

Scientific discovery: powerful,



Dr Raymond Orbach, Director of the Department of Energy's Office of Science, talks to the Editor in Chief of the *SciDAC Review* about his views on science, its future and SciDAC.

Editor: *As the Director of the Office of Science and a distinguished scientist, what in your view are the fields where we might hope to see the most remarkable advances, both in the near future and in the long term? For instance, referring to the DOE's Facilities for the Future of Science and other plans?*

Dr Orbach: I've been a scientist long enough to know that one cannot make predictions about scientific discovery. So though I may disappoint you, I have to say that no-one knows where the really fundamental discoveries will come from. At the same time, I will say that what we hope to do is to build an infrastructure for science that will enable great discoveries to happen.

You refer to our "facilities for science." While no-one can predict where the most exciting discoveries will happen, what I can say is that without the facilities to explore unknown regions, we would probably miss some major opportunities.

It was our intention to create a plan for the facilities that we anticipated would be most effective in enabling scientists to "do their craft" and to make the discoveries that will excite us all. The difficulty, of course, is prioritizing, because none of us really know the capacities of scientific instruments or the pace of developments — and we won't know, very far into the future. So we have to weigh which facilities might be most effective to enable discovery to take place as a function of time and projected developments.

Can you expand on this with reference to your own experience?

One remarkable example of "growth in unexpected directions" has been in high-end computation. This is now one of the most important facilities. Yet, in the past, this was not even regarded as a facility where one would go to pursue scientific discovery. I think we need to give the Japanese credit for recognizing the power of this field. It was really the Earth Simulator, which was announced in the spring of 2002, that opened people's eyes. At least, it opened my eyes — to the possibility of doing things on a scale that we had never done before. What has astonished me is the speed — the incredible rapidity of performance of high-end computation that uses architectures conducive to science. Whereas I was thinking in terms of half

a decade for significant progress in the past, I am now thinking in terms of a year or two...

So you are surprised at the progress?

It is beyond all expectation. These things are working faster than I had imagined. And it's not just the size. It is also about what I consider benchmarks or plateaus that we need to reach in order to make discoveries. My "mantra," if I can use that word for it, is 50 Tflop of speed, because we believe that at that speed one can start to do simulations that have a chance of discovery on a major scale. This speed needs to be accessible to scientists. By this I don't just mean a facility that is physically accessible — I mean *scientifically* accessible.

Can you explain the type of science we may see at your "mantra" level?

Yes, but I would first like to clarify that to reach a sustained speed at that level, with the typical efficiencies that we experience, one has to in reality get peak speeds in the vicinity of 150–200 Tflop. In the past we did not think this could happen, but now it looks feasible within a year or two.

Now to return to your question: this may get a little technical but I will try. At the speeds we are talking about, the electrons in a fusion device can be considered as real point particles and do not have to be treated in mean field approximation. So for the first time at 50 Tflop one will be able to do simulations of high-density, high-temperature plasmas that were never possible before. This will have a significant impact on the treatment of these highly nonlinear systems. These systems are not subject to analytic examination and there may be instabilities that no-one has thought about. This has already been found to be of profound importance for ITER, for fusion science in general (see feature "Simulating star power on Earth," p40), and for interplanetary and space studies.

There are similar opportunities for discovery in other areas. This takes us to topics such as protein folding that most people expect to be able to simulate at petaflop speeds. These are an order of magnitude faster than the level we discussed, but they are no longer unreasonable. It's very possible that within half a decade we will be at those speeds — not just realized at peaks but as sustained speeds. This did not seem possible a couple of years or so ago.

These advances and the possibilities they project are really astonishing. Another exciting area with immense opportunities for discovery is cosmology and its interface with particle physics. I like to quote Prof. David Schramm: "The study of the very large (cosmology) and the very small (elementary particles) is coming together." This was a very astute remark because one of the real surprises of the end of the last century and beginning of this century has been the subject of dark energy. We haven't a clue what it is, but it amounts apparently to more than 70% of the energy budget of the universe. That's what I meant by surprises. No-one could have predicted that. One of the facilities that we're building is a billion-pixel telescope that will be cre-

unpredictable and aesthetic

Biography in brief

Dr Raymond Orbach, Director of the US Department of Energy's Office of Science, manages an organization that is the third-largest federal sponsor of basic research in the US, the primary supporter of the physical sciences in the US, and one of the premier science organizations in the world. Prior to this, Dr Orbach served as Chancellor of the University of California (UC), Riverside, for 10 years (1992–2002). Under his leadership, UC Riverside doubled in size, achieved national and international recognition, and led the University of California in diversity and educational opportunity.

