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A Perspective from the Los Alamos Fellows

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# Future Research Directions for Los Alamos: A Perspective from the Los Alamos Fellows

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## OVERVIEW AND RATIONALE

Dramatic changes in the global political and economic environment have occurred in the last decade that have impacted Los Alamos National Laboratory at every level from the way in which we do business to what business we do. The political and economic changes have impacted the societal view of the role for science and technology in general, and the role of the national weapons laboratories in particular. With the end of the cold war, the long term strategy for research in the national weapons laboratories is being reassessed in a climate of increasing concern about economic, environmental, and health security whereas previously the focus was on a dominant superpower opponent. Our nuclear mission now must support the nation's need for nuclear

deterrence without testing. As we look toward the future, the Fellows wish to begin a dialog with the Director and the new Deputy Director for Science, Technology, and Programs and with the entire Executive Team. We wish to contribute to ensuring the Laboratory's scientific and technological competitiveness in areas that will be essential for addressing future threats to our national security. Drawing upon our collective experience we can contribute ideas to the development of major new scientific themes for the Laboratory of the future.

In the Ehlers report to Congress by the House Committee on Science (September 24, 1998) four main themes are emphasized in looking toward a new national science policy. They are:

- \* Ensuring the flow of new ideas by the support of fundamental research, recognizing that important discoveries often come from unexpected avenues;
  - \* Transferring new discoveries and knowledge to applications;
  - \* Providing sound technical and scientific data for government decision making;
- and
- \* Fostering education and communication.

The long-term future of the national weapons laboratories will depend upon our success in each of these four areas. Importantly, these broad goals must be achieved in the context of sustaining critical ongoing programmatic roles that maintain our national security supremacy.

The United States of America has enjoyed great benefits from a forward looking science policy in which fundamental and applied research, encompassing programmatic and curiosity-driven research, have prospered. In the current climate of rapidly changing priorities, a forward looking and vital national defense research program is required to ensure we will be in a position to defend against increasingly diverse technological and natural threats. Key elements to our being able to develop technological solutions to threats to national security will include:

- \* The ability to redirect our efforts rapidly in response to new threats;
- \* Multidisciplinary approaches to understanding complexity and the development of solutions to complex problems;
- \* Developing and harnessing our computational power for predictive power, including prediction of errors and uncertainty;

Our increasingly sophisticated understanding of the physical universe has enabled scientists and engineers to tackle increasing complex problems. This increased complexity has required specialists to diversify and collaborate across disciplinary lines to find innovative solutions. The boundaries between physics, chemistry and biology have been blurred. Science and technology are beginning to tackle the once unimaginable challenge of having a complete molecular level understanding of the chemistry and physics of living systems and astounding progress has been made in theoretical modeling and prediction in biology. We are tackling mammoth computational tasks such as modeling the global climate in order to predict long term changes. Computational power has unleashed spectacular possibilities for modeling and simulation of complex phenomena that underpin the new world order in which nuclear weapons tests are banned. The importance of experimentally validated simulation of complex phenomena has become paramount in this era of test bans. True scientific and

technological superiority required for national security must also push on the frontiers of fundamental theoretical understanding of complex phenomena.

## **SPECIFIC TOPICS**

To initiate our dialog we have developed short white papers around six topic areas. The Fellows formed teams to work on each topic. Imprinted on the output of these teams is the diversity and individuality of the Fellows, with attention paid to issues spanning from what may seem mundane but of great importance to the almost fanciful but with great potential to unleash capabilities that could revolutionize our lives. The topic areas were chosen are those in which, at this point in time, we see major scientific opportunities or imperatives. We have endeavored to focus, although not exclusively, on the long-term future (~10 years out). In doing so our discussion by necessity builds upon the insights obtained within this current snap shot of time and is therefore expected to evolve.

The six topic areas we chose have overlapping elements and common themes. We have not attempted to compartmentalize the topics by eliminating overlap because the different teams each bring different perspectives within the context of their topic. The focus of the **Bioscience** topic is on the importance of having a molecular level understanding of biological processes and utilizing that understanding for biotechnology applications in the environment and in human health security. **Cybernetics** discusses the potential civilian and military applications of advances at the man machine interface, as well as in microrobotics, prosthesis, biocomputers, biosensors, self wiring computers, and robotic sensing. In the **Energy** topic nuclear approaches to energy sufficiency are considered along with the potential of biological systems for providing "clean" energy. The contributions of integrated computational and experimental approaches to energy and the environment are discussed in reference to climate modeling, combustion, as well as catalysis and separations. The **Materials** topic emphasizes the depth and breadth of materials research at Los Alamos. While materials are of central importance to the nuclear weapons program there are also opportunities for fundamental and applied research in materials for energy applications, bio-materials, electronic and optical materials. **National Security** deals with our central mission responsibilities regarding the stockpile, and expands into our roles in defense against weapons of mass destruction, tactical and theater missile defense, computational weapons, and protection of our infrastructure and environment. In the **Neutrons** topic the importance of our competency in accelerator technology and the science that it serves is emphasized from fundamental nuclear and materials science to accelerator transmutation of waste, production of tritium, and radiography applications.

With these collective thoughts we hope to begin a forward looking and productive dialog that will be of value to the Laboratory.

## **BIOSCIENCE**

The focus of modern biology is moving increasingly toward the goal of understanding complete molecular networks in living systems. Understanding the structure and dynamics of biomolecules and their molecular networks, how they operate, and how signals are communicated to obtain the desired response to a stimulus or to maintain involuntary functions is a challenge to which Los Alamos can make key contributions. Importantly, specific molecular networks can be chosen for study that will have broad

impact in a number of programmatic areas, as well as providing insights into underlying principals that drive forward basic science.

Biology has undergone a revolution this century due to our increasingly sophisticated ability to manipulate and probe biomolecular structures in more complex systems. During the first half of the 20th century, molecular biology was concerned primarily with discovering biological macromolecules and determining their make up. In the 1950's, Watson and Crick deduced the structure of the DNA double helix. This discovery led to the deciphering of the genetic code and to the fundamental dogma of modern molecular biology; that genetic information is stored as the sequence of nucleic acid subunits in our DNA, translated by messenger RNA, and ultimately expressed in the linear sequence of amino acids in each protein molecule needed by a cell to carry out its functions. In the latter half of the 20th century we developed the ability to express almost any protein in simple host systems and to manipulate its amino acid sequence to modulate its functions. We also developed the technologies to study the structures of individual proteins and their complexes. With these data we began to understand basic biochemical mechanisms. We also came to understand that the dynamic fluctuations and conformational transitions within biomolecules are also key to understanding biological function. There are of the order of 10<sup>5</sup> genes that code for specific proteins whose sequences are projected to be available from the Human Genome Project by the year 2005. As more genomes are sequenced we will acquire information about the gene functions. Gene expression and protein levels will be known in a variety of tissues, developmental, and disease states. Information on polymorphisms (different gene sequences that code for the same protein) will be available. We will gain new insights into disease and the new opportunities for biotechnology development will be profound. Continued advances, however, will depend upon an increasingly sophisticated understanding of how proteins, along with DNA and RNA, operate in complex molecular networks in a regulated manner to achieve coordinated function in response to a myriad of physiological stimuli.

#### *IDENTIFICATION OF KEY AREAS*

In the near term, completion of the genome sequencing projects will require innovative sequencing technology that Los Alamos could play a role in developing. In the longer term, Los Alamos needs to be expanding its activities focused on the study of biomolecular structure and dynamics, biomolecular networks, and the biotechnology applications derived from them. With this foundation, Los Alamos can make key contributions in:

#### **1) *Biotechnology applications in national security, the environment, and economic competitiveness.***

Our microbial and molecular bioscience capabilities combined with the gene sequence data from many microbial genomes and informatics capabilities are powerful tools for addressing a wide range of national priorities with biotechnology approaches. These approaches utilize the unique properties of biological molecules and/or organisms for technological applications. The study of microorganisms that survive in extreme environments holds great promise for further expanding the utility of biological systems in a wide variety of industrial and military situations. For example, understanding how thermophilic bacteria maintain functional proteins at high temperatures may reveal general rules that could be exploited in the design of more robust enzymes or receptor molecules. Areas in which biotechnology approaches are going to be important, and which are appropriate thrusts for Los Alamos include:

\* **Chemical and biological threat detection and intervention.** Los Alamos is in a unique position to integrate chemistry, physics, and biotechnology approaches for addressing this problem. The development of biomolecular based sensors for threat detection, characterization, and disabling is an obvious initial focus area.

\* **Bioremediation/global climate change.** The use of biological molecules or organisms to clean up soils contaminated by a variety of toxic agents, including those arising from activities within the DOE complex, is another obvious focus area. The microbial ecology of soils is extremely complex and poorly understood. It has been estimated that a typical gram of soil contains ten billion bacteria representing five thousand species of which less than 1% have ever been cultivated or characterized. Systematic study of the microbial ecology in soils will prove rewarding in establishing a scientific understanding of bioremediation. Biosystems are also efficient at converting CO<sub>2</sub> into biomass. The engineering of plants to do this with even greater efficiency has huge potential for impacting global climate change.

