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# FELLOWS' ADVANCED PROJECTS INITIATIVE

## WHITE PAPER


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With the end of the Cold War, the Los Alamos National Laboratory offers a wonderful new opportunity for our nation. The major resources which the country has assembled in Los Alamos can now be devoted, in part, to the solution of civilian peace-time problems. The Laboratory, with government support, is in an excellent position to tackle many important problems of major national importance in the areas of industrial technology to enhance our international competitive position, energy and environmental preservation.

To pursue these opportunities, and at the suggestion of Professor Hans Bethe, the Laboratory Fellows have requested and screened staff-generated ideas for new initiatives. We have identified a number of promising projects. In making our choices, we attempted to do more than simply identify technically sound projects having substantial funding potential and a high probability of success. While these criteria were heavily weighted, we tried in addition to identify ideas that could make a big difference to critical problems of national concern. Ideas were selected having a high degree of originality, a complex and multidisciplinary nature, a component of vision that we believe to be aligned with trends of the future, and which were not previously identified in the normal course of program development. In particular we tried to identify projects having clear potential benefit to the U. S. national or industrial development, and projects which by reason of scale, complexity, or level of risk are not appropriate for industries or academic research programs. Finally, we sought initiatives not exclusively related to nuclear or conventional weapons programs. The objective is to attract to the Laboratory major support for critical long-range opportunities which are of a dimension and importance to be suitable for a large, multi-disciplinary national laboratory.

The projects that we agreed upon fall into seven major categories. These categories were not pre-determined, but are instead a reasonable grouping of the projects that emerged. The categories are, in general, mutually reinforcing. In some categories more than one project is described. It is noteworthy that most (but not all) of the categories are related to, or in some cases identical with, Laboratory thrust areas as defined in the Strategic Plan.

The categories we have identified are 1. Theory and Applications of Large Scale Computing, 2. Nuclear Energy Generation and Waste Disposal, 3. Designer Materials, 4. Alternate Fuels, 5. Environmental Science and Global Modeling, 6. Health and Biosciences, and 7. Automation.

## 1. Theory and Applications of Large Scale Computing.

Now more than ever before, progress in many areas of science, engineering, defense and even education depends on the skillful use of more powerful computers. Scientific computation is an enabling technology; it is important not only for its own sake but also for the opportunities it opens up in diverse areas. As we shall see, it is a critical component in many of the focus areas described elsewhere in this report. To meet the demands for increased computing power will require progress across a broad front including computer hardware, software and algorithm development. Advances in the scientific theory underpinning various application areas is also essential for the overall success of most of the projects to be described here. With our long experience in large-scale computing, our extensive distributed computer network, our strong supercomputer center, our cutting-edge, advanced computing laboratory with its massively parallel computers, and our Center for Non-Linear Studies, Los Alamos National Laboratory is extraordinarily well positioned to undertake complex problems involving large-scale computing. In particular, the use of massively parallel computers is important to both projects proposed below.

**Turbulence project.** Research on fluid turbulence is valuable because of its application to atmospheric and oceanic studies, areas which tie in with our environmental science and global modeling initiative, because of its industrial and engineering applications, and because it is a fundamental physical and nonlinear mathematical science. Los Alamos possesses both the computer facilities and the scientific expertise for work in this area. As an example of its potential usefulness, a project is proposed to study how significant reduction in drag or enhancement of heat transfer on an aerodynamic surface is achieved by means of arrays of cavities (dimples) on the surface (like a golf ball). The project would involve theoretical fluid dynamics, turbulence modeling, theoretical and experimental study of heat transfer and drag, and numerical simulation. There are credible claims that up to a 30% reduction in total aerodynamic drag and about the same improvement in heat transfer can be achieved. This project is a worthy challenge to LANL because (a) basic scientific questions are raised – on turbulence and how to model it, on the role of turbulence in quasi-periodic burst phenomena, and on how arrays of surface modifications may have a cooperative effect, (b) one of our best codes is already appropriate to this problem, and (c) the potential practical benefits for drag reduction and/or increased heat transfer seem too promising to be ignored. An important step towards achieving these benefits, and similar benefits which would result from the correct modeling of turbulent flow in a host of other engineering applications, would be to establish a turbulence project at Los Alamos.

**Information from large data sets.** The problem of extracting information from very large digital data sets is a general one of broad applicability. A short list of some of the data sets of interest would include: medical records such as text description of patient encounters, medicare financial records, epidemiological data, information from earth scanning satellites, the enormous data sets expected from the Super-Collider, non-proliferation data such as export license records and on-site inspection reports, financial records of large banks and credit card companies to detect fraud and to detect money laundering, the human genome data base, and computer security audit logs.

