Advanced Computing: Scientific,

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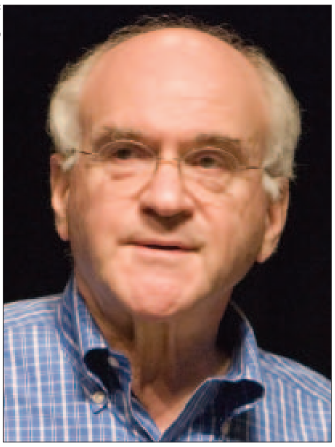

Dr. Victor H. Reis, Senior Advisor, Department of Energy talks to Dr. Lali Chatterjee, Editor in Chief of *SciDAC Review*, about computational science in national security, nuclear partnerships and more.

Dr. Chatterjee: *Introducing high-end computing as an effective mechanism for addressing large-scale, specialized problems has been one of the signatures of your leadership role in national security matters. Please comment on your vision for ensuring national security through the use of computational science and large-scale simulations.*

Dr. Reis: National security involves people with a wide variety of backgrounds and motivations: it is an interactive multi-dimensional problem and as such it can never be absolutely ensured. The unique advantage of using simulations is that we can sample multiple levels of human interactions. We can allow people to interact in very different ways and this allows security analysts to anticipate and understand situations in greater depth.

So, you can sample a complex sub-space of people's interactions as it were?
Yes, to some degree, because we can use simulations to create scenarios. We can ask "what if" questions in some measure of detail and examine the outcomes. For example, a very relevant national security issue today is that of the nuclear weapons stockpile. The current President and others want to maintain our nuclear weapons stockpile—preferably without underground testing. It is not clear whether the current weapons are satisfactory or we need a new weapon that can be developed and certified without testing. Advanced simulations play a critical role in answering these kinds of questions.

When you say "people", I assume you are referring to decision makers?
Right. It is critical to reach the decision makers. They could be tactical decision makers, policy decision makers, business decision makers, economic decision makers and so on. The point is that high-performance computing can really make a major difference in how leaders make decisions. It can facilitate informed, and hopefully improved, decisions.

Returning to your comment about the weapons stockpile—how exactly could the simulation be utilized in order to ensure that the weapons could be maintained without new testing?
One example is to examine the effects of long-term storage on weapon safety and performance. Materials change in a radioactive environment. Little cracks or changes in the material configuration may arise. Are these small effects going to make a difference in safety or performance? How would we know? In the past, underground testing determined such effects. In the absence of testing, detailed validated simulation provides added knowledge upon which better judgments can be made.

Is it possible to take the human element into account in simulations? For example, what if somebody makes a mistake while they are working?
That is a good question. A computer allows you to factor in various types of mistakes. This allows us to train and to learn.

Moving on to the next question, Dr. Raymond Orbach has identified advanced computing as the third pillar of science. What is your perspective on this?
I think he is absolutely right. Advanced computing bridges the gap between theorists and experimentalists. It allows theorists to do experiments in a very realistic way and it allows experimentalists to try their experiments beforehand. I think this advance testing is extraordinarily important. People sometimes miss the point: it is as much about people as it is about computation. It is not that computation is replacing the human being in making the decision. It enables human beings to make better decisions, to understand the science better, and to design better experiments. Obviously, we can achieve these goals much faster, and move into otherwise inaccessible realms.

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Since you are talking to the readers of the SciDAC Review, a compelling question to consider is one about the philosophy and power of programs like SciDAC. Do you think this idea of the three groups of people (computer scientists, applied mathematicians, and discipline scientists) working together is also conducive for the type of large complex environment that includes "people" components?
Very much so. In fact, that is how we started the ASCI (Accelerated Strategic Computing Initiative), program in Defense Programs—now the NNSA (National Nuclear Security Administration). That program was organized around just such collaborations. When we started the Stockpile Stewardship program it was obvious we needed a lot more computing power. But when I visited the laboratories, I noticed that the computing people were separated from the designers. So, when I brought in Gil Weigand from Sandia to run this program, I said, "Gil, don't talk to the computing department. Talk to the weapons designers, the people who actually

Biography in brief

Dr. Victor H. Reis is a Senior Advisor in the Office of the Secretary at the Department of Energy. His primary responsibility lies with the Global Nuclear Energy Partnership (GNEP), part of President George W. Bush's Advanced Energy Initiative. He is also a member of the Strategic Advisory Group of the U.S. Strategic Command. Dr. Reis led the development of the Department of Energy's Stockpile Stewardship Program when he was Assistant Secretary for Defense Programs in the U.S. Department of Energy and he created the Accelerated Strategic Computing Initiative (ASCI) program at the National Nuclear Security Administration (NNSA).