\* **Energy conversion, transport, and transduction.** Biological systems are remarkably efficient at capturing energy from the environment, then transporting and converting it to useful forms for cellular functions. Los Alamos has a strong fundamental program in this area which provides a foundation for biotechnology approaches to harvesting energy from the sun, or new ways of using renewable energy for processing of waste.

\* **The development of new complex materials with novel functionalities.** Biological systems are unique in that their molecular systems can replicate, mutate, and evolve against environmental pressures such that they come up with novel functionalities that optimize their survival. The development of new materials based on biomolecular structures or principles, or biomolecules that can perform novel functions in extreme environments, for example, are frontiers that remain largely unexplored and which are likely to hold remarkable new resources. The multidisciplinary environment at Los Alamos is optimal for bringing together theory, computation, materials design, bioscience, and complex experimentation to open these frontiers.

**2) Health effects research.** The human health effects associated with production of pollutants within the DOE complex and by industry leads naturally to the need to study molecular networks mediating the recognition and repair of damaged DNA and regulation of cellular activities. These areas are appropriate for Los Alamos given our current capabilities, the fundamental importance of these systems in biology, and their significance for the DOE mission.

**3) The origin of life.** With the deluge of sequence information coming available, a systematic comparison of the genomes of organisms nearest to the root of the phylogenetic tree of life may prove rewarding from the perspective of understanding the most fundamental question in biology: what is the origin of life? Thermophilic organisms are of interest in this regard as they originate from some of the deepest evolutionary branches of heterotrophic archaea and bacteria. It is possible that some non-culturable soil bacteria may be extremely primitive and knowledge of their genomes would provide information on the fundamental root of the origin of life.

#### **IMPLEMENTATION**

Success in the key areas identified above requires integrated experimental and computational capabilities with diverse scientific approaches. The integration of cell and molecular biology with chemistry, physics, engineering, theory and computation will be essential to develop solutions to the very complex problems being addressed. In order to

be a major player in this field, Los Alamos also will need to strengthen its technological base in:

- \* Biological technologies for generating sequence or expression level mutants and assaying biological functions, and for providing the materials needed for structure and dynamics studies, with isotopic labeling where needed.
- \* X-ray and neutron techniques, NMR, as well as optical and laser spectroscopies to probe molecular structure - with the theoretical codes for interpreting and refining results.
- \* Kinetic and dynamical analyses using flow cytometry, spectroscopies, and time-resolved techniques.
- \* Cellular level analyses to identify and characterize molecular networks, and to determine sites of molecular interactions using NMR, spectroscopies, and image/flow cytometry.
- \* Theoretical calculations of the free energy of interaction of the molecules in their environment.

Bioscience is a rapidly advancing and highly competitive area. In order to solve the complex problems we are challenged with in national security and the environment, Los Alamos must maintain a competitive basic bioscience program that can feed our applied research efforts as well as attract leaders in the field. We must cultivate, integrate, and add to our expertise and resources. A coordinated multiagency program is needed to realize the potential of Los Alamos' impact in bioscience. We must aggressively explore where DOE and other agencies' interests lie in a strong bioscience capability in the national defense laboratories. It is also critical that we encourage our scientists to compete vigorously for NIH funding, and we must evaluate the impact of our program using measures that include peer-reviewed publications and citations. The rigorous peer review proposal system of NIH is a critical quality control check for our bioscience activities, and the rapid expansion the field is undergoing means we must calibrate our accomplishments continuously against the wider national and international community.

#### *THE LOS ALAMOS ADVANTAGE/MISSION RELATEDNESS*

Los Alamos strengths in interdisciplinary research will be central to our competitiveness in the future of fundamental research on biological systems, biotechnology development and application, as well as health effects research. Our breadth of capabilities in molecular biology, cell biology, microbial biology, biochemistry, biophysics, theoretical, and computational biology provide us with the resources to address what will be some of the most challenging problems of the next century when national security will be focused more on health and environment issues. Los Alamos must foster the personnel and facilities to be a major player in this crucial area.

### **CYBERNETICS**

#### **Man-Machine Interface**

A computer does many things better than a human. Even the most gifted idiot savant cannot approach the machine's arithmetic speed, memory, or search abilities. Some things are done better by humans: the simple, nearly unconscious, tasks of visual awareness remain well out of the sphere of current computational engines. In some tasks, computers and humans are about equal. Deep Blue's defeat of Garry Kasparov was hardly a glorious victory for the machine --- the decision was 3 1/2 to 2 1/2.

It is clear, however, that a great advantage will accrue as the human mind becomes more intimately connected to the machine. In the early days, humans had to pour over endless listings of "zeros" and "ones" to glean what the machine was telling them. Similarly, instructions to the machine could be accomplished only by the tedious wiring of panels. Soon after, computer memories grew large enough to store programs side-by-side with data, the process of loading the program was as easy as loading data. Similarly, output could be cast in easily intelligible units and symbols. Graphics revolutionized the interface for both input and output. Results of a calculation presented in graphical form rather than a list of numbers allowed humans to use their formidable powers of visualization to glean abstraction of magnitude, trend, slope, shape, and even certain kinds of homomorphism from the primitive string of bits. Similarly, with the advent of Visual Basic and other *gooeys* (Graphical User Interfaces), much of the input process has moved from the keyboard to the mouse.

The other senses may be used as well to augment the man-machine interaction. Microcomputers already have audio output to supplement visual output. Three-dimensional displays and audio input are gaining in popularity. Virtual Reality, although still primitive and somewhat over-touted, is a technological imperative and will mature in the next decade. Although holographic displays with touch and kinesthetic-sense interaction will likely be first realized by the entertainment industry, they have enormous potential to facilitate rapid understanding of abstract scientific and mathematical results.

Finally, the greatest power of the human mind is to conceptualize. Conceptualization is intimately related to consciousness and a range tenuous existential substance that science can neither measure nor detect. The infrequent human experience of epiphany is well beyond scientific description: it is easy to know both a theorem and its proof for many years before the day you realize what it is all about. This is ultimate understanding.

Can we find ways for computers to relate concepts directly to humans without requiring laborious mentation or the agony of analysis? Similarly, can we find ways to relate concepts to computers without the tedium of explicit instruction?

Improvements in the techniques of input and output through the familiar sensors and actuators of the human body may have a long way to go. Undoubtedly there are many innovations to be realized for expediting the process of transferring a concept from man to machine and vice versa.

Perhaps we can develop algorithms to read 'body language,' likely in concert with the dilation and constriction of the pupils and the furrow of the brow, to recognize the degree to which the user is understanding, and throttle or reformulate the information-rate or format accordingly.

Ultimately we want to reach into the mind and extract or deposit concepts, bypassing the frailties and ambiguities of the sensory and muscular systems. Los Alamos already has a leg up on the problem, or at least a primal notion. The magnetoencephalography program, pioneered by Ed Flynn at Los Alamos, was in part motivated by the dream of controlling a machine directly with the mind. In a future era when physiology of the brain is so well understood as to make such control practical, perhaps we will find noninvasive ways of inputting the brain as well.

### *THE LOS ALAMOS ADVANTAGE*

Los Alamos has a singularly pronounced profile in the history of computing as the science of computing grew-up with the hydrogen bomb. ASCI and the Delphi Program ensure that we will be at the forefront of supercomputing for the foreseeable future. Many of the machine-man interfaces were either invented at Los Alamos or used at Los Alamos early in their development, e.g. color graphics ~1965, holograms ~1973, multivoice audio ~1985. Los Alamos is a leader in magnetoencephalography, which may shape the far future of computer interfacing.

### **Microrobotics**

Micron-scale sensors and actuators are already under active development, and that nano-scale devices will follow is an article of faith. The impact of such devices will be felt in the national security and intelligence arena as well as in the commercial sector.

Perhaps the most compelling need in the "new world order" is for an effective theater missile defense. A small but wealthy and fanatically ruled nation can acquire missiles with substantial range. Because chemical and biological agents can be dispensed in submunitions shortly after burnout, the offensive missile must be intercepted in boost phase. Thus only 30-90 seconds are available from launch-flash to intercept. Theater tactics at realistic ranges (200-500 km) mandate intercept velocities of about 10 km/sec. This high speed strongly suggests a large rocket in the role of interceptor. But the energy required to disrupt the offensive missile in boost phase is only about a megajoule, so the mass of the kill vehicle need be no more than 20 gm.

If such a tiny vehicle could contain all the sensors, actuators, and data processing apparatus necessary for homing, the total mass of the interceptor could be fantastically small. With specific impulse of 300 sec, the idealized single-stage rocket equation would give a total mass of 8 kg. Realistic structure factors and multiple staging would still allow a mass under 50 kg. What a truly just nemesis for a 10-ton missile!