An important and pervasive informatics problem arising in the use of such data bases is the detection of "anomalies". Currently, progress with detecting anomalies in very large data bases is severely limited because of the sheer manpower needed to solve the many trivial problems specific to each new data set. These problems include such things as parsing a variety of related data sources, validating the data, combining fields into conceptually relevant concepts, fusing data of different formats, evaluating the relative success of different techniques, etc. Only after these problems are solved can techniques such as statistical profiling, rule learning, clustering, expert systems, or feature selection, be applied and the results presented. The complete process is currently so expensive, and so specific to the particular domain, that even though everyone knows that computers should be able to detect important anomalies in huge data sets such as those collected by the IRS, they can not currently do so. We propose to attack the underlying problem – how to make important progress in specific areas in a way that can be easily used by many workers and that will generalize to new data sets as they are presented. Basically this involves the careful construction of a properly modularized, object-oriented toolkit with an easy to use graphical user interface, that permits the processing of data located at remote sites, and does the analysis in a distributed fashion.

Another important problem to be tackled is the document retrieval problem. The basic question to be addressed is "Which documents in the data set are similar to this one?" The idea is not to use the fundamentally limited keyword approach but rather the more flexible $n$-gram approach. Our preliminary success with this method suggests that the goal can be accomplished in a rapid and effective fashion. Basically an $n$-gram analysis matches the probability of sequences of $n$ letters in the two documents. If they match, it is because the same root sequences have been used, and hence the documents are about the same topic. This technique is computationally efficient, insensitive to errors in the text, and not dependent on "stop lists", grammatical parsing, nor semantic analysis. For these reasons it is ideally suited to messy data sets. What is needed, but not yet accomplished, is the application of hierarchical clustering techniques that will minimize the number of comparisons that need to be made.

The Laboratory's traditions, infrastructure, and current capabilities provide an ideal environment for the necessary match of the informatics community with the supercomputer community – which is essential to accomplish these projects. Furthermore, Los Alamos has the necessary scientific expertise, the computing resources and a reasonable spectrum of appropriate data bases to carry out these projects.

## 2. Nuclear Energy Generation and Waste Disposal.

Over the next ten to twenty years there is going to be increasing pressure to draw more of the national and international power requirements from other than fossil fuel sources.

There is presently no clear alternative to the use of nuclear fission power as a considerable resource. The French currently draw about 70-80% of their electric power from nuclear sources. It seems likely that the U.S. will resume nuclear power plant construction in the next decade. A large part of the world will take this nuclear power route whether we do or not, so if we are to lead and keep abreast of developments, and place a high priority on safety, we must make a considerable effort in this area. For any nuclear power capability to grow in the U.S., matters will have to be conducted very differently than they have been in the past. The American public is increasingly concerned with the environmental problems in the country, in particular air and water quality. These concerns have been manifest in a near-absolute opposition to nuclear power, among other reasons because of the perceived environmental dangers of the plants themselves and also because of the perceived environmental problems associated with ultimate disposal of the waste generated by the production of nuclear power. Recently, increasingly serious environmental concerns have focused on global environmental problems such as the "Greenhouse Effect" caused by carbon dioxide emissions and the acid rain problem caused by sulfur emissions from coal fired power plants. These problems have caused the Sierra Club, as an example, to review their earlier anti-nuclear power position.

**Ultra-safe nuclear power.** Barring a severe accident, nuclear power is the most environmentally compatible commercial power source currently available. Because of the absolute need to have public acceptance of any new reactor concept, new efforts should consider a joint study with environmentalists groups such as the Sierra Club, from the start. In essence the joint group would be tasked to evaluate and standardize the new reactor technologies that provide implicit safety features acceptable to the public. Although the manufacturers of nuclear power plants are making considerable progress on designing new, cheaper and safer power plants, Los Alamos National Laboratory could be the central factor in creating a technology and environment in which U.S. nuclear power could develop. It would require one organization to take responsibility for nuclear power from cradle to grave, in a manner similar to what we now do for a nuclear weapon. The economic analysis requires consideration of all costs from first obtaining the fuel through to the final disposal of the waste products, including those from reactor decommissioning.

In addition the very long range problems associated with extension of our nuclear fuel supplies, perhaps by breeder reactors, in a secure and non-proliferating way should be carefully studied. Our long experience with design together with current efforts such as our Accelerator Transmutation of Waste program, enables Los Alamos to fit very well into this broad program. The designs used in power plants need to be assessed and evaluated, materials capabilities need to be available for materials used or proposed for use in plants, operational methods need to be evaluated and tested over extended life cycles. The question of using fuels such as Pu from the stockpile or $^{235}U$ in the fuel cycle, the monitoring of these materials in the cycle, the methods for monitoring other nations commercial fuel cycles for nonproliferation, and similar questions all fit into Laboratory competence areas. Another important question is the use of mixed uranium and plutonium oxide which is relevant to the denaturing of the plutonium coming out of Soviet warheads. The Laboratory expertise in handling hazardous materials in general, and special nuclear materials in particular, would be well suited for both direct involvement and for establishing methods and standards for others to use. The emphasis of this effort should be on speaking to the entire origination-to-final-disposal cycle and to ensuring the integrity of the entire cycle. The Laboratory need not execute the whole cycle, but should be the broker for all parts. It is essential that any organization involved in this broad perspective have an excellent reputation for scientific and technical integrity, and also have no conflict of interest.

