characterization approaches. A key challenge will be to "pin" the most active, highest performance physicochemical state of the nanoscopic material even when exposed to thermodynamic forces (temperature, pressure, electrical potential, photochemical energy) that would otherwise drive restructuring, crystallization, or densification. Although nanoscale matter increases the number of surface atoms relative to bulk, these materials still require analyses that can distinguish the physical, chemical, and structural character of the surface from that of the interior. And if disorder is good, especially on the nanoscale, almost all of our standard analytical and materials characterization tools are inadequate—including x-ray diffraction and EXAFS. Medium-range structural information (beyond first- and second-nearest neighbors) is vital for materials that express transport properties; atomic pair density functional analysis [20,31] offers one way to obtain the nature of structure at these length scales.

4.2.7 Operational Signatures

Concomitant with the performance required of power sources during counterterrorist missions is the need for minimal signature during operation. Of the power sources listed in Table 2 some potential signature concerns arise (Table 3), which will require strategies to counter such signatures and will involve materials considerations and system design.

Table 3. Possible signatures from power sources relevant to IC counterterrorist missions.

Power Source	Nature of the Signature: Thermal	Acoustic Noise	Electrical Noise	Nuclear (γ, n)
High-rate batteries	X			
Electrochemical capacitors	X	X		
Fuel cells [a]	X	X	X	
Biofuel cells implanted in plants and animals				
Thermal-to-Electric	X			
RTGs and beta cells [b]	X		X	

[a] These signatures are relevant unless the fuel cell is low power, air breathing, and gravity- or capillary-fed.
[b] For low-power applications, beta cells may be easily camouflaged.

4.3 Concluding Comments

4.3.1 NSF-Unique Opportunities

The Energy Break-out Group also discerned four areas in which the NSF can improve infrastructural and professional aspects to ensure that NSF-MPS investment in fundamental research will ultimately lead to improved IC-relevant power sources.

- Workforce issues
  - Provide highly cross-disciplinary training
  - Re-establish necessary expertise, e.g., the U.S. is nearly out of nuclear chemists
  - Reverse the decline in numbers of undergraduates majoring in science and engineering
- Ameliorate peer-review hiccups
  - Ensure that promising blue-sky/outrageous proposals get past the peers
- People integration
  - Continue to foster chemists talking to engineers talking to physicists talking to materials scientists talking to mathematicians talking to biologists …
- Facilitate R&D transitions
  - Set up the means for a smooth hand-off to systems engineers
  - Establish mechanisms to infuse funds for pre-development research

4.3.2 Timeliness

NSF, DOE, and NAS workshops in the past 15 months have emphasized the importance of research on the nanoscale for improvements in materials, nanoarchitectures, and charge transfer. Energy and power have been important considerations at all three meetings. Breakthroughs in materials, nanoarchitectures, and charge transfer on the nanoscale will promote improvements in power sources of interest to the intelligence community. The reports from these meetings are good source materials that address the challenges and opportunities awaiting the multidisciplinary community interested in energy storage and conversion [32,33,34].

- Develop materials with multifunctional architectures consisting of nanoscale building blocks, with particular emphasis on nanostructures that self-organize.
- Demonstrate methods to achieve reversible storage of greater than 0.5 electron and

insertion-cation equivalents per transition metal center in battery insertion compounds.

- Discover high activity electrocatalysts for fuel cell electroreactions that also tolerate chemical foulants present in fuels and oxidizers.

- Design charge-insertion architectures that match or exceed the high specific capacitance of hydrous ruthenium oxide (without the use of platinum-group metals) and which exhibit minimal self-discharge.

- Develop new classes of nanostructured thermoelectric materials with high electrical conductivity and low thermal conductivity.

- Discover new classes of semiconductors that self-heal under alpha or beta irradiation.

- Develop computational modeling programs for testing novel materials concepts for electrical energy generation and storage.

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5. Image Reconstruction and Analysis

5.1 Introduction

The Image Reconstruction and Analysis (IR/A) group was tasked with studying the contributions that image processing basic research could make to combating terrorism.

A broad outline of our conclusions is given in Figure 1. This list identifies the broad issues and the corresponding opportunities for basic research. We have noted the possibilities for cross-disciplinary research in the right hand column. An immediate conclusion is that all of these issues call for substantial inter-disciplinary involvement across a broad range of disciplines. This is analogous to recent national and NSF-based initiative in computing technology. In NSF, therefore, the highly visible Information Technology Research (ITR) program (http://www.itr.nsf.gov) offers an analog to the type of interdisciplinary research that we envisage in IR/A.

- Dimensionality reduction

The volume of images and associated information is a substantial problem. Many large format images are taken daily and must be analyzed promptly and thoroughly. Submitting each image to an analyst is simply impossible: many Terabytes (10^{12} bytes) must be viewed daily and compared to previous images. Preprocessing must be applied to images in order for the analysts to focus on possible targets.

- Data management

Large dimensionality implies substantial data management problems. Not only must large amounts of data be stored and retrieved but the corresponding metadata must accompany each image. In addition, different agencies must be able to interoperate and exchange information seamlessly.