The development of such a "brilliant bullet" would have far broader implications than theater missile defense. True surgical strikes may become possible, ending the ideal war with one shot. The technology may allow a broad range of military nanorobots, whose motility includes atmospheric hovering, jumping, and swimming. The opportunities for surveillance and intelligence gathering are manifest. The deterrence and concomitant opportunities for peaceful settlement of disputes are clear.

DARPA has recently coined the term "micrite" for a microrobot with some self-organizing abilities strangely akin to the self-organizing abilities of certain subspecies of slime mold. Here are some words from an advertisement for a workshop at the end of April 1998.

*The workshop is to exchange information and opinions on the potential for developing sub- millimeter to sized micro-robots ("Micrites") for use in penetrating and surveying hard targets.*

*Hard targets are those entities and facilities that pose a threat to US National interest, but that with existing technology are extremely difficult or impossible to detect, localize and target. Hard targets include clandestine drug manufacturing facilities, terrorist*

*strongholds and facilities employed in the creation of chemical, biological, or nuclear weapons of mass destruction.*

*The micrites we envision are of the order of one cubic millimeter in total volume, self propelled, and are capable of carrying a sensor payload equal to approximately 10% of its total weight. Micrites will be capable of simple social behavior when activated: recognize activation, then propel to form an observable group. Large populations of micrites could be introduced into hard targets, carrying in exotic taggant materials that would allow the US to remotely identify the facilities, to differentiate them from civilian facilities and to target them with precision.*

This description is closely related to the "floating fink:" a concept emerging from a *Delphi* study at RAND about four years ago.

Perhaps the area of greatest near-term benefit from these technological developments will be medicine. Microfabricated sensors for analysis of blood samples are nearing commercial application. Sensors that can continuously monitor various biochemical agents and can be fitted to the point of a hypodermic needle are presently under development. Sensors that can be swallowed to monitor and telemeter information about chemical balance in the gastrointestinal tract are already being used. No stretch of the imagination is required to believe that sensors could be developed to travel in the circulatory system, perhaps to lodge at specified locations and provide biochemical monitoring, perhaps to locate trouble spots, aneurisms in the brain, constricted blood vessels in the heart, cancer foci throughout the body.

Once accepting these possibilities, it is not a much greater leap of the imagination to envision fitting these medical robots with actuators and tools so they could repair the aneurysm, chisel out the plaque, isolate the cancerous regions. Perhaps they could even diligently close off the blood supply to inoperable tumors. Nanorobotic surgery seems fantasy, but is far from being limited by physical laws. It is a logical extension of technological trends.

#### *THE LOS ALAMOS ADVANTAGE*

We have a very small microrobotics program in P-Division, which is oriented toward robots of relatively small scale (<1 kg) with the intent that they will eventually be realized at the mm scale. We seem to have lost our edge in microlithography, a technology essential to construction of sensor, actuators, and logic for such critters. Perhaps our best bet is to form an alliance with Sandia for microfabrication.

#### **Prosthesis**

The development of prosthetic devices for the benefit of the sensory-impaired certainly a grand challenge for cybernetic technology. A serviceable substitute for a "seeing-eye dog" appears to be within the scope of near-future technology: requiring development of sensory-fusion algorithms to interpret signals from an array of range finders, audio and video inputs, and perhaps detectors for electric and magnetic field anomalies. Research is currently in progress on embedding conductor matrices within sensor nerve fiber bundles to investigate prosthetic simulation of sight and hearing.

Prosthesis is also province of nanofabrication technology. Researchers are already considering incorporating microsensors for glucose monitoring into an artificial pancreas.

Hearing aids with spectral correction fitted to the auditory response of their owners are already available. That they could also be enhanced to produce feedback signals to damp-out the oscillations of tinnitus seems a straightforward task of microprocessor programming. Eyeglasses that change their focal length (according to range sensed by sonar or infrared) by either mechanical or electrical adjustment of a fluidic lens seem a developmental possibility. Cataract surgery has become so routine that the possibility of implanting an automatic focusing lens only touches on science fiction. In this application, a gelatinous lens focused by piezoelectric polymers seems a reasonable approach.

#### *THE LOS ALAMOS ADVANTAGE*

Los Alamos has a no particular charter to investigate "cybernetic" prosthesis, but we have many of the component technologies. It could possibly fall out of an enhanced program in microrobotics.

### **Biocomputers, Biosensors, Self-Wiring Computers**

This is an agglomeration of potential thrusts sharing a bio-imitative motivation.

The brain is a very plastic and adaptive organ, and the nerve cells of which it is comprised are continually in the process of producing new connections through their axons and dendrites. This ability to self-organize and become greater than the sum of its parts shares a lot with the micrites discussed above, except this desired outcome would not be specified in advance. Rather some kind of reinforcement would be administered in the event of a favorable outcome. This notion shares many features of neural nets.

The mammalian eye preprocesses much information within the retinal nerve tissue itself before sending the signals on to the brain. Can this function be mimicked in silicon? Surveillance cameras already do data compression so signals can be transmitted through ordinary telephone lines, a primitive form of predigestion for a specific purpose. The retinal nervous system, however, can distinguish moving horizontal and vertical lines, a form of perception, and perhaps more complex forms of perception occur in that vicinity as well.

#### *THE LOS ALAMOS ADVANTAGE*

Los Alamos has a no particular charter to investigate "bio-imitative systems," but DARPA and other agencies are quickly discovering the importance of such research.

### **Robotic Sensing**

Mammals have a number of senses that serve them in a very useful manner. The construction of devices that include sophisticated interpretation of the input of the camera, the microphone etc has in fact been vital to mammals. Without them the value of their senses is very considerably reduced.

Among the senses, first let us mention hearing. There is now commercially available speech recognition software, as in the "you-talk, it-types" category of programs. (These programs of course have no notion of meaning.) The ears however go beyond this very important ability. They can also perceive the direction of the sound, recognize non-verbal sounds, discern pitch, distinguish various multi-pitched sounds. The ear can easily distinguish a trumpet from a violin playing the same note, for example.

Another sense is smell. There is progress, (aimed at drug smuggling intervention) in creating a mechanical nose. Here there are various sensors aimed at different categories of molecules, which describe a smell as a point in, say, 15 dimensional space. So far, dogs are better, but as I understand it the experimental mechanical noses are not too bad at the tasks they have been designed for. Taste, is a combination of smell and detection by the tongue of sweet, sour, bitter and salt. That is, smell is enhanced by a further four dimensional descriptor. Texture may play a role as well.

The kinesthetic sense should be relatively simple to model (strain gauge). The sense of touch revealing hot and cold, pressure, injury, and texture, should be possible to model as well, however duplicating the density of these sensors might provide some problems. There are low technology means to implement the sense of up and down (plumb bob).

Finally a most important sense is vision. It may well be that it is vision that is decisive in our conceptual organization of the world around us. Current simulations of vision are like the model where a little man inside the head looks at a TV screen that shows the input from the eye. The eye has (at least) four types of receptors (3 different types of cones corresponding to different colors of light, and also rods for seeing in dark places). There seem to be receptors that are directly sensitive to motion, and to edges oriented in different directions. Behind the retina are, we have been told, three layers of processing neurons which preprocess the incoming visual signal. The result of this preprocessing is sent to the brain via the optic nerve, where further interpretation is done. In addition, vision allows depth perception and automatic focusing by the lens on the retina. The construction of an artificial eye may be the most challenging. Input from a TV type camera or charge-coupled devices could be fed into a two dimensional array of microprocessors which would be cross connected to two more layers in to form of a neural network. From there a high capacity channel would transmit the information to an additional neural network for further processing, recognition and action decisions. Note that orientation and size do not impede the mammalian eye-brain system in recognition. Since many things in our environment are flexible, these distortions of the image are normally handled as well. Also there has to be feedback to focus the lens and there is additional information on the position of the two eyes to give depth perception.

#### *LOS ALAMOS ADVANTAGE/MISSION RELATEDNESS*

Besides the aforementioned prosthetic work, the construction a mechanical eye, which has the ability to recognize various things, could be very helpful. For example, watching our Plutonium storage area is tedious and boring for people, but a suitable mechanical eye, which could tell the difference, say, between an intruder and errant tumbleweed, could be very helpful. Checking the printing of money at the bureau of printing and engraving for flaws is now done by people, but could be done by a mechanical eye. Proof reading type set material is another application. Watching a battlefield from a point too dangerous for soldiers, and sounding an alert when called for is another of numerous possibilities.

#### **ENERGY**

Energy sources that are readily obtained, inexpensive and environmentally acceptable are key ingredients that affect the quality of life for all societies. As a leading technical resource for the country Los Alamos must make substantive contributions to ensure acceptable energy supplies. Our forte is certainly in the research and advanced concept

arenas. We have been active in many aspects of the energy question. These have ranged from fission and fusion nuclear reactor designs through solar and fossil fuel programs. We have also been very active in environmental issues associated with energy running the gambit from site remediation through waste storage and transmutation. Through all of this the strength of Los Alamos has been the great technological diversity we bring to the problem. We have the expertise in all of the fundamental scientific disciplines and the multidisciplinary infrastructure that will be required to attack the wide range of energy related issues. Our emerging emphasis on advanced computing technology will give us a method to pull these fundamental studies into real world applications.