### 3. Designer Materials.

A Presidential Initiative on Advanced Materials and Processing was proposed to address the need for an integrated approach to develop present and future complex materials. We propose a theoretical and experimental materials-by-design program. This program would efficiently select, improve and synthesize new advanced electronic and structural materials. Present and future advanced materials are either nanometer-scale materials or composite materials, and are frequently used under hostile and complex service conditions (*e.g.*, high electric and magnetic fields, high temperature, corrosive environment). The fabrication, stability and performances of these materials are frequently tested and certified in a lengthy process. For example, the developmental stages of new turbine blade materials for aircraft engines last about 20 years before the materials reach the market place. This initiative aims to use our scientific knowledge, experience and computers to help industry by shortening the development time for the introduction of new advanced materials. This effort will require assembling a group of qualified theorists and experimentalists who are experts in first-principle calculation, molecular dynamics, Monte Carlo simulation, fracture mechanics, mesoscopic scale modeling, and continuum mechanics modeling. It will also require state of the art experimental facilities like the atomic force microscope (in which a very sharp point on a flexible arm floats over a surface and measures the field in terms of deflections of the arm), scanning tunneling microscope, transmission electron microscope, neutron scattering, high magnetic field and shock experiments. This team will bring to bear many hierarchical approaches using results obtained in theories and experiments in electronic properties, atomic simulations, microstructural properties, materials properties and system performance for the future rational design of advanced materials at many levels of scale. This proposed initiative would enable us to challenge a core group of competent scientists who will build a fundamental understanding linking the phenomena associated with electrons to real world materials, while being capable of responding quickly to the emerging need for novel materials.

This type of long-term, high-risk and multi-disciplinary approach to materials problems, at a level of several score theorists and as many experimentalists and many postdocs, is not possible in industrial research centers where the aims are short-term payoffs, or in a university where the emphasis is on individual researchers. The Los Alamos National Laboratory has one of the most powerful and productive computing environments in the world, along with a competent group of theorists and experimentalists whose fields range over the areas of materials sciences, metallurgy, ceramics, polymers, metals, semiconductors, materials theory and modeling, materials synthesis and processing, materials characterization, quantum physics and chemistry, statistical physics, liquid flow, and solid state transformations. The behaviors from electrons and atoms up to a system engineering size of kilometers are constantly being studied by multi-disciplinary teams at Los Alamos. For example, the Los Alamos National Laboratory has been involved in several successful materials-by-design type of projects for the solution of the ductility problems of boron-doped $Ni_3Al$ for high temperature structural materials, and metal-halogen polymer chains for electronic materials. Succinctly, it is necessary to combine many skills in this field and Los Alamos has them. This proposed initiative will couple strongly to the DOE's Advanced Industrial Concepts programs, BES programs including our state of the art neutron scattering facility, Technology Transfer efforts, NSF's National High Magnetic Laboratory at Los Alamos and Los Alamos National Laboratory's Materials Science Laboratory, Advanced Computing initiatives, Materials Modeling program and Nano-technology initiative. These programs and our shock experimental capabilities enable us to study the materials under all kinds of service environments. The initial focus of our program would be building up hierarchical models of materials properties and the study of turbine blade materials of NiAl intermetallics, electronic materials of metal-halogen chains polymer, metal-semiconductor hetero-junctions, catalysis, high temperature $MoSi_2$ composites, damage-resistant ceramics, and self-assembling polymers.

## 4. Alternate Fuels

The world production of oil is projected to peak in a decade or so. Clearly, the problems of substitution of power sources for stationary users and railroads is much less demanding than that for automotive and aviation uses where the fuel supply must be carried in the vehicle. To gauge the scale of the problem, the energy equivalent of 3000 Megawatts, the size of a large power station, is about 2 million gallons of gasoline per day, and we use several hundred million gallons of gasoline a day in this country. The development of a replacement for transportation fuels should be a high national priority because of the large financial burden placed on the nation and uncertainty in supply caused by our reliance on foreign sources. Given that oil is a finite resource, it is clear that this problem must be solved eventually if we are not to change our lifestyle dramatically. A suggestion that has been "on paper" for some time and is now being seriously pursued in Germany and other European countries is the use of hydrogen as a basis for substitute fuels. An initiative based on the thermochemical production of hydrogen using either an accelerator transmutation of wastes station or a nuclear reactor as a heat source is described. This initiative is closely related to (2) above and similar social and political considerations apply. Conversion of coal and light hydrocarbon gases to useful transportation fuels is also considered. An additional initiative in this area focuses on fuel cell technology and its relation to hydrogen as a fuel base.