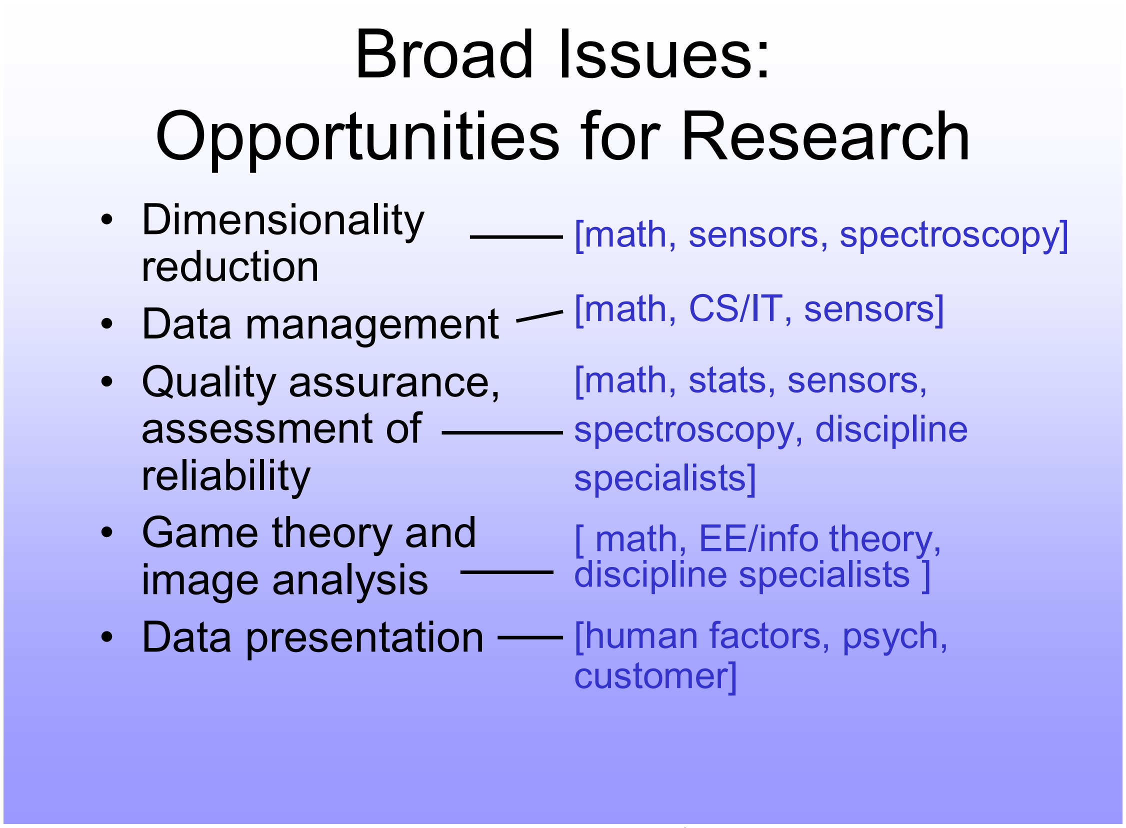

Figure 1 Broad issues: opportunities for research

- Quality assurance, assessment of reliability

Image analysis is inherently probabilistic. This requires that probability be a central part of all image analysis tasks, and that probability must be propagated throughout any resulting decision trees right up to any final decision point.

- Game theory and image analysis

Since decision theory is an important part of image analysis, game theory must also be. Opponents have an interest in concealment and misdirection. Our IR/A work must take this into account.

- Data presentation

Analysts are faced with severe problems in viewing images. For example, our visual system did not evolve in response to large format hyper-spectral images and consequently visual analysis of such images is highly demanding. Tools to aid in the presentation of such data are urgently needed.

In addition to these topics for basic research, we have some comments on the necessity for a systems approach to IR/A. Finally, we conclude with a discussion of areas that we believe are important to the mission of combating terrorism but which were either omitted from the briefing presentations or seem to be under-developed in the IC.

5.2 Research Opportunities

5.2.1 Dimensionality Reduction

Dimensionality reduction is vital to reduce the analysis task to a manageable size. The vast flow of data (in the form of images and accompanying metadata) must be reduced in dimensionality and thence volume. Thus, many stages of analysis may be required until a human analyst would be called upon to look at a specific image or set of images. Automated analysis would look for key signatures that would be used to alert an analyst to the possible presence of an important occurrence.

There remains much work to be done in image analysis, both in transform and non-transform forms. In natural space, segmentation and classification continue to be key developmental areas in many applications of imaging. In transform space, the applications of wavelet transforms have been particularly rich leading to new variants such as ridgelets, curvlets, and brushlets. These and future associated developments are likely to produce important tools for image analysis. Such basic research should be encouraged.

Similarly, an important area of research is the registration of images from different times and modalities. Registration of such images onto a single coordinate system is vital for automated analysis but can be extremely challenging. The lack of robust image registration algorithms remains a limiting factor in many fields.

Hyper-spectral images are a potent source of information. Although one given wavelength can often be spoofed, doing so for a range of wavelengths is very much more difficult. Hyper-spectral data can also aid in the identification of chemical plumes in an environment. The problem with hyper-spectral imagery is one of analysis. Often only highly trained individuals can fully extract information from hyper-spectral images. Advances are needed to allow less trained individuals to interpret such images to, for example, identify chemical or heat plumes.

Work is needed on feature and pattern discovery and recognition. Patterns can occur in a wide range of spaces. For example, patterns in space and time may be as illuminating as patterns in space alone. However, to be most useful, such patterns must be captured in a searchable database. For example, one may benefit from applying segmentation and classification operators to images and then looking for patterns in the changes over times. Similarly, rare events must be captured and maintained for subsequent searches.

5.2.2 Data Management

The volume of relevant data is staggering (many Terabytes per day) and likely to swamp resources for many years to come. Images are large in format and may be hyper-spectral and repeated often in time. Metadata may be voluminous and complex. Think, for example, of the description of a pattern in time and space as described above. With such complicated information, the computation required for metadata queries may be limiting.

Similar problems occur in a couple of areas within the NSF/MPS purview: particle physics and the astronomical community. Both are developing "Data Grids" for distributed computing involving large volumes of data. The National Virtual Observatory (see http://www.us-vo.org; funded by NSF under the ITR program described above) has the task of providing technology for the federation of astronomical databases from multiple sources. All aspects of this endeavor (including metadata, grid computing, and interoperability) are likely to be of direct relevance to the federation of IC-based image databases. Of particular importance is the discovery of patterns in metadata space. This requires new types of analysis and visualization tools adapted specifically to metadata.

5.2.3 Quality Assurance, Assessment of Reliability

Image analysis is fundamentally a probabilistic realm. Classification in particular is probabilistic in nature rather than being a simple binary decision. Usually a multilevel decision tree must be followed to draw a conclusion. It is possible to track the propagation of probabilities through the necessary complex decision trees by using, e.g., Bayesian or Dempster-Shafer approaches. Further research within the context of image segmentation and classification is likely to be very helpful.

Assessment of reliability requires approaches that are independent of the decision tree itself. For example, the analyst will wish to know the stability of feature vectors and classifications under minor changes to the imaging. If seen with a different illumination, for example, does the classification change? Such work calls for simulations including, for example, the construction of fake or known test images with embedded test features. Full end-to-end simulation capability is therefore a valuable tool for the analyst.

5.2.4 Data Presentation

The presentation of image data has been a limiting factor in many areas of science. Substantial work has been invested in data fusion, whereby different information sources are presented in one simple graphical form. Perhaps the most successful automated data fusion occurs in remote-sensing where large format images from different modalities are combined with various sensor measurements, such as temperature, to provide an integrated display of a wide range of related information. This is an advanced field with much to offer.

It is important to emphasize that data presentation can either limit or enable the analyst. Images of dimension > 2 may have to be displayed, together with overlays of metadata such as activity patterns. Fundamental human factors research is needed to understand how best to perform such displays. We must understand how best to match display formats, display devices, and operator training to maximize the effectiveness of the analyst. Research and development of large format displays (both conventional and radical such as electronic papers) must be pursued.

Uncertainties and probability estimates must be propagated throughout and must be displayed as part of the data presentation.

5.2.5 Near-target imaging

In this report so far, we have concentrated on distant imaging where the imaging sensor is far removed from the target area. There are important situations where human targets are nearby and must be recognized. Recent experience, post September 11, has shown that face recognition is still very unreliable. Identification from mug-shots is still somewhat unreliable, whereas for natural scenes, even the preliminary task of finding a face in a static photograph is difficult (see for example the demonstration page at http://vasc.ri.cmu.edu/cgi-bin/demos/findface.cgi). We suggest that research into this and other forms of biometrics via imaging, such as identification by gait, should be funded.