Specific areas that are worthy of consideration for strategic investment include: nuclear approaches to energy self sufficiency, bioenergetics, and computation and modeling for energy and the environment.

### **Nuclear Approaches to Energy Self Sufficiency**

Increasing world energy demands will necessitate revitalization of the nuclear option. Los Alamos should position itself to assume a leadership role to increase public confidence in nuclear power. We should focus on achieving transparent nuclear reactor safety and waste management protocols that reduce waste volume and activity, and minimize the accumulation of fissionable materials of purity appropriate to clandestine use. Accelerator Transmutation of Waste and Accelerator-Based Fission Reactors are two approaches. Los Alamos can further underwrite its leadership position in nuclear power by sponsoring international conferences that chronicle progress and change in nuclear safety, environmental issues, and economics.

***Accelerator Transmutation of Waste (ATW).*** Studies at Los Alamos, and elsewhere, suggest that Accelerator-Driven Transmutation of Waste prior to repository storage is a promising approach that may lead to substantial economic and environmental benefits. Analysis suggests that a commercial nuclear economy that includes ATW treatment of spent fuel will release waste to repositories that decays in 300 years to a level of radioactivity and radiotoxicity that requires 100,000 years without ATW.

### ***IMPLEMENTATION***

Los Alamos, and other research institutions, have made substantial progress in answering criticisms of ATW and now promote the technical superiority of pre-repository processing from a strong analytical base. The Laboratory is fortunate to have many of the necessary components for broadly based research programs to demonstrate ATW technologies. Among them are unrivaled resources in spent fuel treatment, materials science, computer modeling of nuclear systems, and an operating high-power linear accelerator. At a beam power of nearly 1 MW, LANSCE can be commissioned as a 1/20 to 1/40 scale prototype of the first ATW processing plant.

***Accelerator-Based Fission Reactors.*** Conventional nuclear reactor technology, which has many advantages for environmentally clean electrical energy production, is based on the use of  $^{235}\text{U}$  as fuel. Alternative fuels which have potential include  $^{232}\text{Th}$ , natural uranium, spent fuel uranium and even depleted uranium. In particular, most heavy element reaction products from the thorium fuel cycle decay in a few hundred years to levels that are below the levels of natural uranium ores, and plutonium is produced in smaller quantities, reducing the risks of nuclear proliferation.

## *IMPLEMENTATION*

Conventional thermal-neutron reactors using non-highly fissile fuel will not operate in a satisfactory way because of insufficient neutrons. An external supply of neutrons would remove this problem and enable the efficient use of  $^{232}\text{Th}$  or non-enriched U as a nuclear fuel. Neutrons could be produced by a proton linear accelerator of similar design to that required for accelerator tritium production or accelerator transmutation of waste. Further work can be done to evaluate this concept with an initial goal to produce a conceptual design that allows a cost comparison of an accelerator-driven non highly fissile reactor fueled system with conventional and breeder reactors, including cost savings for fuel enrichment and nuclear waste management.

## **Bioenergetics**

Most human activity is powered by biological energy sources. These activities include the life processes themselves, which are driven entirely by bioenergetics, while many of our industrialized functions such as transportation, communications, and manufacturing rely primarily on fossil fuels as their energy source. The biological processes themselves are models of clean and efficient energy production and conversion. However, the use of biologically generated energy sources by humans (that is, primarily, the production and consumption of fossil fuels) is subject to many serious and well-documented problems including exhaustibility of resources, social and environmental acceptability of production, and pollution associated with consumption. A major challenge and opportunity is to use the lessons provided by bioenergetics (the production and conversion of energy in life processes) to conceptualize clean and efficient new energy sources to power the industrialized functions of human activity. The next challenge will be to design practical devices that are based on these concepts and capable of meeting large-scale energy demands.

Modern technology, well developed at Los Alamos, puts these goals within reach. This technology is of three types. First, the biological systems need to be characterized well enough so that the mechanisms of production and storage of energy are understood. This involves significant efforts in structural biology and in functional characterization by spectroscopic and computational approaches. Second, the biological system needs to be rationalized (or simplified) so that the essential features (in terms of practical devices) of the energy production and conversion processes are identified and the "parasitic" processes which are necessary for life functions but not for practical applications are discarded. This problem is seen primarily as a computer-modeling problem. Third, a practical energy conversion device must be produced. This accomplishment requires bringing together the techniques of molecular biology, genetic engineering, synthetic chemistry, and materials science to realize the concepts developed in the first two steps. The ability to focus very sophisticated and diverse modern technologies on a problem of this magnitude, with the objective of producing end products that meet national needs in national security through energy independence, is uniquely available at Los Alamos.

## **Computation and Experiment -- Energy and the Environment**

The Laboratory's capabilities in modeling and computation can help provide solutions for national problems involving energy and the environment in the next twenty years. As the worldwide demands for energy continue to grow pressures to reduce the amounts of pollutants and greenhouse gases from these technologies will intensify. Similarly

experimental capabilities can also make substantial contributions to these areas. Underscoring the difficulties the U.S. and the world will face in maintaining energy usage for a growing economy while reducing the adverse effects on the environment are the commitments of the industrialized countries made to the Kyoto Protocols to reduce emissions of gases contributing to global warming below projected levels. Several areas are outlined below in which the Laboratory could play an even stronger role in the coming years, and strategies in pursuing such a path are briefly discussed.

**1) *Climate modeling.*** Modeling of the earth's climate through atmospheric and ocean simulations represents the most prominent area at present where computational activities are playing an important role in the international debate on global warming. There remain, however, large uncertainties in the interpretation of the observational record as well as limitations in the current atmospheric and ocean models currently in use. These issues make a compelling case for increased computational efforts to achieve greater spatial resolution as well as more reliable predictions over longer time periods.

**2) *Combustion.*** Approximately 90 percent of the manmade CO<sub>2</sub> released into the environment each year comes from the burning of fossil fuels, hence accounting for the bulk of man-made contributions to global warming gases. The results of improved modeling of combustion processes could lead to greater efficiencies and reduced environmental impact from fossil energy usage. The Laboratory has an established track record in the development of computational techniques in hydrodynamics for combustion applications and in the dissemination of these codes to the automotive and other communities.

**3) *Catalysis and separations.*** The transformation of chemical feedstocks into commercially useful products such as polymers, the refining of petroleum feedstocks to fuels, and the treatment of automotive exhaust emissions all involve the use of catalysts, which carry out chemical transformations without being consumed in the process. These economically important processes have achieved increased emphasis in the chemical industry, where these processes are being carried out with less energy consumption and fewer environmentally undesirable byproducts such as greenhouse gases. Processes involving catalysts have typically been modeled at the bulk level by chemical engineering approaches. The development of improved catalysts will involve modeling efforts on a variety of levels as well as coupling with a strong experimental effort in characterization and screening of catalytic materials.

Gas and liquid phase separations constitutes another area of technological significance where large amounts of energy are currently required. These issues assume even larger importance in cases involving global warming gases, which one does not want to discharge into the environment. Modeling activities can address important problems such as the design of selective membranes, predictions of thermodynamic properties of multi-component systems, and unraveling the mechanisms of transport in liquid media and in membranes.

**4) *Hydrogen Economy.*** Using hydrogen as a fuel produces no CO<sub>2</sub> during combustion, however current methods of hydrogen production involve either the use of electricity (produced by a power plant) or the use of fossil fuels with the concomitant CO<sub>2</sub> release. It is thermodynamically more efficient to use the heat from the power plant directly to

produce hydrogen rather than converting the heat into electricity first. Hydrogen could be produced

by pyrochemical methods from the heat of an appropriately designed ultra-safe, accelerator-based fission reactor. The work to be done here involves the refinement of the chemistry cycles, and the design of an appropriate heat source (reactor, for example).

#### *IMPLEMENTATION*

The Laboratory already has significant activities in several of the areas identified above, often involving collaborations with other national laboratories and universities. The DOE Strategic Simulation Plan would build upon the current ASCI infrastructure with applications targeted towards non-defense problems in global warming, combustion, and other important technological areas such as materials. While the Laboratory has very credible competence in the energy and environmental sector, because it is outside our traditional defense mission we will face stiff competition from other national laboratories and universities for new programs and initiatives in these areas. It is therefore important to initiate partnerships with those laboratories whose expertise complements our own, and to define clearly a limited set out of the many potential targets of opportunity in which to invest Laboratory resources in the future.