A distinguished scientist, Dr

Orbach has received numerous honors nationally and internationally for academic scholarship and scientific contribution. His research in theoretical and experimental physics has resulted in the publication of more than 240 scientific articles.

In addition to his vision and leadership role in advancing frontier science, Dr Orbach maintains a love for science and its appreciation that communicates readily in conversation. Dr Orbach received his BSc in physics from the California Institute of Technology in 1956, and his PhD in physics from the University of California, Berkeley, in 1960.

ated for discovery in cosmology. I wish I could tell you about the discovery. We know the opportunity and potential for it is certainly there and it is very exciting to anticipate what it may reveal.

So you think we should be ready for discovery and try to identify the areas where it may occur?

We know we need to ask the questions. And we know that it is so exciting when there is a question that is fundamental, but we don't know how or where to start. Yet, we have to be ready. We can only make the preparations so we do not miss it when it comes. That is what the billion-pixel telescope in space will give us — readiness.

There's another instrument that I wanted to focus on in terms of creating the infrastructure, and that is the Linac Coherent Light Source; we call it the LCLS and it will turn on in 2009. It is an X-ray free electron laser and it will operate in the hard X-ray range so that one will be able to probe at the molecular level. It will have enough brightness so that one will be able to see structures of individual molecules. There are proteins, for example, that do not crystallize. These are the proteins that make up the surface of the cell. There's no way to determine their structure precisely because they do not crystallize, so one can't use the conventional structural methods that we have. But we now have the capacity [with this new instrument] to control the ability to see one molecule at a time. And so for the first time we will be able to determine the structure of the molecules that really

regulate cell function and allow drugs to pass through the cell walls, and we will learn some very important lessons in biology from understanding these structures.

And that's just the beginning. That instrument will offer a large number of photons and a timescale shorter than any facility of its kind has ever probed. This will be at one-third of a femtosecond (a femtosecond is 10^{15} s) and what it will do is it will freeze chemical reactions in time, just like a stroboscope does, so that we will be able to see how the chemical bond forms in time as the reaction takes place.

This is completely new. No-one has ever probed that region of science before. And again, I can't tell you what is going to happen, but it will be in a time domain that has not been accessible at these X-ray energies before. So, in principle, one will be able to follow a chemical reaction in real time so that one can really understand how the valence electrons are reorganizing themselves as the reaction takes place.

Theories for these exotic time scales are still in their infancy and the opportunities here are unlimited. It will finally enable us to break away from rate equations and really get down to the fundamentals of how chemical reactions occur and the nature of the chemical bond and where it comes from. Again, I can't tell you precisely what will happen because it's never been done before. The instrument gives us that opportunity.

In your address to the AAAS Fellows in February 2005, you said: "Science provides much of our intellectual nourishment. The excitement of discovery persuades not only our psyche but our very language." And in 2002 you said: "Science in the Office of Science is beautiful." How important do you think this feeling of "excitement" and inspiration is?

Well, it is the reason that we all do science. Science can be very difficult and very frustrating at times, and most of the time, our ideas do not work. But when they do, the experience is so satisfying that this is what drives us. I like to think of science as an aesthetic experience. Scientists recognize that research is not easy. But whether it is discoveries made by ourselves or by others, the experience is so beautiful that it opens a sense of satisfaction and excitement that is uniquely "science."

One of the advantages of science is the opportunity of doing experiments which provide validation, or otherwise. It's also a quantitative subject, and the precision we aspire to adds to the aesthetic satisfaction. Expressing that excitement to the public is what draws people into science. The reason I am in science is because of this excitement of discovery. When I talk to young people — high school kids, junior high school kids — about science, I say to them: "First of all, science is beautiful. Secondly, it's you, it's your contribution." In science, one can make a contribution to society that is authenticated by the accuracy of measurement, and is immutable although interpretations may change and evolve. Unfortunately, we typically teach science in a very dull way that does not propagate this excitement. I try to share the excitement and beauty of science when I can. ▷

Moving on to SciDAC's mission and message, I would like to ask about one of your quotes about computational science on the DOE website: "In the last decade, the power of computation — our ability to model and simulate experiments that we have not conducted in a laboratory — has become so great that it must now be considered a third pillar, along with theory and experiment, in the triad of tools used for scientific discovery." Do you think computational science has established (or even surpassed) itself as truly the third pillar of science?

