

"HERDING CATS" —

A NEW INTER-INSTITUTIONAL SCIENCE NETWORK

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I'd like to talk to you today wearing two hats. One I wear as a computational scientist specializing in condensed matter physics, or more generally, materials science, and the other as an administrator and organizer of a new national network to promote interdisciplinary research among groups within the Department of Energy (DOE), universities, industry, and other government agencies. We have heard many of these themes expressed in earlier talks and comments, so some of the motivations and ideas for fostering such a network will be familiar.

Of course a solution to our problems is funding, additional funding. But with budget caps, tax cuts, defense, and social programs, the funding for science may be approaching a zero-sum game. Strategic areas will be identified for increased funding, but other areas will likely be pinched. The current priority areas identified by the National Science and Technology Council (NSTC) include (1) Information Technology, (2) Global Change, (3) Climate Change Technology, (4) Emerging Infectious Diseases, (5) Protecting Against 21st Century Threats, (6) Aviation Safety, Security, Efficiency, (7) Plant Genome, (8) Food Safety, (9) Integrated Science for Ecosystems, (10) Educational Research, (11) Nanotechnology. While I will speak about research relevant to high performance computing under item 1 and dealing with phenomena under item 11, there is no guarantee that there will be major increased funding for computational materials science.

Within the Materials Science Division of the DOE it is recognized that additional funding to provide each national laboratory with all the new resources to compete is not possible. One way to pursue new science is to assemble teams of experts from various groups and to share resources from different laboratories. The question is how we get scientists to work together across institutional and interdisciplinary boundaries. This is the problem of "herding cats," according to a friend who recently retired from Argonne National Laboratory. John Wesley Powell, the one-armed civil war veteran and geologist who first explored the Grand Canyon, wisely knew that coercion was not the answer. In testimony to the Allison Commission in 1885 he said: "Scientists spurn authority. They are as a class, the most radical democrats in society—patient, enthusiastic, and laborious when engaged in [absorbing] work ... but restive and rebellious when their judgments are coerced by superior authority."

Even the simple answer—*money*—is not enough (although it sure can help). A large cooperative project needs important, relevant, and big ideas. The Manhattan Project and the Mission to the Moon are at one end of the example spectrum, and even High Energy Physics Accelerators have been based on big ideas. Today the mood of the country and the mood of Congress is to denigrate *big* projects, for example, the F22 fighter plane (too expensive), the Superconducting Super Collider (too expensive, and management problems), and perhaps the Spallation Neutron Source (management problems).

Before describing the compelling argument, the important vision, for investing in computational materials science, let me start the story a little over a year ago when panel meetings were taking place. At that time the DOE had started plans for a Strategic Simulation Initiative (SSI). This was to be a non-defense sister project to the Accelerated Strategic Computing Initiative (ASCI) that has placed the world's fastest supercomputers at the weapons laboratories to simulate the properties (e.g. aging) of nuclear weapons. When actual testing was banned, ASCI was proposed and funded as part of Nuclear Stockpile Stewardship. The computers employed are massively parallel, with thousands of processors. They are not at all easy to use. Not wanting the future of supercomputing to be completely dominated by the Department of Defense (DOD), the non-classified part of DOE was inclined to start SSI. Other agencies have joined and the interagency IT**2 initiative is generally slated for funding this next fiscal year (although there is now some funding trouble). The SSI was aimed at big projects and both the global climate modeling and the combustion components were identified early. A small remaining part of SSI is designated "basic science." Materials Sciences were welcomed to compete for part of the basic science piece of the pie. There were several national panels convened to discuss what computational materials science would propose as its main thrust, and a rather natural vision arose; however along the way it was clear that our community was not accustomed to working in large teams. We were called a "cottage industry" by some, and indeed the discipline is filled with single principal investigator groups, many competing against each other rather than working toward any single goal. We had to induce a cultural change to assemble a large team and agree on a project worthy of these remarkable computing resources. This new collective cooperation is not meant to replace single principal investigator groups which continue producing outstanding research, but rather the goal is to foster cooperation in order to work on truly large scale projects requiring multiple talents and disciplines.