**Hydrogen from heat.** There are two well-known problems with this suggestion. First hydrogen is very bulky and hard to store. It may only be liquefied at very low temperatures and it tends to diffuse into the walls of its storage vessels with concomitant deleterious changes in their material properties. Storage as metal hydrides presents a large weight penalty. The use of hydrogen compounds such as alcohol or ammonia, currently used in large quantities in agriculture, simplifies this storage problem at some cost. The second problem, from our point of view, is its production. Currently, aside from electrolysis, the principal methods for the production of hydrogen all depend on the use of fossil fuel. If the power for electrolysis is to be generated from a heat source, rather than renewable electrical sources such as solar cells, hydroelectric or wind turbines, it is surely more efficient to generate the hydrogen directly from the heat source rather than to include an intermediate conversion step. We here propose to investigate the development of an alternate procedure, which is the direct production of hydrogen from water by the application of heat through pyrolytic chemical processes. Temperatures up to 700-1000° C are expected to be required, and can be produced, for example, by a solar furnace, an accelerator transmutation of wastes station or a high-temperature, gas-cooled reactor. Since sunlight is rather diffuse, we would need something like a six-mile square to produce the equivalent of our 3000 Megawatt power plant, when efficiencies are taken into account. The other sources seem to us to be more feasible than solar, and are directly in the area of expertise of the Los Alamos National Laboratory. We know that there are sets of reactions which will produce hydrogen from water at the aforementioned temperatures while recycling the other reaction components. However there are significant high temperature chemistry problems to be solved. What needs study is the chemical kinetics, appropriate catalysts, and the most optimal set of reactions from the point of view of efficiency, economy of operation, and avoidance of scarce or toxic substances. In parallel with this study, the question of the design of the heat source, as discussed above for a nuclear power station, and its adaptation to these processes will be undertaken. One likely candidate is the high-temperature, gas-cooled reactor upon which Los Alamos did the original work. It would need to be redesigned, however, to produce the proper working temperatures. The heat source aspect will become more focused as the answers to the chemistry questions are learned. As a very rough guide, the cost of production of the energy equivalent of a gallon of gasoline (around 35 kWh) from such a process can be estimated from the current wholesale cost of electricity by considering the expected relative efficiencies, to be approximately one dollar. This estimated cost looks potentially competitive for the future.

**Energy Conversion and Storage.** Our large supplies of coal and natural gas present an alternative to our reliance on foreign oil, if ways can be found to utilize them for transportation in a cost effective and non-polluting manner. Chemical kinetics measurements and modeling have pointed to conditions under which the conversion of light hydrocarbon gases to alcohols is significantly enhanced by using large quantities of free radicals to produce partial oxidation at low temperatures. Other catalytic techniques are also possible. Alcohols are proven transportation fuels and there is a large domestic supply of light hydrocarbon gases available from natural gas and coal gasification. Laser techniques can also be applied to assist the catalytic reactions for coal liquefaction, and to produce useful products such as kerosene and methane. Admittedly, such developments would not free us from a dependence on fossil fuels, but should be viewed as an important bridge, and are synergistic with fuel cell and related technologies that will be important in the future independently of the ultimate source of hydrogen-rich fuels. The transition to alcohol as a transportation fuel would be greatly accelerated by the development of electric vehicles ("green cars") powered by fuel cells. Fuel cells with energy conversion efficiency twice that of the internal combustion engine and output of 5 kW per gram of catalyst have been developed. These fuel cells utilize a carbon-supported platinum catalyst on thin ionic conducting polymer membranes that have produced significant improvements in electrochemistry by providing simultaneous access of protons, oxygen, and electrons to catalytic sites. Another benefit of fuel cell technology is the absence of toxic pollutants. $CO_2$, with its attendant problems *vis-a-vis* global warming, is a byproduct if alcohol is the fuel. Even this problem can be eliminated if a way can be found to carry safely sufficient quantities of hydrogen without a large weight penalty, leaving only water vapor as the effluent.