I don't think it's surpassed itself but it is certainly now a comparable [pillar]. The advent of fast computers opened up what I call the nonlinear world. It's the world that conventional theoretical approaches simply cannot cope with. It is not a world that's reached by perturbing slightly your existing world. It's a whole new world and while there are some formulas which can help one understand it, it was really opened by computation. So I don't feel one is more important than the other, [it's] just a question of different worlds as investigative tools.

The nonlinear world is a fascinating area, and so also is the random world. In the absence of conventional cartesian structure, these worlds can only be explored by simulations, as we do not have sufficient analytic tools yet. We have some, but very few that are capable of describing phenomena in these new worlds, and here is where computational methods offer opportunities that we can't get any other way. My own research focuses on random systems and computational simulations. It was discovered that there was actually order in these systems. There was a correlation length, which I had never imagined possible in a random system — truly random — and I wouldn't have been able to realize it in any other way. Subsequently, through a set of experiments we were able to show that nature really does behave that way. That discovery was driven and led by simulation, and there are many other examples, especially in the nonlinear world, where simulation has led the way. So, it's not a question of being more important or less important. It's another set of tools we have available to explore issues that do not yield to our current theoretical structure.

The SciDAC program has been a major initiative during your leadership of the Office of Science. Has SciDAC been effective in strengthening the role of high-end computing as a means to discovery in science?

First of all I would like to claim credit for SciDAC but it was here when I got here ...

But I think it has grown in your time ...

Well I hope so. SciDAC is unique in the world. That's one way to answer the question. There isn't any other program like it anywhere else, and it has the remarkable ability to do science by bringing together physical scientists, mathematicians, applied mathematicians, and computer scientists who recognize that computation is not something you do at the end, but rather it needs to be built into the solution of the very problem it is that one is addressing. As a consequence, it can best be done in that format and it has been a format that has proven itself over the years to be very attractive, and to literally define whole new fields for discovery.

And so it is "Yes" to your specific question — SciDAC has strengthened the role of high-end computing in furthering sci-

ence. In good part this is due to the fact that it is unique and brings together teams that are able to create a structure for addressing what previously have really been intractable problems. We will have to see what happens when those are actually implemented on these large-scale facilities. But it is the only way to go forward.

There is another angle to this. As with all new and innovative programs, I am not too sure people have really come to terms with SciDAC yet. First of all, it is a group of people, not an individual. Secondly, they need a facility of sufficient scale and magnitude to be able to deal with the issues at hand. This refers to the fact that the computer is no longer one person's domain. Rather, it has now become an instrument for a group to work on. Hopefully, this group is of the right structure so that they can work most efficiently as it needs to change the nature of computation.

Computation, in my view, will become very much like our other large-scale facilities. For example, [computers] will become user facilities like our high-energy physics accelerators, our light sources or our neutron sources. If you think about those facilities, they tend to be worked at and developed by

My own research focuses on random systems. Computational simulations led the way to the discovery of order in these, and I had never imagined this possible.

teams of investigators. Furthermore, they are not all just scientists, but people who are experts in electronics and people with mechanical devices expertise, and in general a very complex group of individuals who are able to take maximum advantage of that particular facility. I believe computation now has reached a point where it has become a similar enterprise, and I believe SciDAC is the vehicle for approaching these new facilities. What I anticipate in the future is competition for computational cycles at computer facilities based on the quality of the science, but also based on the structure of the collaborative groups competing for the time in order to achieve discovery.

This is going to change the way we allocate computer time. It is going to change the nature of our investments in these computers because they are no longer a small part of a person's research portfolio. They are now the "big iron," if I can call it that. They are the massive devices that we need to invest in, in order to give these collaborative teams the opportunity of working on them. I find it unlikely that a single individual will be able to approach these machines and compete for time because of the necessity for that individual to be an expert in their subject field, as well as the quantitative methods to be used in this computational structure and the visualization of the results that may emerge. I think teams that have experts in each of those individual fields will be more common than they have been in the past in terms of utilization of these facilities. We have to start thinking about how to operate the very large-scale computational structures as user facilities which will offer their properties to users. The reason I used that phrase is that we have a well-established structure for user facilities, like the ones I

mentioned earlier, within the Office of Science. My belief is that we are now at a point where we are going to be doing this in computation as well.

Do you also see participation from other countries in relation to the user facilities into which the computer sites will evolve?