#### **MATERIALS**

Materials research and technology has historically been a strong element of the Laboratory's technology base. The nuclear weapons program drove the need for expertise in metallurgy, low-temperature/condensed-matter physics, materials under extreme conditions, polymer composites, and high explosives. As our mission has broadened to include aspects of energy, non-nuclear defense, and industrial competitiveness, expertise has grown to include ceramics, highly-correlated electronic materials, materials for sensor applications, fiber composites, electronic and nonlinear optical materials, and, recently, biomimetic and biomolecular materials. The materials community at Los Alamos, in addition to providing an extremely broad and deep competency, is a fertile arena for multi-organizational research at the interface between traditional disciplines of ceramics, metallurgy, solid-state physics, materials chemistry, polymer science, and biology.

The early focus on weapons materials and classified research has evolved into a more open materials research effort, resulting in integration of the Laboratory's materials scientists with the broader national and international community. Today, our materials community has several world-class efforts and overall strong collaborations with researchers from industry, universities and other national laboratories. As the Laboratory's expertise and interests in materials research have grown, there has been a precipitous decline in the level of effort of large industrial materials research laboratories such as IBM, Bell Labs, Exxon, and US Steel. The broad materials research base and the culture of working on large complex problems utilizing a cross-disciplinary approach positions Los Alamos to assume a national leadership role in materials research. By the same token, advances in materials synthesis and characterization techniques provide great opportunity to address current Laboratory problems in weapons science, threat reduction, and energy. The scientific strengths in materials research are augmented by a number of important research facilities including large ones such as LANSCE and the

National High Magnetic Field Laboratory and smaller facilities such as the Ion Beam Materials Laboratory, the electron-beam microscopy facility, and the ultra-fast spectroscopy laboratory.

#### *IDENTIFICATION OF KEY AREAS*

Materials issues are ubiquitous in the Laboratory's missions from nuclear weapons and threat reduction to fundamental science. Nuclear-weapons programs provided a strong focus for materials research in areas such as plutonium structure, materials under extreme conditions, and high explosives. Nevertheless, our evolving mission and the emergence of new national security issues will drive the future evolution of materials research. We discuss the future of materials research from the combined perspectives of programmatic areas and traditional materials research disciplines.

**1) *Materials for Energy.*** The increasing demand for energy and the call for reductions in fossil-fuel emissions, stemming from concerns over global warming, offer a wide range of opportunity for materials development. High-temperature materials such as metal/ceramic composites and advanced intermetallics/ceramics are needed to increase the energy efficiency of engines and enable new high-temperature industrial processing. Energy conservation and space-based applications suggest the need for low-density structural materials such as alloys of magnesium, a very abundant lightweight metal. Energy efficiency will also drive development of longer-lasting materials that can be recycled.

In addition to using energy more efficiently, there are options for alternative sources of energy. A possibility to replace the carbon-cycle economy of fossil fuels is a hydrogen-based fuel system in which the safe and economic storage of hydrogen will be a major issue. Recent advances in non-silicon based materials have demonstrated high efficiency for electron-hole pair separation and subsequent energy conversion and storage through water dissociation. Fuel cells also play an important role in energy conversion, as do alternatives such as novel battery technology.

Although nuclear energy has been in a decline in the United States for decades, near-term conditions may signal a reversal of that trend. Accordingly, there is a need for a new generation of nuclear reactors that have been redesigned to optimize efficiency and safety while minimizing waste. Of more pressing concern is the ability to treat/store nuclear fuel waste. The ATW Program is one attempt to deal with these problems. Paramount in such programs is the development of new materials for radioactive and corrosive environments.

**2) *Electronic and Optical Materials.*** From flat panel displays and electronic processing devices to fiber-optic communication and optical data storage, electronic and optical materials have and will continue to fuel the technological innovations of our time. Further, these materials open up exciting new frontiers in fundamental understanding of the coupling of electronic and magnetic excitations with lattice and optical processes. Understanding and controlling competing interactions and cooperative phenomena on multiple length scales pose outstanding scientific challenges, crucial to producing novel materials properties with technological functionality. Recent examples include colossal magneto resistance materials with potential magnetic-recording application and coherent coupling of vortex excitations in high-temperature superconductors which limits the critical currents in practical superconductors.

Organic electronic and optical materials are a rapidly developing field where increased understanding can have important impact on key technological areas including information display and optical communications. Major advantages of organic materials are their ability to be processed economically in large area, the tunability of their electronic and optical properties, and their flexibility in materials and device design. As in other electronic materials, the theme of competing interactions provides a unity at the fundamental physics level among these classes of materials.

**3) Biomimetic and Biomolecular Materials.** An exciting area for future materials research is programmable and/or adaptive materials. It is likely that such novel materials will emerge at the interface between traditional disciplines of life and physical sciences. One area is biomolecular materials that build from and incorporate biological molecules. An example is biomineralization where systems develop intricate high-strength structures through the growth of metastable inorganic phases that are controlled by proteins. By isolating the genes that code for these proteins, scientists are beginning to use them to grow artificial organic-inorganic hybrid structures.

Biomimetic materials are materials that mimic biological function. For example, biological systems convert energy by coupling photochemical or redox processes to the creation of a proton gradient. If such coupling mechanisms can be determined and mimicked in synthetic materials, it may be possible to take energy from arbitrary sources and convert it to a standard form. Another example of biomimetic materials is artificial membranes that incorporate recognition molecules selected from biomolecular combinatorial libraries. These functional membranes can be made to mimic stages in olfaction to produce highly selective elements for chemical and biological sensors.

**4) Materials & Nuclear Weapons.** An important materials expertise essential for the nuclear weapons program is the study of materials under extreme conditions, e.g. shock compression, ultra-high temperatures and pressures, dynamic stress, and high magnetic fields. Such studies provide key feedback for a fundamental understanding of materials by probing interatomic potentials at ranges and energy levels far from normal conditions, thereby assisting in establishing accurate electronic and molecular-dynamic models. In addition, new materials-related problems have arisen in the context of SBSS, three of which we mention here: the evaluation of materials aging phenomena in stockpile weapons systems, the remanufacture of weapons materials and components, and the incorporation of materials-related properties (equation of state) and behavior into weapons computer codes. Examples include aging effects in high explosives, new processes for plutonium-pit remanufacturing, and modeling of the deformation behavior of materials under extreme conditions.

#### *IMPLEMENTATION*

To maintain existing areas of materials research while at the same time developing new promising directions will require coordination of diverse efforts, integration of materials synthesis and characterization with simulation, and theory, and some stability in core funding of outstanding materials programs as well as of important facilities. Specifically Los Alamos should:

\* Maintain excellence in selected materials research areas as close connections and interactions with outside communities are crucial to have access to state-of-art advances in rapidly moving materials areas and to attract the "best and brightest" to the Laboratory.

\* Support medium-scale facilities and capabilities that are essential for the continuing health of materials research and which are often overlooked in the overall funding picture. Examples include techniques in laser spectroscopy, surface modification and analysis, thermodynamic and electronic transport measurements, high static and dynamic pressure, and a wide variety of electron-beam and atomic microscopies.

\* Develop and maintain unique world class experimental facilities for materials research *and* also fund the science base necessary to utilize the facilities effectively. Examples include the LANSCE neutron scattering facility and the NHMFL magnetic facility. Without an active scientific program coupled to the capabilities, facilities can be more of a detriment than an asset because they demand high levels of resources.

\* Make use of evolving capabilities in large-scale computing to address important problems in materials behavior. Integration of modeling with experiment and theory and more access to computing resources is critical.

Materials research at Los Alamos is extremely diverse and we have not been able to address all the exciting science and technology represented. Many of the issues that are needed to ensure the continuing overall health of materials research and some of the opportunities for future growth have been presented.

#### *LOS ALAMOS ADVANTAGE/MISSION RELATEDNESS*

Los Alamos needs to capitalize on its unique combination of facilities and scientific researchers to develop and maintain a world class materials research effort in focused areas. We already have some large facilities that are central to materials research: neutron scattering at LANSCE, high field pulsed magnets at the NHMFL, and large-scale scientific computing. Neutron scattering and computing is also key facilities for nuclear weapons work. Materials research can benefit tremendously from a synergy of effort that cross cuts major facilities, interdisciplinary research, and complex problems. The role of materials across the Laboratory remains vital to nuclear weapon and threat reduction as well as furthering fundamental science and bringing the latest and best ideas, techniques, and people to the Lab to provide a firm foundation for programmatic efforts in national security.

#### **NATIONAL SECURITY**

Since the establishment of the Manhattan Project in 1943 to address the urgent World War II national defense requirement, Los Alamos has continued its preeminent role and responsibility in the U.S. nuclear weapon program. In addition, we have engaged in a broad spectrum of activities supporting the U.S. defense establishment in other, non-nuclear areas. Approximately three-fourths of the Laboratory's \$1.2 billion annual budget is devoted to these activities, in the Nuclear Weapons and the Nonproliferation and International Security Programs, under the responsibility of the Associate Laboratory Directors for Nuclear Weapons and for Threat Reduction, respectively.