A parallel initiative focuses on the development of a medium scale, cost-effective, electrochemical energy conversion and storage system that could be used, among other applications, in residences and small businesses. The essential elements of this concept can include hydrogen storage, a solar cell array, a reformer and, at its heart, a bifunctional fuel cell/electrolyzer. This unit could either be used to convert solar electric power to hydrogen, or to convert hydrogen or reformed hydrocarbons to electricity. Coupled to the fuel cell/electrolyzer is a hydrogen storage system and a reformer. The hydrogen storage system allows reasonable amounts of hydrogen to be safely and efficiently stored and to be retrieved. The reformer allows alternate chemical fuels such as natural gas or methanol to be converted into hydrogen rich gas when the hydrogen storage is insufficient for the electrical demands. To realize the benefits of this system will require applied research, engineering, and development. The significant obstacle is cost. Each of the elements of this system has been technically demonstrated. However, the current cost of the technology puts this system completely out of reach for the consumer market. The objective of this initiative would be to attack each of the elements of this system with the goal of reducing the cost by a factor of 10 or more. The fuel cell/electrolyzer is envisaged as a polymer electrolyte membrane system with bifunctional electrodes, capable of both hydrogen oxidation (fuel cell operation) and water electrolysis. To achieve the goal at a cost affordable to the consumer will require significant optimization and innovation in the electrode structure and cell design. The hydrogen storage system is envisaged as a metal hydride system, although other storage technologies would be considered. The hydride system would require inexpensive materials that achieve efficient storage and release of hydrogen at temperatures compatible with the fuel cell/electrolyzer. The reformer would utilize partial oxidation of the incoming fuel to provide the energy necessary to convert methane or methanol to hydrogen. Reducing the size and cost of this unit will also require innovative design and engineering. A substantial engineering effort will also be required to integrate the components of this system into a safe, reliable and cost effective whole.

## 5. Environmental Science and Global Modeling.

Concern about changes to the global environment wrought by human activity has become widespread over the past several years. Some of the greatest concerns relate to pollution of the lowest level of our atmosphere resulting primarily from energy generation and its use. There is also a considerable concern that the copious release of carbon dioxide into the atmosphere will cause a global warming that could eventually trigger a long-term change in climate. Such a climate change could have a major impact on the quality of human life, particularly in coastal areas. Conversely, an excessive quantity of smoke and/or dust released to our atmosphere can increase its optical albedo, thereby cooling the Earth and perhaps triggering an ice age. Computer simulations at Los Alamos and elsewhere of n ar winter scenarios have suggested that such cooling is possible; global cooling observed after the eruptions of Mount Pinatubo in the Philippines lends credence to these simulations. Further, we are now aware that human activity is leading to depletion of the atmosphere's protective layer of ozone. Public interest in these and other issues has sparked a number of studies to provide the scientific understanding necessary to chart public policy on energy use and atmospheric emissions. These studies have shown that major gaps exist in our knowledge of the various factors that control the evolution of the atmosphere and climate. As a result of these gaps, the national and international policy decision making process on energy use and atmospheric emissions has become paralyzed. In order to help relieve this paralysis, the international scientific community has embarked on a program of intensive research aimed at achieving a comprehensive understanding of the factors and processes that affect global environmental change.

Although most of the public awareness of environmental issues is focused on the biosphere (the uppermost level of the Earth's crust and the lowest level of its atmosphere), our environment and the factors that affect it extend far beyond the biosphere. We know, for example, that the Sun is the dominant energy source for atmospheric processes. Even small changes in the solar output can cause large changes in climate, which can completely mask human-induced effects. Studies of records of $^{14}C$ contained in historic materials (shown to be a reliable proxy indicator of past changes in the solar output) have revealed several marked changes in our climate history, relatively recent examples being the prolonged hot period between 1120 and 1280 AD and the prolonged cold period between 1640 and 1710 AD. Thus research aimed at understanding the Sun and its variable output is an important component of any comprehensive study of environmental change.

Photographs of the Earth taken from space help emphasize the fact that our environment extends outward through the upper atmosphere, to the ionosphere, the magnetosphere, and beyond. This near-Earth space environment is increasingly a focus of human activity and interest. For example, we have become dependent on satellites operating in near-Earth space for purposes of communications, weather forecasting, national security, and basic research. Yet space is a harsh environment that is subject to major disturbances driven by solar activity, which can and do induce serious failures in spacecraft systems. They have also induced serious (and costly) disruptions of ground-based power grids, most recently the power blackout caused by the March 1989 geomagnetic storm that shut down the entire province of Quebec for 6 hours. However, we still lack a sufficient understanding of solar activity and the mechanisms that link short wavelength and particulate emissions from the Sun to the near-Earth satellite environment, to be able to provide a predictive capability. Whereas in the past, this lack has resulted in economic losses, in the future it will result in insurmountable radiation hazards to personnel operating in near-Earth space. Thus an increasing effort is being made to understand solar activity and the mechanisms that link such activity to our extended space environment.