His past appointments include serving as Director of the Defense Advanced Research Projects Agency (DARPA), Director of Defense Research and Engineering (DR&E) at the Pentagon, and Assistant Director for National Security and Space in the Office of Science and Technology Policy, Executive Office of the President (OSTP). He has chaired and served on numerous high-profile committees and is well known for his contribution to implementation of high-end computing in multiple national projects.

Dr. Reis earned a Bachelor's degree in Mechanical Engineering from the Rensselaer Polytechnic Institute (1957), a Master's degree in Mechanical Engineering from Yale University (1958), and a Master's degree and Doctorate from Princeton University (1962). He has authored numerous scientific and policy publications and his many awards include two Department of Defense Distinguished Public Service Medals.

have to address the problem. Ask them about the important challenges that they are going to have to face in the absence of testing. They are the ones who are going to have to make timely decisions." We were able to get the requirements that way as opposed to talking to the computer people and asking how they can build fast new computers.

So, you wanted need-based development of the computer?

Right, and then we found later we also needed a new set of visualization tools, and we had to broaden the community beyond the laboratories. We put a significant amount of money into developmental interdisciplinary research because stockpile stewardship is an interdisciplinary problem. It wasn't just a physics problem; it was also a materials problem, an engineering problem, a chemistry problem, and a coding and algorithm problem.

And then there is the parallel computer environment.

That is very important. The weapons parts of the laboratories were not using parallel processing very effectively, so we had to build that in as well.

You established communication between these groups of people?

Right. SciDAC's interdisciplinary approach for solving specific problems is essential when dealing with many areas in applied science. It reinforces the approach we took with the ASCI initiative.

We also had to interface and partner with the computing industry because they are the ones who have to build the computer and so they have to understand our computing needs. Solving large complex problems usually involves developing and using the right sorts of tools.

You have talked about the ASCI program. You also initiated novel and interesting explorations of computational structure during your leadership of DARPA (Defense Advanced Research Projects Agency), and you are currently involved in GNEP (Global Nuclear Energy Partnership). We would like to hear about the role of simulation and advanced computing in relation to these programs.

Advanced multidimensional simulation is what we are hoping to apply as part of the GNEP. The nuclear reactor design community has been very conservative and traditionally has not used truly advanced computing as part of their design process.

Don't they use simulations to run their reactors?

But we're talking about designing and qualifying a new class of reactors and more importantly the entire fuel cycle. Remember that we haven't built a reactor in a long time, and the United States is just beginning to seriously consider closing the fuel cycle. This means there are a number of issues involving separation, transmutation and disposition that need to be considered as well as reactor design.

When we started the ASCI program in 1993, the world's fastest computer was at Los Alamos. It was a Thinking Machine computer, and it had less speed than a Macintosh you can buy today. In supercomputers, we are now at 200 teraflops and there is a mature, commercial vendor base that can be applied to the GNEP challenge.

You asked about DARPA. When I first went to DARPA in 1989, it was the leader for developing massively parallel computing. This was a continuation of its role as a major driver in computer and information technology development. During my time there, one of my main concerns was getting mainline computer companies, like Cray, involved in using the massively parallel approach, and applying massively parallel machines to a variety of national security problems. In fact, if we go back a little bit further, the crucial DARPA enabling discovery was packet switching, which allowed computers to communicate with each other. Massively parallel computing is part of that technology heritage.

So, the DARPA research was not classified? It was readily handed over?

Oh, yes. This was started well before my time. And there is a fair amount of literature about it. The book *Rescuing Prometheus* by Thomas Hughes (Pantheon Books, 1997), describes how it all started.

I will quote you on that. Thank you. A related question: How did you develop your own interest in computational science?

Well, when I was a director at DARPA, I asked myself how DARPA can continue to make an impact. This was at the end of the Cold War, and I realized that the DARPA's strength was in the information technology they had been developing. This technology was to be even more important in the new national security environment.

Do you expect a new vision as we go now from teraflops to petascale computing, or do you think we do not need to be at this scale?
I don't foresee that there will ever be a limit to "how much we need." Computing, in particular, high-performance computing, can be thought of as a tool for expanding the brain, and providing for a deeper understanding. It is powerful as a communications tool, and we are learning how to input and output human effects. For instance, we can create pictures and make very effective dynamic imagery.