5.2.6 Non-visual Imaging

While hyper-spectral imaging has evidently shown its worth, multi-waveband imaging seems to be under-utilized by the IC in comparison to the remote sensing community. By fusing together data from quite different wavebands in the Electro-Magnetic spectrum, it is possible to form a more accurate picture of a region. For example, the use of *passive* high resolution radio imaging brings entirely different information. Active radio imaging (via SAR for example) is very widely used in remote sensing. Polarization imaging can reveal unexpected features. Differential SAR is very effective at finding low-level changes in topography, due to, for example, earth disturbance or tunneling.

We also note that passive radio imaging is also possible (though difficult) using either large antennas or antenna arrays.

Acoustic and seismic imagings are also possible using inexpensive deployed sensors. Imagine, for example, laying down a network of inexpensive passive seismic or acoustic sensors over a region of interest.

5.3 Concluding Comments

5.3.1 Game Theory and Image Analysis

Combating terrorism is a deadly game played against very sophisticated and resourceful opponents – both terrorist groups and terrorist nation-states are very capable of misleading and misdirecting intelligence efforts. IR/A is not intrinsically superior in this regard. As a result, every effort must be made to anticipate and counter moves by our opponents.

Game theory itself is of course applicable to this problem. In addition, we suggest two different types of counters:

- **Team A/Team B:** When faced with an intelligent opponent, it is easy to be deluded about the effectiveness of one's actions. A tactic widely used in many different areas (particularly business and military) is the Team A/Team B concept whereby adversarial internal groups are established with the same goals. Either played out in war-games or in longer term engagements, such teams can rapidly leapfrog each other in capabilities.

- **Honeypot:** Computing security in recent years has been strengthened by the use of "honeypots" to attract hackers. Computer systems that are asserted to be secure are made available to all-comers on the Internet. Break-ins are rewarded in some way, either by contracts or financially. We suggest a similar scheme here. NIMA could make typical imagery sets available to researchers with rewards for target identification.

Tools used by terrorists are amenable to such approaches. For example, both cryptography and steganography (hiding a message within an image, video, or audio) are likely to be used for covert communications. Both techniques could be investigated using the approaches described above.

5.3.2 Systems Approach for Image Analysis

It is important to emphasize the importance of the imaging system or systems from which the data are obtained. To get optimal results from imaging systems (including the analysis software) requires an end-to-end design and operation philosophy. For example, astronomical projects such as the Sloan Digital Sky Survey (http://www.sdss.org/sdss.html) are conducted by teams of astronomers, physicists, mechanical, electronic and software engineers. The end-to-end design is developed in a highly iterative way that involves all team members. From our interactions with various members of the IC, we understand that such end-to-end design is rarely possible.

We strongly urge the IC to adopt such end-to-end systems design methodologies.

5.4 Suggested Request-for-Proposal Topics

1. Develop new tools to aid in the analysis and presentation of data derived from large format hyperspectral images, for example to identify chemical or heat plumes.

2. Explore the application of wavelet transforms to image analysis.

3. Carry out fundamental research in methods for the registration of images from different times and modalities to develop robust image registration algorithms.

4. Study the propagation of probabilities through complex decision trees in the context of image segmentation and classification.

5. Develop improved automated data fusion techniques and large format displays.

6. Develop new methods of face recognition and other forms of biometrics via imaging such as identification by gait.

6. Mathematical Techniques

6.1 Introduction

The case for the development of mathematics directed at intelligence issues is compelling. The IC is faced with an overwhelming task of gleaning critical information from vast arrays of disparate data, choosing the best forms of collecting information, developing new data sources and setting up personnel to effectively function in adverse circumstances. Each of these areas demands an intensive effort on behalf of the mathematical community to develop techniques and ideas aimed at resolving these fundamental issues.

The role of mathematics in the scientific advances of the last century, from advanced computing through lasers and optical communications to medical diagnosis, is now widely recognized. Its central role in developing intelligence capacity is equally striking. From new cryptographic schemes to fast data processing techniques, mathematical ideas have provided the critical link. We are now faced with an extraordinary situation in our global fight against terrorism, and this report seeks to encourage the mathematical community to use its full capabilities in responding to this challenge.

The group meeting in Chantilly, Va., in November 2002, considered various areas in which the development of mathematical techniques might impact intelligence operations. A focus was quickly developed around issues dealing with the extraordinary quantities of data received on a daily basis by the IC. The problems faced in sifting through this data, organizing it, processing it and, most importantly, figuring out what is useful, are overwhelming without some effective mathematical techniques. These techniques may derive from a variety of areas of mathematics. While statistics has naturally been at the forefront of data analysis, geometric representations of data suggest the use of advanced techniques of graph theory, topology, geometric analysis, and dynamical systems.
Directing resources at the development of these technologies should have two aims:

1. The growth of these ideas and methods into truly effective techniques of data processing

2. The engagement of these approaches with the needs and challenges of data analysis that face the IC

We list below some of the issues, areas, and approaches identified by the working group on "Mathematical Techniques." The list is by no means definitive, but will show the potential of mathematics to make a significant difference in IC data analysis.

Fundamentally new mathematics takes time to develop and we encourage the IC working together with NSF to be cognizant of this fact. We recommend that the effort be viewed as happening on two levels. Support should be given to projects aimed at quickly resolving pressing needs of the IC, and further resources should be aimed at fundamental development of new approaches that will lead to new ways of thinking about data analysis and will steadily change the landscape of our intelligence capabilities.

6.2 Research Opportunities

6.2.1 Background on Data Processing

Although the needs of the IC are extensive and complex, in this chapter we will focus upon the issues that are driven by aspects of interaction with large and diverse data sets. Typical examples are the areas of data processing and data mining. These areas include data collection, preprocessing, analysis, synthesis, and finally presentation.

There are many varied aspects of data collection. The first involves the location of sensors. What are the optimal locations for sensors, determined by optimization strategies? What are the constraints to placing sensors in optimal locations and how can these constraints be addressed? This area is very rich mathematically and intersects with each of the other research groups in the workshop. Clearly the need for smaller, longer-lasting, adaptive energy sources impacts optimal sensor or detector locations in both space and time. The ability to analyze visual data and to reconstruct images depends heavily upon the spatial and temporal richness or paucity of measured data. The inverse problems involved in image reconstruction and the data distribution necessary to effectively analyze these data utilize known mathematical optimization techniques. The complexity, heterogeneity, and potential lack of integrity of these data greatly complicate the mathematical techniques.

Understanding the connectivity of diverse data sets or streams of data is essential in developing effective metadata that can be used later in data mining algorithms. We must be able to assign efficient metadata to streaming data in order not to be overwhelmed by the amount and complexity of the data in the streams.

Once data is collected efficiently, effective data preprocessing techniques must be developed; this includes filtering, compression, feature extraction, symbolic representation or classification, and data fusion. Research in these data preprocessing techniques is widespread, but not as common in data sets with constraints. For example, feature extraction from a data set with intentional misinformation demands very different mathematical techniques than those used in conventional data mining. The field of needs from the IC community involving image reconstruction and analysis is enormously impacted by the preprocessing techniques used to reduce the dimensionality or the incompleteness of the data. Triage and prioritization of the data is essential for the enormous data sets involving complex linkages and low data quality.