We now recognize that the solar-terrestrial system is made up of many components (some were just mentioned) that are tightly coupled. Small changes in one component can trigger much larger changes in others. This fact has raised a number of practical questions concerning global change for which we, at present, have no answers, yet which deserve serious consideration: How stable is the terrestrial environment? Does the environment have metastable states? What are the mechanisms that drive and return our environment to and from stability? How rapidly do these mechanisms operate? We are aware that the Earth's environment is unique among that of all the Sun's planets - it is the only one capable of supporting life as we know it. All of the other planets, which are subject to different energy inputs from the Sun and have different internal structures, different atmospheres and different magnetospheres, are unlivable. Is it possible that our own environment could evolve to an unlivable state if perturbed sufficiently? Extensive research on all of the factors that control our environment is necessary to provide answers to such questions, and to find ways, either through policy decisions or technological advances, to mitigate detrimental long-term trends.

The potential negative impact of global environmental change on human activities and the present level of awareness and concern by the public on these issues suggest strongly that the time is ripe for a major initiative by LANL in this area. The global environmental field is by nature of large scale and quite complex, and our progress in understanding environmental issues fundamentally demands a multidisciplinary and long-range approach. Scientists at universities, at industrial laboratories, and at the national laboratories (including Los Alamos) are currently working on various aspects of the global environment problem. However, to date this effort has been somewhat diffuse and relatively poorly organized. Nevertheless, the multidisciplinary scientific expertise, personnel, technical capabilities, facilities, and data archives existing at Los Alamos suggest that the Laboratory is ideally suited to take up the challenges posed by global environmental change. Support provided by DOE in this effort would be highly leveraged since other government agencies are also strongly supporting research in this area. Our particular contribution could be to act as a focus and center of excellence for a broad scope of activities on global change, ranging from experiment design and implementation, to the collection, analysis, archiving, and dissemination of environmental data, to the development and testing of computer models of global dynamics. This effort would take advantage of a large base of technology, scientific expertise, management capabilities, facilities, and environmental data archives already existing at Los Alamos.

## 6. Health and Bioscience.

Advances in the basic biosciences and related technologies underpin the prevention and treatment of disease, and the concomitant cost and effectiveness of U. S. health care. Scientific problems in these areas have the highest national priority, and the Laboratory is addressing these issues by defining major thrust areas on both the technological and basic science fronts in health, biotechnology, and biosciences. The Laboratory has substantial strengths and a clear track record of accomplishments in basic and applied biosciences. Moreover, there is high potential for the practical application of developments in these areas to the health care industries. At this point biology appears poised to make the most revolutionary advances in its history in the understanding of molecular functions and the control of disease in the mammalian organism. The past decades have furnished tools of enormous power including the ability to analyze and map the mammalian genome; to identify the biological function of specific genes and non-coding sequences; and to identify, isolate, determine 3-dimensional structure, and ascertain the interaction of DNA with other molecules of proteins, carbohydrates, lipids, and a variety of supra-molecular, cell structures. The time has now come to use these powers to gain a conceptual understanding, which is still lacking, of the nature of mammalian differentiation and the vast array of diseases that arise from its defects. The result will be an enormous increase in the powers of medicine which may even transcend that which developed in the specific area of infectious diseases at the beginning of this century. Another way that the tools of molecular biology, which have been developed during the past decades, can be used is the characterization of microbes found in environmental samples

**Cell differentiation.** This subject embodies one of the ultimate questions in biology remaining to be answered in the twenty-first century, namely: "How does a single cell (the fertilized egg) control its genes and its cell proliferation to produce different cell types that lead to the development of different organs (brain, liver, heart, skin, *etc.*) that make an adult animal or plant?" This question in biology is analogous to that of a "unified field theory" in physics.

Los Alamos National Laboratory is ideally positioned for this new synthesis to occur because of the presence, at a single installation, of great resources in biological techniques, chemical and materials sophistication, enormously powerful engineering and instrumentation skills, and an unparalleled array of resources in the realms of physics, mathematics and computational science. The practical requirements for undertaking this project are of such a scale that it could not, and never would, be undertaken by a university, a single commercial company or even by an industrial consortium. Yet, it would lay the groundwork for technology transfer and great commercial advancement.

Flow cytometry is a method of studying the properties of cells in a flow which uses laser and staining techniques and is capable of separating different types of cells directly in the flow. The original work on this method was done at Los Alamos and our continuing biophysics expertise in flow cytometry in LS-Division and the National Flow Cytometry Resource Center would serve as the experimental heart of the project, supplying differentiated cells for experiments and analysis of cell differentiation progression. The Theoretical Biology Group in T-Division could develop models for cell-cell interactions that lead to tissue structure and shape. The Structural Biology Groups in LS and INC Divisions could focus on understanding the molecular interactions of growth factors with the cell surface receptors leading to signal transduction for differentiation. The biochemistry expertise in LS-Division, which is presently dedicated to understanding protein-DNA interactions, could be expanded to focus on the mechanisms controlling the changes in genetic expression necessary for cell differentiation. The biophysics expertise in P-Division, the laser experts in CLS-Division, the neutron scattering expertise in LANSCE, and the instrumentation engineers in MEE could design and develop new instruments for differentiated cell structure analysis. The mapping of cell differentiation would identify the differentiated cell types, biochemical pathways and molecular structures, particularly susceptible to radiation damage, chemical carcinogens, and other industrial hazards.