A principal activity of the Laboratory is to maintain the enduring nuclear weapons stockpile, those strategic nuclear weapons for which Los Alamos has development, surveillance, and maintenance responsibility. This task is accomplished using a broad-based, science-based, stockpile stewardship program comprised of physics, computational modeling, engineering, and materials science. An associated program supports national objectives in arms control, treaty verification, nonproliferation, intelligence assessment, emergency response to nuclear incidents, production, control,

and disposition of nuclear materials, manufacture and dismantlement of nuclear weapons, and nuclear waste management.

In the post-Cold War environment many of the DoD analysis centers and "Beltway" think-tanks have either gone out of business or greatly reduced their work on nuclear weapons systems and applications. As a consequence Los Alamos needs to return to a more visible leadership role.

An over-riding concept is reducing the global nuclear danger. The Laboratory must continually demonstrate credibility and leadership in these areas. Minimizing technological surprises is an important aspect. The shift from proof testing with nuclear experiments at the Nevada Test Site, to the current state of reliance on archival data, numerical computations, non-nuclear experiments and analyses, and professional expertise, is providing both challenges and opportunities. This is the cornerstone, and should be handled as such.

#### *IDENTIFICATION OF KEY AREAS*

We now list and briefly describe some of the over-riding national defense programs, requirements, and opportunities. We attempt to describe problem or opportunity areas, and suggest possible courses of action or laboratory capabilities that can be brought to bear in those areas. However, because of the limited resources, and space, available to this report, a more detailed "matrix" of capabilities to apply against particular tasks was not attempted. National Security is such a pervasive effort at LANL that the Fellows are currently undertaking more detailed studies on two aspects: the "Science Based Stockpile Stewardship" program and on the "Impact of Technology Developments on the Next Generation of Strategic Forces – 2010-2025 Time Frame".

**1) Nuclear weapons program and the enduring stockpile.** The Laboratory's stockpile management program is well founded and broadly based. It covers areas of physics design, large-scale calculations, engineering design, testing, and manufacturing, materials studies, component aging, and experiment execution and diagnostics. For some areas of supporting activities that need attention, LDRD has taken up some of the slack. Overall difficulties are the general lack of depth in professional staff and funding constraints that limit studies on new works, processes, etc.

The over-riding problem for our nuclear weapons program, in a nutshell, is this: For years Los Alamos and Livermore adopted basically an engineering approach (in the best sense of the word) to developing nuclear weapons. Starting with previous test results modest changes were made and the resultant new design tested. In some fashion or another calculations were made to fit the new results (if they did not naturally do so) and another step was taken. The result is that predictive capability (i.e. physics, chemistry, etc models) developed only within this restricted scenario and reached its own equilibrium with respect to other activities. Without testing this equilibrium is inadequate to fill the void. So what is the problem?

The problem is that things that never entered into the historical design process begin to emerge as potential problems to worry about. The theorist can rather quickly come up with a list of 100 things that may go wrong, never mind that 90 of them are likely red herrings. Different people then seize on their favorite topic(s) to determine what is important to do.

Our stockpile will have to be rebuilt after some period of time. The two outstanding problems, most broadly speaking, are 1) what are the effects of aging on performance (i.e. when do we have to rebuild) and 2) what are the effects of rebuild on performance. As long as our stockpile is "comfortably tolerant" of "small" variations there may be no problems at all. However, remanufactured pits will be made by different processes. The grain size will be somewhat different, changing material strength. The impurities will be somewhat different, changing high-strain-rate flow properties. To deal with such issues we need physical models that describe accurately what we have now (better than currently exist) so that variations can be evaluated. This model development/improvement will have to be accompanied with an appropriate experimental program to keep the theory honest. This partnership will be especially important for plutonium work. We need a vigorous program to learn as much as possible about the properties of Pu alloys, for example

Numerical hydrodynamics is the platform that all our other physics packages operate from. To the extent it is in error, this error is propagated to the other disciplines. The best approach to this problem is a contentious subject, but the need find the best is critical. We believe data base activities such as Equation of State, Opacities, and Nuclear cross-section work will be even more critical in the future than they are today but they face a budgetary fight for survival. Managers cannot believe that we have not already measured and evaluated all the nuclear cross-sections we will ever need.

ASCI is great. But we need to accompany the increase in computing power with a commensurate improvement in physical models (of the type described above for material behavior for instance). There is some movement in this direction but it is a struggle. Validation of ASCI codes is sorely lacking.

Maintenance and enhancement of the Laboratory's capabilities requires attention to such areas as material properties, including aging effects; new, safer, more energetic explosives; operation of weapons on-the-margin; development of robust, non-sensitive components or designs; etc.

Techniques are being developed, such as proton radiography, that have the potential to measure the effects of aging on weapons with enough precision to predict performance using hydrodynamic tests. If successful, these techniques will enhance the ability to respond to questions of stockpile assurance in the absence of nuclear testing. As new diagnostic techniques are developed, there are potential proliferation implications, although the absence of benchmarked nuclear test data may limit the value to proliferants.

The extension of nuclear weapon technologies to weapon effects phenomena and applications is weak and could be strengthened to provide a more forward looking approach, especially for the next generation of nuclear warheads and delivery systems.

**2) WMD (Weapons of Mass Destruction) Proliferation.** It has been an overarching priority of national policy since 1945 to prevent nuclear attack against U.S. soil. To the nuclear threat we must now add biological and chemical weapons of mass destruction. These weapons could kill thousands to millions of Americans at a single blow, while changing for all time our democratic society. In fact, our overwhelming military superiority invites covert attack, because covert attack is one of the few options remaining to a determined adversary.

Deterrence of threats and mitigation of consequences to domestic and international security are addressed in the three principal focus areas of nonproliferation and arms control, technology development, and international technology monitoring and assessment. Important capabilities to support this area are developed via NASA (National Aeronautics and Space Agency) space research.

Monitoring and assisting in control of large inventories of plutonium, enriched uranium, and alternate nuclear materials, remains a major commitment, as does support of monitoring and assessments of actual or possible foreign nuclear weapon-related activities. Response capabilities related to nuclear incidents and accidents fill a national need.

Chemical and biological weapons, both in a battlefield venue and in the hands of terrorist or other directed attacks on the U.S., require continued development of detection sensors, of fast-response assessments, and of efficient and economical means of mitigation. Particularly important are covert and standoff techniques that allow early warning of proliferant activities in denied areas.

If proliferants acquire WMD, we must minimize the chance of their use, and mitigate the consequences if indeed used. Improving our defense at the country's borders, by advanced sensors and processing to detect smuggling, is part of the response to proliferation. So is containment of an attack by civil defense, which includes threat prediction and mitigation. Attribution of the source is essential to any follow-up, whether military or prosecutorial. Laboratory capabilities that bear on these problems include space sciences, mass spectrometry and other laboratory forensics, information science, remote sensing, nuclear and other sensors, modeling and simulation, especially the prediction of threat vectors, and systems analysis. Robotic and biological science will make an increasing contribution to this mission. Intelligence analysis, as always, remains critical to the prediction and attribution of threats.

**3) *Missile Defense.*** Tactical or theater missile defense (TMD) has been long recognized as a defense requirement. Since the end of the Cold War, defense of the continental U.S. has been dismissed as non-time urgent, until the recent Rumsfeld committee's assessment that non-superpower ballistic missiles may be developed or acquired sooner than otherwise anticipated. The laboratory should continue to support missile defense in threat analysis, launch detection, and determining lethality requirements and developing specialized warheads. Critical to this effort will be our capabilities in nuclear weapons, modeling and simulation, sensors, and space engineering.

**4) *Advanced Conventional Weapons (ACWs).*** ACWs are potentially available to industrial powers, where they may already be under development and also to developing or third world states, by means of indigenous development, technology transfer, or outright sales. In order for U.S. and Allied Forces to be prepared for such encounters, the Laboratory should increase its monitoring, evaluation, and technical assessment of such capabilities. The potential application of such technologies in attacks against the U.S. domestic infrastructure should be evaluated and responses addressed. Of particular but non-exclusive concern are HPM (high power microwave) and RF (radiofrequency) sources. Advanced capabilities such as unmanned aerial vehicles could also be configured to carry nuclear warheads or WMDs.

**5) Conventional war fighting.** Laboratory technologies have the potential of increasing weapon effectiveness, in developing precision munitions and precision delivery systems, in target identification, in battlefield management and assessments, in high speed data processing, in developing interdiction methods to preempt adversary actions, etc. These capabilities will be critical in the asymmetric conflicts that the U.S. will face. We have overwhelming technological superiority, but are seldom as motivated as our adversaries, so we need to apply force precisely and remotely with minimal or no risk of casualties to U.S., Allied, or civilian forces.

**6) Infrastructure protection.** The U.S. infrastructure, including utilities, transportation networks, and information nodes and connections, is disturbingly vulnerable to attack. This is true of both DOE facilities and the nation in general. What can go wrong was illustrated in the Southern Hemisphere last year, during which the main electrical power supply was lost for Auckland, New Zealand's commercial center; the domestic water supply to Sydney, Australia was contaminated by giardia; and the natural gas supply to Melbourne failed for several weeks.