Visualization techniques can be critical in aspects of feature extraction. This is a special type of data reduction concept that can quickly pick out special events or anomalies. Clustering is an essential tool in data reduction that is complicated considerably through distributed data sets and complex linkages between data sets.

Given the enormous size and complexity of the required data sets, scalability is an essential attribute for algorithms utilized in these data mining processes. Another critical requirement, often labeled knowledge presentation, is the complex display and integration of disparate data sets that can convey a critical, but complex, body of knowledge that can then be effectively interrogated and understood.

The synthesis of the data is the next essential step. The meta analysis allows information to be grouped, interrogated, and effectively synthesized. Expert systems can be brought into use. The basic interrogation and integration of the different data modules can yield critical new insights. Finally the data analysis needs to be summarized, integrated, and utilized in decision processes. Again, decision making under uncertainty or deliberate misinformation requires new mathematical techniques and interpretation.

6.2.2 Data Mining

Many excellent algorithms have been developed for large, and potentially multi variate data sets. Existing technologies are, however, not adequate for application to enormous, “dirty,” heterogeneous data sets, distributed across disparate and complex databases.

6.2.2.1 Dimensional reduction

Our ability to collect data exceeds our ability to analyze it. Every day, the IC receives terabytes of speech, text, and image data, as well as other forms of raw and processed data. For the purposes of computational efficiency, rapid indexing, and prioritization, there is a critical need for efficient methods for dimensionality reduction.

Different needs will call for different approaches. Dimensionality reduction for computational efficiency might involve finding representations in high, but much reduced, dimensional spaces that preserve, and possibly even reveal, important attributes of the data.

Possibly, linear methods such as principal or independent component analysis can be effective, but the primary focus should be on nonlinear methods which might reveal lower dimensional manifolds that contain most of the data variation.

Dimensionality reduction for rapid indexing might involve a drastic reduction to a handful of highly informative, and possibly symbolic, annotations (such as word, place, and category descriptions). Ideally, these representations would be inferred from a large “training set” comprising examples of data that have already been annotated. It is anticipated that information-theoretic methods, such as classification trees, as well as probabilistic/Bayesian methods will be effective.

Prioritization represents a kind of rapid triage, whereby data of the highest potential intelligence impact is assigned the highest priority. The emphasis is on minimizing “false alarms” while preserving zero or near zero missed detections. Depending upon the data type, the task may involve image or linguistic analysis, or the categorization of more abstract entities represented, simply, by high-dimensional vectors. Approaches might use geometric (shape analysis), statistical (Bayes nets, pattern classification), or information-theoretic analyses. Useful methods require very high computational efficiency.

6.2.2.2 Clusters and other geometric structures

Cluster analysis is probably the number one tool of data mining. Assuming the data is in the form of “p” variables or measurements on each of “n” objects, the primary form of the clustering problem is to partition the objects into “g” groups or clusters such that the clusters are cohesive and separated from each other. The problem is genuinely hard both for theoretical and practical reasons. Hundreds of algorithms exist but a comprehensive understanding of their pros and cons is still lacking. There is no generally accepted “mathematical theory of clustering.”

Notwithstanding this rather sorry state of affairs, the need for effective ways to find clusters in massive (large and complex) data sets continues to be one of the truly compelling challenges of data analysis. It is informative to contrast the “pure” clustering problem, as described, with another traditional problem of classification where the group structure is known in advance and the focus is on assigning “unknowns” to the existing groups. The latter is relatively easy to treat mathematically, while the former is extremely difficult!

One productive way to think about new research in this area would be to contemplate a continuum of problems between pure clustering (unsupervised learning) and pure classification (supervised learning).

In many intelligence applications there may be enough knowledge about the problem, such as a hint that certain things go together or a reason to assume the number of clusters is in a certain range, to allow for new types of approaches that are easier to execute than for the pure clustering situation. A related opportunity would be to develop approaches for finding certain clusters (e.g., ones associated with suspect individuals) without bothering to find all of them.

Another class of mathematical challenges would be to develop corresponding approaches for finding other types of geometrical structures, such as cycles in graphs. Depending upon the application, there may be a wide range of such structures that could be of great interest to intelligence analysts. (See Section 6.2.2.3 on Computational Topology.)

Generally, this area of research would benefit greatly from collaborations among mathematicians, statisticians, and computer scientists. It is not good enough to develop efficient algorithms without proper consideration of the mathematical and statistical structures that will emerge from their application. Nor does it help to propose extracting geometrical structures that cannot be reliably and efficiently computed.

6.2.2.3 Computational topology

The representation of data as clouds making a geometric formation has spurred the use of topological techniques aimed at identifying internal structure of the data set. While it is most natural to use this approach to identify cycles or holes in the data, it has also been developed as a diagnostic tool for other features relevant in image processing, such as corners and edges.

The issues of processing data based on intelligence may be of a very different nature, except those directly representing images, but the point remains that the identification of structure and patterns in data sets is the aim of computational topology. Needed would be an effort directed at adapting the growing body of techniques in this area to the data sets coming out of intelligence operations. Communication of the issues to researchers in this area and collaboration over the development of tools aimed at intelligence data could be extremely fruitful.

At this point, it is hard to see the end-product of this interaction but the promise is great as it brings to bear on intelligence operations a century's worth of high-level mathematical development.

The area of topology is mature and well-developed, but focus has largely been on low-dimensional cases. Considering the kind of data sets that face the IC, the application also promises to enrich the mathematics as it supplies both a reason and a context for developing higher-dimensional techniques.

6.2.2.4 Mining across distributed, heterogeneous databases

New data fusion and linking techniques are needed to enable more effective and efficient data mining. Of particular interest are statistical and mathematical approaches capable of linking data stored in databases that are massive (Petabytes), heterogeneous (in the sense that they contain multiple natural languages, and both structured and unstructured forms, e.g., text, spoken text, audio, video and images), and distributed among disparate networked repositories. Data fusion might be achieved through graphical analysis of semantic networks of metadata, or other approaches to concept mapping, and may involve the exploitation of ontologies, profiles, or statistically-derived concept spaces. Since fusion may cull data from different agencies, means are also needed to ensure the privacy of individuals. At the same time, techniques are needed to infer the use of aliases by suspects. Data must be fused using methods that do not compromise their spatial and temporal integrity; and new techniques are needed that aid data fusion through the recognition of related events and their sequences, through social relationships, and relationship patterns learned through use. Automatic tagging of data with metadata is important to data fusion and exploitation; this tagging also includes logging and exploitation of their lineage and history of use.