The elucidation of cell differentiation will also make fundamental contributions to our understanding of cancer, since this class of disease manifests a pathological differentiated state where cell proliferation controls are lost. Some of the new advances demonstrating the existence of new principles of genome regulation in mammalian cells have involved Los Alamos scientists. A mechanism has been uncovered by which different segments of the genome become exposed at the periphery of the cell nucleus. This region is an active center of RNA synthesis. Another such region of genome exposure has been revealed to lie around the nucleoli of the nucleus, and this is where the "housekeeping" genes are located. It has been shown that cancer cells have lost genome exposure in the peripheral nuclear region, but have retained that in the nucleoli. Therefore cancer is a loss of differentiation. It will be possible to define the genes which are active and inactive in each differentiation state in normal health. This knowledge should allow the understanding of the defects responsible for cancer and other important pathologies, and should lead to a means by which such defects can be prevented or corrected.

**Microbial Characterization.** Environmental remediation is often undertaken by the addition of suitable micro-organisms, as in cleanup of oil spills. It is however, frequently difficult to measure the distribution and abundances of the introduced organisms, and of others occurring naturally, and hence to assess and improve their effectiveness. It appears that the technology of modern molecular biology may provide a new approach. Moreover it has become clear that changes in the genetic content of the microbial flora within the environment have a direct impact on the health of many species of animals and plants. However, little is known of these changes or their specific impact on ecosystems. Previously, the measurement of the genetic content of such samples required culturing viable organisms. This method does not provide an accurate measure of the vast number of different species present. Technology recently developed and refined at the laboratory now provides methods to determine the genetic content of samples by detecting specific DNA sequences (genes). Chemically synthesized DNA probes prime the synthesis of selected DNA fragments using DNA from an environmental or laboratory sample as a template. Amplification of a target DNA by an in vitro DNA synthesis reaction that is primed by the addition of these short DNA sequences implies the presence of the original gene in the sample. This technology is very sensitive – detection of a single DNA molecule within a sample has been demonstrated – and quantitative. Development of a battery of DNA primers that are specific for selected organisms or genes can be used to demonstrate the presence of these within a sample. Use of random DNA primers will generate a DNA fragment "signature" for particular samples. Changes in this "signature" can be easily detected and can serve as a measure of changes in the overall genetic content of the sample. It has been estimated that only ten percent of the organisms present in an environmental sample can be detected using present technology. Development of this new technology should generate more complete genetic profiles. Once developed, the technology can be used to monitor microbial changes in response to abiotic changes in the environment. It can also be used to identify and isolate selected microorganisms that might play important roles in environmental remediation or in the production of pharmaceutically valuable compounds.

Los Alamos National Laboratory is particularly well suited for developing such a program. Several different laboratories within LS division are presently using this technology for characterization of the human genome and for the study and isolation of certain genes from a variety of organisms. However, its application to environment studies will provide a wealth of knowledge concerning changes of the microbial flora in response to natural and anthropogenically-induced environmental changes. Such studies will provide rapid methods of microbial site characterization for the generation of models that accurately predict the impact of environmental modification. The laboratory is developing a data base containing DNA sequences for a variety of different microbial species as part of a program to identify target organisms in environmental samples. The computational expertise of the laboratory will be necessary for managing the large amount of data generated and for the development of environmental models that use this information. Possibilities for technology development and transfer are significant.

### 7. Automation.

**Microrobotics.** To date most of the work on microrobotics has been done at universities. Although a number of industries are very interested in micro-robotics, the long time scales and high risk levels associated with projects in this field make them unattractive for industrial development at present. Now the field is developing to the point where a more complex, multi-disciplinary effort is appropriate. Los Alamos has an extended history in advance computation and the use of microelectronics. The Laboratory also enjoys a broad technical legacy from the Artificial Intelligence Initiative of 1984. During the Cold War, concern for radiation vulnerability of microelectronics provided the impetus for the development of a microfabrication facility for the construction of millimeter-scale thermionic circuitry components. A recently initiated Exploratory Research and Development Initiative has dedicated substantial Laboratory resources to nanotechnology, the study of exceedingly small electronic and robotic devices.

Micron-scale sensors and actuators are already under active development, and nanoscale devices seem likely to follow. We propose both a theoretical and experimental modest effort to explore the design and construction of microrobotic devices. There are both military and commercial applications for such devices. Perhaps the area of greatest near-term benefit would be medicine. Microfabricated sensors for the analysis of blood samples are nearing commercial application. Sensors that can continuously monitor various biochemical agents and 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 these possibilities are accepted, it is not such a great leap of the imagination to envision fitting these medical robots with actuators and tools so that they can repair the aneurism, chisel out the plaque, or isolate the cancerous regions. Prosthesis is another 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. The technology may allow a broad range of military nanorobots, whose motility includes atmospheric hovering, jumping, and swimming. They could be oriented towards a minimally lethal war. The opportunities of surveillance and intelligence gathering are manifest. There are possibilities for deterrence and concomitant opportunities for the encouragement of peaceful settlement of disputes as well.