Last December three of us went to the DOE's materials sciences division and suggested the idea of a network. We had two models in mind. One was already in place among DOE laboratory experimental groups, called the Synthesis and Processing (S&P) Center; and the other was in place in

Europe, called the psi-k network. To foster collaboration among groups in different countries, the European community put up money to support postdoctoral fellows and students in joint projects, provided that they join groups located in a country other than the one in which they were trained. We were given the green light to organize such a network and the Computational Materials Sciences Network (CMSN) was started.

First let me describe the major science theme running through the current proposals for CMSN projects, and then I'll give a few specifics about the network. This information and a more elaborate description can be found on the CMSN web pages at: <http://cmpweb109.ameslab.gov/cmp/ccms>.

As in the automotive and aerospace industries, materials scientists and engineers are beginning to make greater use of powerful computers to help comprehend, design, process, and produce better materials with desirable properties. In many cases bigger computers are not just better, they are vital for simulations of real materials. Today's scientists are starting to calculate the structures and properties of real materials, calculations that were unimaginable just a few years ago. Until recently, our knowledge of materials arose mainly from trial-and-error techniques. Only with information about the atomic and molecular structures have scientists been able to comprehend materials at the most elemental level. Today, extensive computer modeling capabilities can complement and accelerate laboratory development. Computer simulation tools which should be available in the near future could substantially reduce the amount of time required to take a new material from synthesis to product, a process that currently takes a minimum of 10 years, and may take as long as 25 years. In the United States economy, this time lag to market is generally the principal barrier to new materials development.

The key new vision is that we have nearly all of the knowledge and computing power to couple fundamental atomic level knowledge with larger length scale simulations to evaluate and understand materials properties enough to greatly aid engineering designs. Scientists refer to multi-scale modeling when they want to describe interactions and properties at increasingly larger length and time scales. Scientists have a reasonable handle on both the smallest-length scale, which cannot be seen with a microscope, and the largest-length scale, which can be seen with the naked eye. In between is the intermediate-length scale, which scientists call the mesoscale, where there exist particularly exciting materials science challenges. It is the structure at the mesoscale that ultimately determines vital materials properties such as mechanical strength and magnetic behavior.

By accurately modeling and tailoring the mesoscale, scientists expect to:

- Create materials with new and innovative properties, such as polymer lasers;
- Extend the capabilities of existing materials, such as those that underpin silicon-based semiconductor technologies;
- Process materials cheaply and efficiently, reducing costs and waste.

These achievements will impact developments such as:

- Lightweight materials for transportation;
- High-temperature alloys for higher-efficiency turbines;
- Magnetic materials for motors and data storage;
- Opto-electronic materials for communication and information technology;
- Bio-compatible materials for implants, etc.

With this grand vision in mind, the mission of CMSN is: To advance frontiers in computational materials sciences by assembling diverse sets of researchers committed to working together in order to solve relevant problems that require cooperation across organizational and disciplinary boundaries. This project requires scientists with expertise in solving the quantum mechanical interactions, computer scientists skilled in parallel computing, and engineers who can make use of the atomic scale data (suitable averaged) for calculations of bulk material properties and design. The intent of the modest funding is to foster partnering and collective activities among these disciplines. It is expected that scientists who join CMSN projects are already funded (by DOE or other agencies) for work somewhat related to that portion of the project they would be contributing to within CMSN.

CMSN was launched February 3, 1999 when a number of possible project topics were discussed at a meeting of about 60 scientists. So far, four workshops have taken place. Three proposals have been submitted, with one funded; we expect that three or four more will be funded this next fiscal year. The workshops bring together 20 to 30 scientists to focus on specifics. Some of the scientists decide that the topic has narrowed in such a way that they are not interested in pursuing the project, and they decide not to join the effort. This is fine. There is certainly not much additional money at stake, and people have to be committed to the overall goal before the modest funding for travel and shared students and postdoctoral fellows is appealing. So far there has been great enthusiasm, although the exact mechanisms for the large scale collaborations are less well defined and will undoubtedly undergo modification and optimization during the first year or two of operation.

CMSN is a new experiment, one that could lead to a cultural change that may enhance large-scale cooperation in a discipline that is poised for major breakthroughs. It reminds me of many small villages forming a modern city, with common goals for infrastructure and economic prosperity.