6.2.2.5 Accounting for deniability and deception

Data mining with denial and deception introduces significant constraints that complicate the algorithms markedly. By "denial" we mean a target's attempt to eliminate its "fingerprints" from our databases. By "deception" we mean a target's attempt to mislead or misinform us in our databases. The IC faces "denial" for example when targets use an alias in email, or when they talk in a "code" that gets around mentioning targeted topics; or in imaging, when they move objects back to normal positions before the predictable return of a satellite. The IC faces "deception" when targets give us false "nuggets" that cause us to misdeploy resources. How can data mining detect the characteristics of "denial" and "deception"? Can we make models of programmatic, adversarial activity and detect that steps up to a certain point were taken, and that expected follow-on steps were not observed? Can we detect mistakes in attempts to eliminate the adversary's traces? Was the alias not successfully used every time? Were the attempts to mislead inconsistent? Can we distinguish between data that was deliberately eliminated or misinforming, and data that was inadvertently missed or misinterpreted? Could we detect that the target knew we were on to them? What mathematical tasks would help us make these determinations? System identification? Graph analysis? Data clustering and structuring?

6.2.2.6 Data quality

One of the nastier issues in data mining is data quality. This refers to many aspects of the data, not the least of which is simply the raw error rate. But there are many other issues that fall under this heading such as missing data, data precision, and economic questions such as how much investment to make in the data collection process given the purposes to which it will be used. So, in a sense, data quality is itself a "multivariate problem" with many angles to it.

It is also relatively less studied than other aspects of data analysis, and there is nothing approaching a theory of data quality that would guide practitioners.

One approach to data quality is to subject the data to data analysis with the hope of identifying all its questionable aspects. This can be exceedingly tedious even in data sets of modest size. Research is needed to see if automation of such tasks is feasible. Another approach, already well developed in certain directions, is to use so-called robust methods of analysis which are designed to still do sensible things even when a certain fraction of the data (potentially as much as 50%!) is faulty. There is a side benefit to this approach as well: with robust models in hand one can more readily spot the outliers or bad data by noting which ones are not well represented by the model.

This line of thinking could be developed into a strong attack on data quality problems.

6.2.3 Data Manipulation, Approximation, and Modeling

Our knowledge in mathematics concerning approximation in high dimensions is mostly inadequate (even in dimensions as low as 10); most theoretical tools available are useless for effective (fast) computation and processing. Such knowledge would lead to selection of small sets of sampling points in order to model a function to a specified precision. The availability of such approximation theory together with efficient parametrization of low dimensional subsets of high dimensional spaces would enable quantitative regression and estimation of desired empirical functions. The main issue with the current state of nonparametric modeling (neural nets and other schemes) is the lack of ability to quantify errors.

A useful tool for interpretation of data in moderate dimension could be provided by metric perceptualization. To be specific we could try to represent a point in 10 dimensions by a string of sounds; the point is that we would like to compare the auditory perceptual distance with the Euclidean distance between the points. Such metric (bilipschitz) maps between Euclidean space and human perceptual metric could be extraordinarily useful. In particular we would like the analyst to listen to the data and identify certain clusters and their relation. The role of dimensional reduction would be to map empirical data into the low dimensional Euclidean space, which would then be perceptualized for efficient learning.

6.2.3.1 Multiscale geometric analysis

Tools have been developed for assessing the dimensionality of data-sets that ostensibly lie in higher-dimensional spaces. These sets may contain features that lie on lower-dimensional sets and these can be identified using a combination of techniques now under development. Part of this involves the injection of ideas from harmonic analysis into statistical and computational approaches.
When fully developed, it is anticipated that this body of techniques will lead to effective tools for dimension reduction through lower-dimensional feature identification, data compression, and cleaning. These approaches are being developed for large data sets, such as occur in digital astronomical catalogs. Their development could benefit crucially from an effort to handle intelligence data output.

6.2.3.2 Model-based data and outcome analysis

By model-based data and outcome analysis we mean the use of physical, biological, or social network models to provide mathematical structure. This structure can model the generation and evolution of data and can be used to predict or control outcomes given measured data sets. The task is complicated by spatial heterogeneity, temporal variability, nonlinearity and high dimensionality of dependent variables. These models typically take the form of deterministic or stochastic partial or ordinary differential equations, difference equations, or complex or dynamical systems. Mathematical issues include model construction and selection, sensitivity and uncertainty analysis, parameter identification, and controllability.

Examples include: the use of air and water transport models to predict outcomes given measured data; modeling DNA structure to determine identifiers. These identifiers can be for individuals or for disease or toxin identification; model the spread of diseases both to identify new diseases and to determine if containment is possible; model the spread of ideas as they are distributed in space and time.

6.2.3.3 Dynamical systems-based modeling

Time series coming from a system evolving in time can be tested for low-dimensionality using established techniques of dynamical systems (often called nonlinear time series analysis). Models can be created directly from the data even if the user is blind to the underlying physical process. If successful in a particular instance, this approach gives a powerful tool for prediction. While this technique has proved useful in representing univariate series, the total lack of physical input in the modeling has meant that even simple relationships between data streams in multivariate series are not included. Hybrid approaches in which dynamical models can be built that incorporate some underlying known structures could be extremely useful in processing intelligence data sets. This is a major challenge to the dynamical systems community as it will involve rethinking the way the models are constructed.

6.2.3.4 Data assimilation

At the opposite end of the spectrum are physical models that incorporate data through the process of assimilation. The state-of-the-art involves use of the Kalman filter. This has proved successful in atmosphere and ocean prediction. For application in more varied situations, it will need significant development. It is essentially a linear technique, and adaptation is needed for dealing with highly nonlinear situations. There is also an assumption that errors are distributed in a Gaussian fashion and an improved filter is needed to deal with fat-tail distributions.

6.3 Concluding Comments

The extraordinary demand for techniques to process enormous quantities of complex, disparate data on behalf of the IC casts the main challenge to the mathematical community in addressing intelligence needs. The group recommends that NSF and the IC focus effort and resources in this priority area with the goal of encouraging the mathematical community to rise to this challenge.

Mathematics is, almost by definition, concerned with finding structure and patterns in numerically represented sets. Advances in computational and observational technology have compelled the mathematical community to develop techniques for dealing with discrete sets of data, rather than the idealized geometric objects that fueled mathematical thought in the past. This development has led to a vast array of novel techniques, some already developed and some promised, that can aid us in processing large data sets. The goal is then to place this research into the context of intelligence issues so that further development is responsive to the direct needs of the IC. The nature of intelligence data, with its quantity, heterogeneity, and noisiness, demands that we take these advances to a whole new level. The promise is of adaptable and effective techniques for the IC that draw on the insights of deep and advanced mathematics.

Specifically, we recommend the following steps to be taken:

1. Identify researchers who can lead the effort to revolutionize data management and processing. Institute funding opportunities with directed effort to support the identified individuals and groups.

2. Seek projects to fund that reflect both immediate pay-off in intelligence capabilities and others that promise development of totally new approaches to data processing. This should include projects aimed at developing advanced mathematical ideas with future potential for intelligence applications.

3. Develop mechanism for collaborative efforts between the IC and the mathematics community, including the possibility of jointly funded grants supporting team-based research efforts involving individuals from both camps.