Another way that micro- to nano-scale autonomous devices contribute is to the "Warrior's Edge" which is the eighth Science and Technology Initiative within the Office of the Secretary of Defense this fiscal year. The four major technological emphasis areas are enhanced human performance, improved sensing, decision-making and lethality. Microrobotic technology can contribute significantly to the last three of these areas. They can be used to improve vision and hearing, and to sense in other areas, such as atmospheric chemical sensing and electromagnetic field sensing, where human senses are relatively weak. By tying in to the command, control and communications network, the decision-making capabilities of the individual warrior can be considerably enhanced. High-resolution information could also be transmitted to and from the warrior and it could be interfaced with heads-up displays through the use of advanced micro-computers. Examples could include orders, color maps, and positional navigation. Lethality could be enhanced through computerized fire control coupled to the warrior's microrobotic system for target detection and acquisition, thereby enabling more rapid identification and destruction of targets. The proposal here would be to develop the necessary micro- to nano-scale technology to make possible these applications by U. S. industry.

**Dilute source technology.** In order to use dilute resources such as sunlight or wind, for example, a lot of equipment would be required. In order for these efforts to be economically feasible, the equipment must be very inexpensive to produce and maintain. These goals point in the direction of self-diagnosis, minimal-human-intervention maintenance, and robotic assembly. We already see steps in these directions in some computers that have multiple central processing units which will shut down a faulty unit and continue to run with the remaining units, while reporting the fault in order that repairs can be made. Automation in the manufacture of industrial and agricultural goods has progressed during this century to a remarkable degree. While at the beginning of the century it took a large portion of the population simply to grow food, today this portion is a few percent. Textile mills that can operate without workers, as well as fully automated production lines for solar cells already exist. Indeed, it is hard to find a manufacturing process which could not be automated–at least in principle–using today's technology base. This trend towards higher automation will gradually lead towards self-maintenance and self-assembly, whether one states it as an explicit goal or not. Clearly the attainment of this goal is still far in the future. However, by setting the goal of self-assemblying machine systems one redefines the issues in automation in a way that we believe to be fruitful. While the short term advantage in automation lies in increasing the sophistication of manufacturing equipment, the long term gain, pursued here, lies in reducing the cost of this equipment by automating its production. This in-depth approach to automation can be based on currently available technologies and will lead, on a relatively short time scale, to large gains in productivity from partially self-producing factories. Eventually it can lead to a closed system which produces everything necessary to maintain and produce itself.

We propose to explore how one might lay the foundation for a new technology based on self-assemblying machine systems which promises increases in productivity similar to those of the industrial revolution, as well as access to a renewable energy resource which could satisfy even a greatly increased world demand. The Laboratory has the expertise in many of the relevant areas from material to computer science, particularly the necessary theory and chemistry,

## Appendix

The material in this document was drawn from the following proposals:

"Advanced Projects Initiative, Large Programs," C. B. Storms.

"Artificial Mesospheric Clouds," M. T. Sandford II, M. V. Hynes and T. D. Hunkle.

"Bifunctional Electrochemical Energy Conversion and Storage System for Residential and Small Business Applications," R. A. Lemons.

"Cell Differentiation in Human Development," L. R. Gurley.

"Computational Informatics Initiative at Los Alamos," T. R. Thomas, V. Faber and R. Strittmatter.

"Contributions of AMO to National Energy Needs," N. A. Kurnit

"Dimples and Turbulence," C. Zemach.

"Hydrogen from Heat," G. A. Baker, Jr., C. D. Bowman, G. J. Kubas, C. F. V. Mason and W. H. Woodruff.

"Joint Early Warning/Ecological Disaster Distributed Active Archive Center," E. R. Tech.

"Life Sciences at Los Alamos in the Coming Decade," T. T. Puck.

"Materials by Design Initiative," S.-P. Chen.

"Methods of Characterizing Microbes in Environmental Samples using Molecular Biology Techniques," P. J. Jackson.

"Pitman," J. Moore.

"Proposal for a Global Environment Research Center at Los Alamos," J. W. Ogle and M. V. Hynes.

"Self-Reproducing Machine Systems For Global Scale Projects," K. S. Lackner, C. H. Wendt and D. P. Butt.

"The Global Environment," W. C. Feldman and J. Gosling.

"The Motility of Military Microrobots," J. C. Solem.

"Ultra Safe Nuclear Power," S. D. Howe.

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