The GNEP has three simultaneous goals: to provide sufficient nuclear power (1,000–2,000 GigaWatt/year by 2050), dispose of radioactive waste, and reduce proliferation risk, and we think recycling by fuel cycle states may realize this. The GNEP principles emphasize that global issues require global solutions and spent fuel is an asset to be managed, not a waste.

Dr. Victor Reis, SciDAC 2006, Denver, CO

Like virtual reality?
Dynamic virtual reality. It probably depends upon what you mean by "reality." Let me give you an anecdote that relates to this and dates to the time I was at DARPA during the first Gulf War. Right after the war ended, I sent a group of people to Iraq to recreate a battle that had actually been fought. Using the people who participated on the actual terrain and recordings of voice transmissions, we built a simulation of the real battle which could, in principle, allow for continuous interaction of both sides leading to possible different outcomes.

So you have the added dimensions of people's interactions to transform a computer (data) simulation into a "humanized" visualization or a movie?
Exactly. I showed a movie of the simulation, to the then Secretary of Defense, Dick Cheney. His reaction was, if I had had this before, we might have been able to show people the repercussions of their actions, and so used it to avert the war. I think he meant that very seriously. It is important that we provide the proper information in the proper form, in order to help policy makers to make decisions.

The national laboratories have been torchbearers in some sense for advancing science and technology. Do they have a role in GNEP?
The reason we have national labs is not only to advance science and technology, but also to apply their expertise to important national problems. The GNEP is addressing one of the most important national and international problems of the 21st century, and there are significant technical problems that must be overcome. The national labs will be critical in this effort, and in particular, we see them as playing a leading role in the myriad simulation and validation aspects of GNEP. When we work on major national/international problems, they should have appropriate tools. Computing is one of the tools, just like large-sized machines such as the National Ignition Facility, at Livermore, or the Accelerator facilities.

Since you mentioned Livermore, would you like to comment on BlueGene/L? (see "High-Performance Hardware," p40)
BlueGene was designed to solve some specific types of problems. But that is where the art of designing the "tool set" comes in; BlueGene was developed for special focus tasks as part of an integrated program. I should add that it is very good for material science, which is a significant part of the GNEP Research and Development challenge.

So, basically BlueGene/L did come into being because of that whole program?.
Yes. But again, the partnership between IBM and Livermore to create it was important. The labs can't build a computer by themselves and the industry is often reluctant to invest their own money. Collaboration is essential.

Nuclear power has been extremely controversial in the U.S. for decades. Is GNEP ready to face the challenges?
Interestingly enough, a lot of the polls indicate that there is a real difference between what people really believe (they are in favor of nuclear power) and what they think is generally believed (they think most people are against it.) The U.S. has by far the largest amount of nuclear power in the world. It represents 20% of our electricity in this country, and it is running very safely and very efficiently. The whole purpose of the GNEP is to have a lot more nuclear power, not just in the U.S., but around the world. I think we are ready, but time will tell.

Do you think that you need to share more information with the public so that the public is involved in a positive sense?
Yes. It is the public who uses the electricity, and worries about the long-term concerns. I should note that the problem is not in designing the reactors, the problem is in how we handle the waste. If we are going to put this stuff away, it is going to have to stay away, safely for long periods of time. Because we can't wait 2,000 or two million years to experiment, we have to simulate. And here we return to policy makers. Simulation has to be convincing not only to the scientists, it has to enable policy makers to understand what is happening and feel comfortable that they are making the right decisions. This takes us back to our earlier discussion where I talked to Vice President Dick Cheney—absolutely a policy maker—and he said, I can help make better decisions using this. Simulation has long been in