4. Facilitate ongoing two-way communication so that the mathematical community is aware of IC needs and technology is transferred to the IC. This can be achieved through targeted workshops, visits, and exchanges of personnel, IC briefings to leaders of the mathematical community, etc.

5. Make (sanitized) data available to the project leaders. This may be disguised data or data run from a realistic model.

6. Make funds available to support graduate student training and research, with focus specifically on issues of concern to the IC. This is a particularly efficient mechanism for seeding a spectrum of relevant long-term research programs.

The group felt optimistic that the mathematical community would respond to this challenge, and that, if the resources are made available, the prospects for real advances are very high. To summarize as a single objective: the goal is to guide the research on data analysis toward addressing intelligence needs through constructive engagement of the mathematical community with the IC.

6.4 Suggested Request-for-Proposal Topics

1. Support general areas of graph theory, topology, geometric analysis, and dynamical systems applied to data mining and analysis.

2. Develop mathematical methods for feature extraction from enormous, "dirty," heterogeneous data sets distributed across disparate complex databases with intentional misinformation.

3. Develop efficient methods for dimensionality reduction, with emphasis on nonlinear methods that might reveal lower dimensional manifolds that contain most of the data variation.

4. Develop effective means to find clusters in large and complex data sets.

5. Develop new approaches for finding geometrical structures such as cycles in graphs.

6. Explore statistical and mathematical approaches capable of linking data stored in databases that are massive, heterogeneous (in the sense that they contain multiple natural languages and both structured and unstructured forms such as text, spoken text, audio, video and images), and distributed among disparate networked repositories.

7. Explore whether automation of the task of assessing data quality is possible.

8. Develop mathematical techniques that will lead to effective tools for dimension reduction through lower-dimensional feature identification, data compression, and cleaning.

9. Develop novel mathematical techniques that can aid in processing large data sets.

10. Develop the mathematical foundations of agent-based modeling.

6.5 Appendix: Overview of Mathematical Techniques for Counterterrorism

In this appendix we give a general overview of mathematical techniques in the arena of counterterrorism. In the first subsection we illustrate, by example, how a wide variety of mathematical methodologies can play a role in the combat of terrorism. In the following subject we briefly review a wide range of techniques which have been or are being applied.

We note that this appendix is included as a survey of mathematical techniques that are applicable to counterterrorism, and thus can be very useful to the basic research community. However, some of the areas covered are applicable in the homeland defense context, rather than in the intelligence context, and thus will not be included in a joint NSF/IC request for proposals; clearly support can be pursued in other channels, since the problems are important in the overall national security picture. The sections on bioterrorism preparedness (6.5.1) and mathematical epidemiology (6.5.2.2) are examples that fall outside the scope of the intelligence community's responsibilities. Inclusion in this workshop report may also serve the purpose of stimulating other applications of the mathematics to social network issues that fall within the IC's purview (e.g., how loosely ordered organizations connect, how ideas propagate, how communities of interest self-organize, etc.)

We also emphasize that certain areas may not be supported in open environments, such as universities. The introduction to the report (section 1.0) notes that this workshop seeks the areas of intersection between the IC's needs for enabling science and technology and the academic community's norms of carrying out research in an unclassified environment. Consequently, there are again some areas that, although appropriate for inclusion in a broad review of the applicability of mathematical techniques to counterterrorism, will not be included in the NSF/IC request for proposals. A good example of this is cryptology (6.5.2.1), a core discipline in the intelligence community but one that by policy is not pursued in academia under IC sponsorship.

These points have been made because it is important to avoid misunderstandings as we seek to define important areas for collaboration between the IC and the community served by the NSF. On the other hand, it is more important to emphasize the richness of collaborative opportunities so amply demonstrated in this volume.

6.5.1 An Example: Bioterrorism Preparedness

Biodefense preparation and response planning provide an example to illustrate the relevance mathematical modeling and analysis to the combat of terrorism. We can separate two main aspects of biodefense preparedness. First, there is the process of gathering intelligence to help predict likely events and to detect events as soon as possible after the release of pathogenic agents. This includes both the development and deployments of detectors and sensor networks and the exploitation of these and existing data streams. Second, there is the aspect of planning and policy-making. There are many questions related to stockpiling, allocating, and distribution of resources such as vaccines, hospital beds, critical personnel of various sorts, morgue capacity, etc. How much is needed? Where should it be stored? When and how will it be distributed? And so forth.

Another aspect of policy-making includes the development of protocols for vaccination, quarantine, and evacuation. For example, when will vaccination occur for various groups in the population. How much prophylactic vaccination should occur? In what stage of bioterror event detection should vaccinations be administered? How widely? If supplies of vaccine are limited, how should they be allocated? Yet another set of policies concern the modifications to infrastructure, such as the road system, public transportation system, and postal system, in the event of a suspected or confirmed bioterror attack.

A great variety of mathematical techniques can be used to help support effective intelligence gathering, planning, and policy-making. The development of new sensors is almost sure to involve modeling with differential equations and simulation with computational algorithms. The optimal deployment of sensor networks may well involve sophisticated constrained optimization problems and possibly game theory. The effective exploitation of information falls under the rubric of data mining, which has been approached with a variety of mathematical techniques including, of course, probability and statistics, but also linear algebra, approximation theory, graph theory, neural networks, and optimization. For studying the effects of various plans, policies, and protocols under various scenarios, an essential ingredient will be the modeling of the dispersion of various sorts of bioagents in various environments (the atmosphere, a subway system, the postal system), and, even more importantly, the modeling of the spread of disease. Such modeling involves ordinary and partial differential equations and integral equations, dynamical systems, and numerical analysis. The mathematical modeling of disease spread in the case of naturally occurring pathogens is in fact a well-developed discipline called mathematical epidemiology.

Finally, once the effects of various defensive protocols for various attack scenarios are successfully modeled, the evaluation of policy options brings into play optimization, operations research, game theory, and control theory.

The utility of such mathematical approaches has already been demonstrated. Mathematical epidemiology has had a significant effect on how we deal with a variety of naturally occurring diseases, such as AIDS in the human population and foot-and-mouth disease in the bovine population. In the arena of bioterror planning, recent work of Kaplan, Craft, and Wein (KCW) [1] modeled the effectiveness of different vaccination strategies in limiting the consequences of the intentional introduction of smallpox in an urban area. Using a combination of mathematical epidemiological modeling and queuing theory to model vaccination administration they made the case for mass vaccination over a ring vaccination strategy.

This work has already had substantial influence in a rethinking of vaccination protocols by the Center for Disease Control and other governmental agencies.

6.5.2 Mathematical Techniques for Counterterrorism

We now review a variety of mathematical techniques with relevance or possible relevance to counterterrorism.

6.5.2.1 Cryptology

Certainly the most established of these is *cryptology*. Cryptography and cryptanalysis, based on mathematical techniques, were developed in the 19th century. The deciphering of the German Enigma code by British mathematicians working at Bletchley Park during World War II is well known. The breaking of Japan's PURPLE code by American cryptologists also involved the application of statistical and mathematical techniques in novel ways. Together these victories probably shortened the war by two years and saved countless lives. The National Security Agency was born as a direct outcome of these intelligence successes. It is now the largest single employer of Ph.D. mathematicians in the world.