Oh, it has to be international. What we have learned from all of our facilities is they have to be open to everyone, and by the way, they have to be open and without charge.

Without charge?

That is right. The facility should be open and available without charge on a worldwide basis, solely on the basis of the scientific quality of the program. I mean this in the context that our high-energy physics machines or light sources are free to all users. However, whatever is needed to carry out specific projects will be the responsibility of the driving groups.

You mean they need to get their own projects and detectors for their experiments, like specific experiments at Fermilab or SLAC do — but there is no charge for the facility itself?

Precisely. The detectors in line of the light source are the responsibility of the users — the accelerator is the facility that we run. For example, some group may have an end-station. Another may have a visualization facility, or something that is quite specific to their particular project. These will be the responsibility of the team, although obviously in many cases they will be our responsibility to fund. But this will be separate from the core facility, which in this case will be the high-end computation facility.

Could we then interpret these user facilities as an expansion of the role of SciDAC?

We have been facilitating this in an experimental fashion via a program called Innovative and Novel Computational Impact on Theory and Experiment (INCITE). What we have done for the last three years now is to open this on a worldwide basis to anybody. You do not have to be a Department of Energy (DOE) grantee to get time. In fact, we are funding people with NSF grants, who compete for time. When we started this, we did not have much computer time — just 10% of the National Energy Research Scientific Computing Center (NERSC). Since then, we have obtained other machines, like the LCC at Oak Ridge, for example (see “The experimental apparatus of computational scientists,” p 38). Now we can carve out more time and allow competition for this computer time. Interestingly, we are finding that we did not need to require that teams be created. In fact, for these very large-scale problems, teams are convening together to do what I just described — in the spirit of SciDAC.

I have not heard of any computing facility anywhere else in the world that is treated as a user facility in the way you have just described. Do you think we can provide a world leadership in this?

We would like to think so. Frankly, I feel that we are pioneering this effort and to my knowledge it has not been tried anywhere else in the world before. It is also important that the results be freely available in the open literature. This would make it “perfectly American.” I mean especially [that] the openness is American.

Please comment on the creative integration across programs in the Office of Science is involved in the SciDAC program.

In my view, it is one of the beauties of the Office that we do multidisciplinary science. We are in the DOE and we support biology, high-energy physics and materials research, to mention a few. We are doing all of these because they are fascinating fields and the Office of Science brings them all together.

What is your perspective on the role of the Office of Science within the broader umbrella of the DOE?

The Office of Science needs to be thought of as being as broad as the DOE. Therefore, it has the responsibility of working on the mission of the DOE, and this means including applied research in its purview along with basic research. In turn, the basic research conducted through the Office of Science strengthens the assistance the DOE can provide to its programs.

The Office of Science also profits from the applied programs of the DOE because they have fascinating overlaps with science, and in my view enliven research in the DOE. So I look at the Office of Science as being an integral part of the DOE and inseparable from its applied responsibility.

The next question is about something we have touched on before.

How do you think we can reinforce your comment “Science is good for you” at the AAAS meeting this year, in relation to non-science students and the public at large?

Yes, I think science is good for you. I think that, first of all, the discipline of science is an intellectual exercise that is shared by many other fields of endeavor. The scientific method is beautiful and structured in itself and it has an intellectual core fully as vigorous as any other in the academic disciplines. Secondly, it has a great advantage in having experiment available to guide it, and this can inform scientific enterprise. I am no smarter than the physicists at the time of Newton or any other time. They were just as smart, maybe smarter than I am. But I have the advantage of new opportunities provided by experiment that they did not have. I find that physics for me is realizable and I have been able to make original contributions, partly because I have the unfair advantage of experiment as compared to some other academic disciplines. Probably this is not something that you expected to hear, but it’s the way I look at my life.

I try to convey these advantages of science to young people and to the community at large. It has profound consequences for our economy not because we do it for the economy, but because we want the consequences of science. Science influences the way we live and I firmly believe that the quality of life in our country, and the improvement in that quality, has resulted from scientific discovery. The very computers we have talked about over this past hour would not be possible without the transistor. Yet the transistor was really invented after World War II, that is, about 50 years ago. When you think of the laser and the impact it has had, and when you think of microelectronics and the impact it is having, these were things that nobody even dreamed of. But they are now just routine. Children who are using XBoxes have computer capacities never dreamed of 10 years ago, and it will probably increase further in the future. So we are enabled in our society by the fruits of science. That, to me, is something very exciting and beautiful about our field. ●