Such events have large economic and security impacts. The best tool against such events is prevention, guided by detailed systems studies made possible by large-scale simulations. The computer side of the threat is particularly compelling, and lends itself to offensive and defensive actions derived from Laboratory computer capabilities.

The focus of ASCI thus far has been dominated by the nuclear weapons program. The goals of the projected enhanced performance and the related complexities of operation have applications to missions of NSA. The Laboratory's ASCI experience could be integrated and utilized to enhance the future posture of NSA in their programs.

**7) Environmental security.** Resource limits, especially food supplies, energy and water availability, have the potential of leading to international instability and conflict. Alleviation of these problems can assist in preserving U.S. national security. Capabilities that are critical to these problems include large-scale environmental modeling and remote sensing.

**8) Underground facilities.** During the Gulf War, and again in Afghanistan and Sudan, the U.S. demonstrated an overwhelming capability to locate and destroy surface targets. Adversaries are responding by going underground, especially as regards their most critical and dangerous facilities: command and control, ballistic missiles, and all aspects of WMD. To a large extent, we neither can find, characterize, nor neutralize these facilities. Improved tools are needed, and the Laboratory can make a significant contribution. Capabilities important to this mission include remote sensing, earth science (especially seismic sensing), information science, advanced sensors, and detailed computational simulations.

#### *IMPLEMENTATION*

**Customers.** Our customer base is limited to the defense establishment, supporting agencies, and national policy makers. Among these are DoD and OSD, e.g., STRATCOM, USASMD, Joint Chiefs, Navy, Army, Air Force, DTRA, DIA; CIA, e.g., OTI, NPC; DOE, DP, IN, and NN; DOS; NSA; FBI; NRO. Collaboration as opposed to competition is a recurrent issue, particularly in times of diminishing resources.

**Infrastructure needs.** Maintaining competencies and capabilities has been recognized as critical. Mentoring and training of personnel, and establishment of new experimental facilities, is being addressed as part of the core weapons program; however, small-scale experiments are suffering. LDRD projects make limited but important contributions.

### **A. Personnel**

Key to long-term success is developing trained, competent personnel. This requires continual effort, in recruiting new degreed scientific and technical personnel, and technical support staff, and in upgrading the competency of the staff. The X-Division TITANS course, to develop qualified, "certified," designers, is an excellent example of such an approach. Comparable professional development in other defense-associated areas should be developed. The nominal 20% time available for self-directed, but relevant, work and studies attempted in X-Division is a good principle, potentially providing an incentive to broaden experience and also providing an opportunity to do interesting and challenging non-directed work.

Professional development must be encouraged. Although the new Performance Appraisal (PA) process specifically addresses this area, results in the past have been decidedly mixed. An overall, Laboratory-wide, viewpoint must be established, in developing and employing standards. The conflict between highly individualized performance evaluations vs. the necessity for collaboration and teamwork, with perhaps "lower importance" work assignments, is an issue.

More advantage in national defense programs should be taken of Laboratory retirees. The "Associate," "Affiliate," or "Guest Scientist" status is being applied inconsistently. We should assume that Group and Division line management recognize the desirability of bringing on staff new personnel – Nuclear Weapon Programs annual sponsorship of four post-doc fellowships is a promising means of recruiting, and that retirees are only a short-term solution to staffing needs. However, a more accepting attitude on the part of Division and Program Office Management would allow a better response (more timely and more accurate work) to Laboratory programmatic requirements, by using retirees. The position of Laboratory HR (Human Resources) requiring that retirees, who have been retired for more than one year, be accepted only as "contractor" personnel shows no understanding of working-level operations and should be rescinded. Would an "emeritus" category finesse this problem?

### **B. Facilities**

Weapon-associated facilities and operations, such as ASCI (Accelerated Strategic Computing Initiative), DARHT (Dual-Axis Radiographic Hydrodynamic Test) facility, the Atlas high-energy pulsed power source, LANSCE (Los Alamos Neutron Science Center), the ARIES (Advanced Recovery and Integrated [plutonium] Extraction System) process, the expansion of TA-55 for plutonium processing, and APT (Accelerator Production of Tritium) and ATW (Accelerator Transmutation of Waste) studies, are the most obvious examples of the Laboratory's commitment to develop and implement new technologies in support of defense needs, and are to be commended.

However, general laboratory facilities and infrastructure are aging and not being replaced. Others are being decommissioned, in part because of "space taxes" that are perceived to be excessive and which cannot be supported by programmatic cost codes.

These issues must be addressed; they exacerbate the problem of promoting computation over experimentation, at the expense of validation of calculations.

### *LOS ALAMOS ADVANTAGE/MISSION RELATEDNESS*

Since its inception, the *raison d'être* for Los Alamos has been nuclear weapons, from invention, to engineering for deployment, to maintenance of the stockpile in the absence of full testing. In the coming years, new threats to security will require responses based upon a variety of scientific capabilities. To fulfil our national mission we must have the capabilities needed to defend against biological and chemical agents, conventional weapons and missiles, attacks against our environment and infrastructure, including computer networks. Our computational capabilities and diversity of scientific disciplines provide us with significant advantages to take on these challenges, although there are areas we will need to strengthen.

### **NEUTRONS**

An important component of the research program at Los Alamos has been centered on the use of high-intensity linear accelerators and the science they support. A major component of the national nuclear physics research program was centered at LAMPF, using the 800 MeV, 1 mA proton linac to produce pions, muons, and neutrinos. This accelerator now is used in conjunction with the Proton Storage Ring (PSR) to produce spallation neutrons for condensed matter science and defense programs applications at the Los Alamos Neutron Science Center (LANSCE). The Accelerator Production of Tritium (APT) project is currently using the linac as a test bed to demonstrate technical feasibility of this approach in support of the nuclear stockpile needs of the country. The linac is also being used to develop proton radiography for stockpile stewardship. In addition, the linac provides the basis for a first-class research program in fundamental neutron and neutrino nuclear physics. A number of other high-intensity accelerator designs have been developed in support of the national fusion program, neutral particle beams for national defense, the Superconducting Super Collider (SSC), and presently for the National Spallation Neutron Source. Plans are being developed to use the LANSCE accelerator in applications of the accelerator transmutation of waste (ATW) and possibly accelerator production of energy. The materials science, nuclear physics, and weapons physics communities have made great use of the LAMPF/LANSCE accelerator. The research program using this accelerator has led to new radiographic techniques to study dynamic physics phenomena, advanced instrumentation to handle extremely high data rates, and new discoveries in nuclear science. The accelerator complex has served as a magnet facility to attract outstanding researchers to Los Alamos. We fully expect that the complex will continue to be a magnet facility in the future with an even broader research program.

Neutrinos have had an anomalous history at Los Alamos. They are indubitably part of the basic research agenda. The initial effort in this area came from the realization that nuclear weapons might be such a prolific source of neutrinos and that they might afford a chance for their direct detection. This effort moved to the use of a reactor devoted to defense concerns and the neutrino was observed there by a Los Alamos group directly for the first time. Since neutrinos interact so weakly, the LANSCE accelerator with the highest intensity anywhere offered opportunities that were unparalleled for neutrino studies. The sign of the interference term between W and Z was established here, a

fundamental part of the verification of the standard electroweak theory. Los Alamos is also a source of expertise in the handling of radioactive materials which was definitely a factor in the experiment to attempt to see evidence of neutrino mass from tritium decay. At the time, this limit on the electron neutrino mass was the best in the world. More recently, the Liquid Scintillator Neutrino Detector (LSND) at LANSCE has seen evidence for flavor changing neutrino oscillations, which when verified, will have profound effect on the view of the world of particle physics, astrophysics and cosmology. A follow up experiment is approved at Fermilab, BooNE, a collaboration of premier US university groups as well as Fermilab itself to attempt to verify the LSND result and to provide detailed and precise measurements of the parameters. Los Alamos too has had seminal impact on the solar neutrino problem with the SAGE collaboration and now with the US-Canadian collaboration SNO. This collaboration is virtually certain to have a major impact on the solar neutrino problem.

There has been a continuing tradition of using high-intensity accelerators for both programmatic and basic research efforts. One example of this synergy is the use of the LANSCE accelerator for APT, neutron scattering at the Manuel Lujan Neutron Scattering Center, the Weapons Neutron Research (WNR) facility, proton radiography, neutrino physics (LSND), and fundamental nuclear physics with cold and ultra-cold neutrons. It is essential to maintain this type of synergy between the programmatic and basic research efforts at Los Alamos. The current push by Senator Domenici for increased use of nuclear energy in the United States provides a good example of how energy policy, national security, and high intensity accelerators (through ATW and the accelerator production of energy) are brought together as part of our mission. Los Alamos is a leader in the design, construction, and operation of high-intensity accelerators. It is important to retain this capability and to expand its applications into new research areas. Neutron science plays an important role in this future, as it is certain that no research reactor with higher fluxes than available at present will be built in the foreseeable future. Thus, spallation neutron sources must meet the needs of research requiring intense neutron beams or intense neutron fluxes. Los Alamos will be able to play a key role in this future only if the MLSNC becomes a viable national user facility and only if the expertise in linac design at LANSCE is retained and nourished.