Cryptology remains an active research field. There are several scientific journals, such as the Journal of Cryptology and Cryptosystems Journal, dedicated to the subject, and numerous others for which cryptology occupies a large proportion of their articles. There are many conferences each year and a professional organization. The subject is taught in many mathematics departments, even at the undergraduate level. The field, which is now highly mathematical, is undergoing rapid development. The cracking of DES, a de facto encryption standard, in 1998 highlighted vulnerability. Moreover, some in the scientific community believe that the replacement standard AES is probably not secure. Quantum cryptography, which involves a very different model of computing, is now the subject of intense study and may eventually change the entire cryptography landscape.

6.5.2.2 Mathematical epidemiology

Mathematical epidemiology is also a well-established field, as evidenced by journals, textbooks, courses, and conference series. In a nutshell, it models disease spread by dividing the population into groups and modeling the movement of individuals among the groups via differential and integral equations. The resulting model can be studied analytically and solved numerically.

Practical epidemiological models have much in common with the SIR model, but tend to be much more complicated. The population may be segmented into many more groups according to age, disease stage, course of treatment, etc. Terms are added for mortality, from the disease or other causes, and for births and aging of the population. An area of contemporary research is to incorporate more sophisticated models of interaction between the groups which take into account spatial variation, travel, time delays, etc.

In the context of counterterrorism, several additional issues arise. Deliberately released biological agents may differ from naturally occurring ones in various ways, such as simultaneous or near-simultaneous appearance in multiple locations, non-natural modes of dispersal, and genetically-engineered virulence or resistance to vaccines and treatment.

Agent-based models furnish an interesting alternative to classical continuum-based epidemiological models, and are beginning to receive a lot of attention. In these models, the spread of disease is simulated through the interaction of a large number of software agents representing individuals. The mathematical foundations of agent-based modeling (in all fields) is in its infancy and is of high potential.

6.5.2.3 Data mining

The terms data mining, data fusion, and information integration refer to methodologies to extract useful and predictive information from collected data. This area encompasses a vast range of problems that vary greatly from one another. For example, some problems may be data-rich and others data-poor. Or the feature of interest may be anomalies involving a small part of the data, or trends involving much of it. There are many evident applications in intelligence and counterterrorism--in fact this is likely to be the arena where research in mathematical techniques has the greatest payoff. Of course data mining is of great importance in many other application areas as well, from astronomy to sociology, business to medicine.

Data mining is a huge and flourishing, though not yet cohesive field. Many different mathematical techniques are being applied. These include statistical methods like clustering, classification, decision trees, and Bayesian networks; discrete mathematics including graph theory and combinatorial optimization; algebraic methods like latent semantic analysis and neural nets; and many computer science techniques like database design, various machine learning schemes, and high performance computing techniques. Much of the contemporary interest (but certainly not all) focuses on problems involving massive, heterogeneous, noisy datasets. This is of evident relevance for counterterrorism.

Since 2001, the Society for Industrial and Applied Mathematics has held an annual data mining conference. This spring the third such conference will be held. In conjunction with it, there is a planned workshop on Data Mining for Counter Terrorism and Security. The following topics of interest are given in the workshop description.

- Methods to integrate heterogeneous data sources, such as text, internet, video, audio, biometrics, and speech
- Scalable methods to warehouse disparate data sources
- Identifying trends in singular or group activities
- Pattern recognition for scene and person identification
- Data mining in the field of aviation security, port security, bio-security
- Data mining on the web for terrorist trend detection

Another topic, of critical importance to the intelligence community, is the nascent subject of *privacy-preserving data mining.* Privacy-preserving algorithms can be based on a one-party query to a database controlled by another party without getting full access to the database, or on the injection of noise into a database designed to disguise information which is not to be revealed but not to disguise the information being sought.

6.5.2.4 Imaging

An image may be loosely defined as data in a natural geometric arrangement. A lot of intelligence data is imagery, e.g., satellite imagery, seismic imagery, and radar imagery. Imaging can be divided into three overlapping and inter-related parts. *Image reconstruction* refers to the creation of images using data from physical devices such as optical instruments or sensors. Computerized tomography algorithms are a well-known example, and others arise in MRI, seismic imaging, acoustic imaging, synthetic aperture radar, and astrophysical imaging. Image reconstruction generally involves the solution of an inverse problem in partial differential equations and often involves a significant amount of geometry, especially differential geometry *Image processing* is the processing of transforming images into images which are in some sense better or more suited to the purpose at hand, e.g., by reducing aberration, enhancing certain features, compressing, fusing multiple images, etc. Harmonic analysis, partial differential equations, information theory, geometry, and optimization all enter. Finally, *image interpretation* is the process of extracting using information from images. (Thus it is a class of data mining.)

A difficult set of problems in image understanding which is of great importance for national security involves face detection and recognition. These problems have been attacked by many researchers and a variety of different methods have been used: deformable templates, basis expansion methods such as eigenfaces, statistical learning methods, multiscale representations, graph-theoretic methods, etc. Nonetheless the results are still not satisfactory for many applications. Even the problem of scanning a picture and identifying the faces in it, regardless of orientation, shadow, expressions, etc., remains very challenging and still only partially solved.

6.5.2.5 Social network analysis

Mathematical techniques are increasingly being applied in the social sciences. One example of this which is being applied also for counterterrorism is social network analysis, a quantitative approach to the analysis of interpersonal relationships using a graph-theoretic framework. In this methodology a community, organization, or social group is described as a graph in which the vertices are the individuals and edges connect vertices to indicate various types of relationships or connections among the individuals. Then a variety of graph-theoretic measures can be used to assess the significance, centrality, and similarity of different individuals and subgroups.

Social network analysis is most commonly studied in sociology departments and has been applied in many situations including primitive societies, disease networks, and corporate cultures. Recently there has been significant efforts to apply such techniques to terrorist networks [3]. Significant challenges arise both in determining relevant measures of significance, and in dealing with relatively large and dynamic networks, knowledge of which is very incomplete and uncertain.

6.5.2.6 Game theory

In dealing with terrorism, the outcome will depend not only the decisions we make, but also on the decisions our adversaries make. This is precisely the situation contemplated by game theory. The present of an intelligent adversary has implications for almost all the problems and methodologies discussed above. For example, some datamining algorithms may prove more robust to disinformation. While game theory has been long used in military planning, a new thrust, in which it is combined with some of the methodologies discussed above, could have a large payoff.