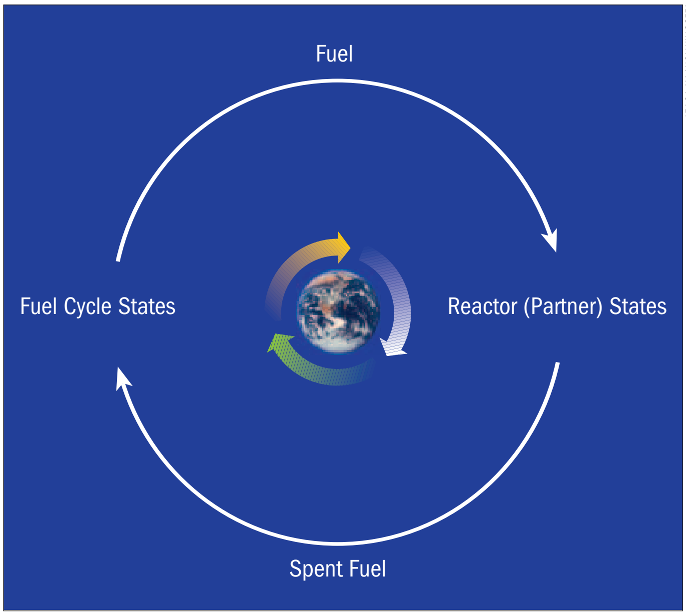

ILLUSTRATION: A. TOVEY

Figure 1. *Fuel leasing is an integral component of GNEP plans. This chart has been developed from Dr. Reis's talk at SciDAC 2006, Denver, Colorado.*

use for training people who were in battle for instance. What we are doing is taking it to another level and using it in policy making. The people in the GNEP, the national laboratories and the computing people are going to contribute to this development and this is really where the simulation is going to play out.

But you have a complicated situation here because, as you said at the start, this effort involves so many different countries and cultures.
Right. The one thing all these other cultures are interested in is simulation. But they all do it differently. This is a global effort that must incorporate the different approaches to this problem. When I go to Japan to discuss this, I have to understand their constraints. When I go to France, I have to prepare for a different set of conditions. Large-scale simulation is headed to becoming an international communication tool.

So you visualize computational and simulation science as communication at many different levels?
Exactly, and that's where I think SciDAC can help. For example, a SciDAC-like problem is the long-term disposition of waste in the global context.

Our planet is for all, so it makes sense that waste disposal should be addressed at the global level.
Right. The problem of waste disposal is a global one, and the solution must survive many hundreds and thousands of years, or eons as it were. Remember one of the keys to the GNEP is the whole idea of fuel leasing—even Hans Bethe suggested it thirty years ago, ("The Necessity of Fission Power," *Scientific American*, 1976).

It isn't just U.S. fuel leasing; it is fuel leasing around the world. Geologies are different, and the geochemistries are different. We want to be able to design waste repositories in forms conducive to the geology that they will be embedded in. We don't do that now.

In some ways this is similar to the problems we faced with stockpile stewardship. What can we do if we can't test? How do I get people to understand what the problems are? Not just the weapons designers, but the people who have to make the decisions.

It is also a major task to get the public—the global public—to accept the long-term waste issue concurrent with a major expansion of nuclear power. So it is broader than just a science problem, it is a socio-political problem. How do we convince policy makers around the world that our approach to waste disposition is safe and secure? Remember, different countries have diverse cultures. They have different ways of looking at these problems. We must understand and respect their varied responses.

The United States has been out of the game (research and development of nuclear power) for over a decade. France, Japan, the U.K., and other countries have continued the research and development of the construction of nuclear power facilities. What role can we effectively play given that we may be fifteen years out of date?
While others are certainly better prepared in some ways, we have a major strength—simulation power. Secondly, we really do have the national laboratories that have been involved in the technology, and we also have a lot of very good universities that people aspire to come to from all over the world. And recall, the GNEP is a global effort, so the emphasis is on partnership.

Are our current reactors all old designs?
Yes. The current reactors are old, but I think we will get new reactors. Again, the mission of the GNEP is to create a global partnership to solve global problems such as climate change. Nuclear power is the only real source of energy that can produce baseload electricity without greenhouse gas emissions or other pollutants.

So, solving the greenhouse problem is part of the "big picture plan"?
Yes. Globally, there is enough coal around to provide energy for some length of time. But coal is also synonymous with pollution, climate change, and other crucial problems. Nuclear energy—on sufficient scale—is a primary means of dealing with greenhouse gases.

You have a history of initiating new wave projects as you said, and now you have to go beyond just getting computer companies interested—you are going to have to get the whole world interested.
With the end of the Cold War, nothing is more important than getting an international approach to the energy, climate change, and proliferation challenges. The GNEP is an approach to attacking all of these issues simultaneously. Our initial discussions with international partners have been very encouraging, but I am reminded of the Japanese proverb:

"A vision without action is a dream. Action without a vision is a nightmare."

I think we have the global vision. Time will tell whether the global community has the will to act. The people and institutions that participate in SciDAC can help.

Thank you for speaking with us.