Another important area that has developed largely due to the nuclear physics program at Los Alamos has been the development of large, sophisticated detectors, intelligent data acquisition preprocessing, pattern recognition algorithms, and transfer, handling, and analysis of immense amounts of data. The expertise in detector technology in the pion physics program at LAMPF led directly to the development of proton radiography. This technique offers that ability to provide good contrast between low Z materials inside high Z materials (such as within the core of a plutonium pit) with high resolution ( $< \text{mm}$ ) with good time resolution (nsec) at repetition rates of an image every few tens of microseconds. Thus, one can study dynamic processes such as the shock wave propagating through a piece of high explosive which is inside a high Z material. The defense program has rated this as a "must have" capability and a strong R&D effort using the LANSCE and AGS (at Brookhaven) accelerators is underway. Los Alamos is also the lead laboratory for construction of the silicon micro vertex detector in the Phoenix experiment that is under construction for use at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven. This detector has positioning tolerances of a few microns, has  $> 10,000$  silicon strips, must withstand intense radiation fields, and the data acquisition system must handle multiplicities in excess of 20,000 particles per heavy ion collision. Novel detectors based on a variety of detection techniques are under

development at the Laboratory within the field of nuclear science. It seems likely that many of the techniques that have been developed in the nuclear physics program could be of benefit to a wider range of research fields including stockpile stewardship, threat reduction, and potential applications in medicine and industry.

Nuclear science depends upon the ability to sift signals out of large and noisy data sets. In some applications, this feat requires development of preprocessing electronics to be able to handle high data rates in which it is essential to reduce the data prior to recording without loss of the desired information. In other applications, the analysis of large data sets in nuclear and particle physics is often related to the ability to recognize patterns. This need is also present in many other fields of research at Los Alamos. There is currently an effort in advanced computing to develop models and make quantitative predictions using very large sets of input data. However, we feel this is only the tip of the iceberg and that a concerted and coherent effort at the Laboratory to pursue pattern recognition development would be of direct benefit to both programmatic and basic research efforts. In this case, it is often necessary to develop the ability to reduce massive amounts of multidimensional data to a form that can be readily interpreted by the human mind. The human mind is still our best tool for finding order within apparent chaos, but one needs to develop the data reduction and analysis efforts to make optimal use of its capabilities.

#### *IDENTIFICATION OF KEY AREAS*

We see four areas in which support is required in order to have Los Alamos become a world center for neutron science:

**1) *Development, construction, and operation of high intensity accelerators.*** The present LANSCE accelerator complex currently provides the basis for a broad research program in both programmatic and basic research fields. It clearly will continue to be an important component of the program for the next decade. Beyond LANSCE, efforts to develop high intensity accelerators with possibly higher energy beams are an important component. This would allow advances in both programmatic applications (such as APT and ATW) and in basic research as well (neutron scattering and nuclear physics).

**2) *Progress in nuclear science requires not only high intensity accelerators, but also the presence of a vital research program that is central to the mission of the Laboratory.*** Foremost among these is the use of spallation neutrons for research in programmatic fields. Specific examples are neutron scattering to study aging effects in nuclear weapons, neutron capture measurements on unstable radchem detector isotopes, and the ability to do dynamic experiments with techniques like neutron resonance spectroscopy which provides a means to measure temperatures generated by the shock waves in a high explosive. Another area of vital concern is the development of programs linked to the increased use of nuclear energy in this country. Research programs such as ATW can play a crucial role in supporting the Nation's energy reserves. In order for this to succeed, it is absolutely essential that LANSCE be a success and become a national center for a wide range of neutron physics.

**3) *The development of radiography plays a special role in the future research program at the Laboratory.*** Proton radiography can address uniquely a number of weapons physics issues making this technology a high priority for the weapons program. However, other techniques (including gamma ray and neutron radiography) also serve important and complementary roles in addressing issues ranging from weapons physics

to medical technology and industrial applications. It is important that we have a coherent and broad effort in radiography in the future.

**4) Advanced instrumentation plays a critical role in the future science program at the Laboratory.** A great deal of instrumentation has been developed within the nuclear and particle physics fields at the Laboratory. Significant advances have been made in handling vast amounts of data, both in terms of hardware preprocessing of data as well as analysis techniques. This type of technology development can have potential impact on many applied and basic research efforts within the Laboratory. One of the challenges the Laboratory faces in mapping out a bright scientific future is the ability to integrate research developments from one field (such as nuclear physics) to other fields (such as neutron scattering and medical technology). The transfer of technology from nuclear science to other fields can provide one means of meeting this challenge.

**5) Neutrino physics.** Neutrino physics with its technical complexity, use of techniques which are at the limit of the nuclear and particle physics art, offers an opportunity for Los Alamos. We can claim that not only do we bring technical excellence to bear on the problems we deal with but we can also have substantial impact in areas that are of preeminent interest in the scientific world at large. Excellence is our primary scientific product, and the establishment of quality should be seized whenever a clear opportunity exists. Neutrino Physics has been such an opportunity and it should continue.

#### *IMPLEMENTATION*

Neutron science covers a very wide range of research fields at the Laboratory. It is a field in which the future health of both the national security program and basic research are intertwined. A first-class research effort in neutron science can, and should, strengthen the research capabilities within a wide range of other research areas at the Laboratory. In order to have a healthy and vital Laboratory 10 – 20 years in the future, several steps must be taken.

\* **LANSCE, and in particular, the MLNSC must be a national success.** We believe that it is critical in the short term to resolve issues at LANSCE that may prevent achieving this goal.

\* **Over the next 10 years, new programs such as ATW must be strongly supported.** The development of new capabilities, both in terms of new high intensity accelerators and new technologies in nuclear science, must be a priority if neutron science is to be a central component of the Laboratory.

\* **Over the longer run, it is important to provide a solid base of stable support research within the area of nuclear science** (which includes neutron scattering and related science, radiography, and nuclear and particle physics). The developments that come from this area are likely not only to help keep Los Alamos as a world leader in basic science, but also has direct (and likely unexpected) benefits to many other areas of research at the Laboratory.

\* **It is important to the long-term vitality of neutron science that the programmatic and basic research efforts be closely linked and fully integrated.** There has been some progress made in this respect, but such efforts are somewhat random and sporadic. It would be of real benefit to the Laboratory to have better communication and interactions between staff in the programmatic and basic research efforts. There is interest on the part of a number of the researchers in neutron science to close this gap and the Laboratory should undertake to drive these connections. One means might be to form a neutron science weapons working group.

\* ***The neutrino physics program must be supported.*** The follow up experiment to LSND, BooNE, at Fermilab has no immediate competitor, and the return to Los Alamos for a successful verification is immense. In SNO Los Alamos has been a key player in this work from the start. They are identified with the neutral current part of this work which is likely to have dramatic impact on the solar neutrino problem and hence the whole view of particle and astrophysics.

The first component carrying out these steps is to integrate LANSCE into the national user community. This requires that reliable beam be available both at the MLNSC and for other applications such as APT. The Laboratory should provide assistance in solving regulatory problems which impede meeting this goal. The Laboratory also needs to strive to meet the needs and desires of the LANSCE users. A closer coupling to leading figures in the neutron science community would be valuable in this respect. A second important component in carrying out these steps is to provide discretionary support (either LDRD or program development funds) in support of neutron science. Obviously, one needs to strive for stable DOE funding that will be sufficient to meet the goals discussed above, but discretionary funds are also essential in laying the groundwork for future efforts. Finally, the Laboratory needs to take specific actions to bring the basic research and programmatic side closer together. If management makes the commitment to take these actions and carries them through to completion, we believe that we will indeed be able to become THE Neutron Laboratory as one vital component of the Laboratory's mission.

#### ***LOS ALAMOS ADVANTAGE/MISSION RELATEDNESS***

The Los Alamos Neutron Science Center (LANSCE) is the flagship research facility at Los Alamos. Its neutron beams and new instruments have the potential for creating strong links to academic and industrial science in a variety of research areas - structural biology, condensed matter physics, accelerator science, nuclear physics, materials science, isotope production, and more. LANSCE is also strongly connected to our future in national defense areas - accelerator production of tritium, neutron and proton radiography, advanced neutron cross section measurements (use of unstable targets), and accelerator boosted transmutation and energy production. By 2000 Los Alamos will be in position to become a center of excellence in areas of science related to LANSCE capabilities provided that LANSCE has become the right kind of facility. Accelerator transmutation of waste and accelerator-boosted subcritical power generation are good ideas. Their associated complex technical and political issues are fertile ground for imaginative thinking about the future (Energy Subsection). Los Alamos has the broad range of knowledge required to make intellectually credible contributions to these nuclear issues.