6.5.3 References

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7. Participants

7.1 Sensors and Detectors

- Prof. Thomas C. Baker
  Iowa State University
- Prof. Philip Bucksbaum
  University of Michigan
- Prof. Ananth Dodabalapur
  University of Texas at Austin
- Prof. Catherine Fenselau
  University of Maryland
- Prof. Jiri Janata
  Georgia Institute of Technology
- Dr. Sallie Keller-McNulty
  Los Alamos National Laboratory
- Prof. Chad Mirkin
  Northwestern University
- Prof. Dan Prober
  Yale University
- Dr. Alan Rogers
  Haystack Observatory
- Prof. Michael J. Sailor
  University of California, San Diego
- Prof. Richard Smalley, *Group Leader*
  William Marsh Rice University
- Dr. Anthony Tyson
  Bell Labs, Lucent Technologies
- Prof. David R. Walt, *Speaker*
  Tufts University

7.2 Optical Spectroscopies

- Prof. John Baldeschwieler, *Workshop Co-Chair*
  California Institute of Technology
- Dr. Bruce D. Chase
  E.I. Du Pont Nemours & Company
- Prof. Ronald Coifman
  Yale University
- Dr. Brian Curtiss, *Group Leader*
  Analytical Spectral Devices, Inc.
- Prof. William Fateley
  Kansas State University
- Prof. Theodore Goodson
  Wayne State University
- Prof. Chris Lawson
  University of Alabama
- Prof. John Margrave
  William Marsh Rice University
- Prof. W.E. Moerner
  Stanford University
- Prof. Margaret Murnane
  University of Colorado
- Prof. Jeanne Pemberton
  University of Arizona
- Prof. John Rabolt
  University of Delaware
- Dr. Philip Schwartz,
  Naval Research Laboratory
- Prof. Jeffrey Steinfeld
  Massachusetts Institute of Technology

7.3 Energy Sources

- Prof. Hector Abruna
  Cornell University
- Dr. Terrence L. Aselage
  Sandia National Laboratories
- Prof. Gerbrand Ceder
  Massachusetts Institute of Technology
- Dr. Kenneth Davis
  Motorola Labs
- Prof. Mildred Dresselhaus
  Massachusetts Institute of Technology
- Prof. Adam Heller, *Speaker*
  University of Texas at Austin
- Prof. Ernie Moniz, *Workshop Co-Chair*
  Massachusetts Institute of Technology
- Prof. Robert Nemanich
  North Carolina State University
- Dr. Bryan S. Pivovar
  LANL
- Dr. Debra Rolison, *Group Leader*
  Naval Research Lab
- Prof. Leo Schowalter
  Rensselaer Polytechnic Institute
- Dr. Karen Swider Lyons
  Naval Research Laboratory
- Prof. Sarah Tolbert
  University of California, Los Angeles

7.4 Image Reconstruction and Analysis

- Prof. Wolfgang Bauer
  Michigan State University
- Dr. Timothy Cornwell, *Group Leader*
  NRAO
- Prof. Lee Sam Finn, *Speaker*
  Penn State University
- Prof. Ron Gronsky
  University of California
- Dr. Robert Hanisch
  Space Telescope Science Institute
- Prof. Barbara Jacak
  Stony Brook University
- Prof. Sharon Neal
  University of Delaware
- Prof. Naoki Saito
  University of California
- Prof. Guillermo Sapiro
  University of Minnesota
- Prof. John Silcox
  Cornell University

7.5 Mathematical Techniques

- Prof. Douglas Arnold
  University of Minnesota
- Dr. Clifford Behrens
  Telcordia Technologies
- Prof. Richard Ewing, *Group Leader*
  Texas A&M University
- Prof. Stuart Geman
  Brown University
- Prof. Christopher Jones
  North Carolina State University
- Dr. Jon Kettenring
  Telcordia Technologies
- Prof. Shrinivas Kulkami
  California Institute of Technology
- Joyce McLaughlin
  Rensselaer Polytechnic Institute
- Prof. Michael Neubert
  Woods Hole Oceanographic Institution
- Prof. Alex Szalay
  John Hopkins University

8. Workshop Agenda

Approaches to Combat Terrorism (ACT): Opportunities for Basic Research

A Joint Workshop by

The Directorate for Mathematical and Physical Sciences, NSF
and
The Intelligence Community

Monday, November 18, 2002:

Arrival; Participants Receive Workshop Materials at Check-in

Tuesday, November 19, 2002

Plenary Session, Grand Dominion IV

0800-0900 Registration

0900-0915 Welcome Remarks: Dr. John Hunt, Acting Assistant Director, Mathematical and Physical Sciences, NSF and Dr. John Phillips, Chief Technical Officer, Intelligence Community and Chief Scientist, Central Intelligence Agency

0915-0930 Charge to the Workshop: Dr. John Hunt and Dr. John Phillips

930-945 Opening Remarks by Workshop Co-Chairs: Dr. John Baldeschwieler and Dr. Ernie Moniz

945-1030 Keynote Address: United States Intelligence Community Response to Terrorist Threat: Background and Nature of the Threat: Dr. Donald M. Kerr, Deputy Director for Science and Technology, Central Intelligence Agency

1030-1045 Break

1045-1200 Participants receive orientation briefing on Intelligence Community (IC) agencies and areas of responsibility. Examples of two scenarios which illustrate IC problems and technology limitations: Tom Beahn, ITIC and representatives of member agencies

1200-1300 Working Lunch, Grand Dominion IV - Dr. Rita Colwell, Director NSF

1300-1630 Overview Presentations (30 min. each)

1. Energy Sources
   Adam Heller
2. Mathematical Techniques
   Douglas Arnold
3. Image Reconstruction and Analysis
   Sam Finn

Break

4. Sensors and Detectors
   David Walt
5. Optical Spectroscopies
   Phil Schwartz

1730-1900 Reception, Grand Dominion VI

Wednesday, November 20, 2002

08:30- Breakout groups meet as follows:

Sensors and Detectors, Adams
Richard Smalley, *Group Leader*
Fred Ambrose, ITIC Representative
Dave Nelson, NSF Representative

Optical Spectroscopies, Wellesley 40
Brian Curtiss, *Group Leader*
Bill Stein, NIMA Representative
Susan Durham, ITIC Representative
Jim Breckinridge, NSF Representative

Energy Sources, Cumberland 30
Debra Rolison, *Group Leader*
Jim Carrick, IC Representative
Art Ellis, NSF Representative

Image Reconstruction and Analysis,
Cambridge 50
Tim Cornwell, *Group Leader*
Paul Salamonowicz, IC Representative
Brad Keister, NSF Representative

Mathematical Techniques, Marlborough 20
Richard Ewing, *Group Leader*
Mel Currie, IC Representative
Ron Walters, ITIC Representative
Bernie McDonald, NSF Representative

Thursday, November 21, 2002

Check-out

Plenary Session, Grand Dominion IV

0830-1030 Group Leaders Present Reports to Plenary Session: Identify Recommendations

1030-1045 Break

1045-1145 Summary of Workshop, Next Steps: Dr. John Baldeschwieler and Dr. Ernie Moniz

1145-1215 Remarks by Dr. Eric Haseltine, Associate Director for Research, National Security Agency

1215-1315 Working Lunch, Grand Dominion IV

1315 Workshop Closes