Getting to Know DOE's New Under Secretary for Science

DOE

Theoretical physicist Dr. Steven E. Koonin is the new Under Secretary for Science at the U.S. Department of Energy.

SciDAC Review: *Congratulations on your appointment as the Under Secretary for Science. How do you like your new responsibility? How is it different from your role as Chief Scientist at BP, and prior to that, as Provost at Caltech?*

Dr. Steven E. Koonin: Thank you. I'm privileged to serve the nation in this capacity and now that the confirmation and swearing in are done, it's time to get to work. Part of my efforts at both Caltech and BP involved catalyzing and enabling cross-disciplinary ideas and research. This is one of the roles of the Under Secretary for Science in the Department of Energy (DOE). We clearly have an opportunity with the new administration, Secretary Chu, Under Secretary Johnson, Administrator D'Agostino, and the rest of the Department's leadership to make a difference in how the nation approaches energy and environmental issues. Part of my initial efforts will be devoted to defining and enabling science programs that knit the Department together and lead to novel energy research efforts.

President Obama has made energy and climate change a central theme of the administration and hired a dream team of Steve Chu, yourself, Kristina Johnson, and Bill Brinkman to define, deploy, and manage DOE's investment in science to achieve transformational discoveries in sustainable energy and environment. How will you refocus DOE and its laboratories on these important global problems to deliver breakthrough science? What changes do you see in the way DOE pursues science in order to optimally meet our nation's energy challenges? What will DOE look like in a decade, and how will the role of the Office of Science change during that time?

DOE shares the Administration's goal to reinvigorate the American scientific enterprise through a bold commitment to basic and applied research, innovation, and education. DOE is very focused on breaking down stovepipes within the Department, fomenting a revolution in energy, keeping basic science vital, and continuing to innovate in nuclear security in a changing world with a changing environment.

In the context of research DOE is asking, what are we good at? Our strengths in computational science are well-connected to applications, and we will leverage that to support additional energy efforts. We plan to pursue projects that change the way engineers and scientists think about solving energy problems. We will also continue our mission to steward the nuclear weapons stockpile, and we are supporting active research in all energy areas, from nuclear power to advanced biofuels and beyond. We are defining grand challenges to bring the appropriate expertise together to provide solutions to a variety of important problems we face today. We are hoping these grand challenges will inspire collaboration both within DOE and between our national laboratories, universities, and industry partners.

What are your plans to re-energize the national labs as centers of great science and innovation? How will you engage the scientific staff at the laboratories and convince them that there is a new deal, that there is an opportunity to embrace a degree of risk-taking in research?

The national labs have been centers of great science and innovation for many years. Energy is different from other research areas, due to its scale, ubiquity, and incumbency. Energy research, then, requires participation of a wider community, including industry and social scientists. National labs are a natural pillar of this effort, and have always encouraged wide collaborations. Risk-taking research requires the researchers to have a voice. Our challenge is to develop programs that enable scientists to pursue a wide variety of efforts, including high-risk research. We have confidence that transformative research will arise more easily in such an inspired, science-focused environment.

In the early days, the lab directors and senior managers at a laboratory had a great deal of latitude to focus research on delivering transformational scientific outcomes. Do you see some recalibration of the current management model to allow the laboratories to innovate?
I believe innovation is inevitable due to complexity of energy challenges. Increased collaboration will undeniably create a new dynamic, and we are designing problem statements that encourage broad participation. Our energy challenges require transformative outcomes, and DOE is developing multiple programs with different approaches to allow that to happen.

We often perceive a corporation as a top-down management structure, whereas decision making at academic institutions is usually driven by faculty. How do you envision the management at DOE? Is there an optimal medium that would drive scientists to solve important problems while maintaining a healthy level of scientific independence?
In science, management should set the overall vision and goals, and then enable progress. The DOE leadership brings the ability to identify technical challenges in achieving policy goals set for us by the President and Congress. Our job is to translate those policy goals into well-defined scientific and technological goals. We look to the science and research community to meet these goals with creative solutions.

> There is tremendous growth potential in applying high-performance computing to climate modeling and monitoring, and in development of alternative sources of energy ...

In order to best meet our nation's science and energy problems, where is the low-hanging fruit, and where do you see growth potential?
Increasing energy efficiency in transport and decreasing the energy intensity of buildings are two things that immediately come to mind. There is enormous immediate growth potential in developing materials that can address energy issues in a variety of ways, such as lightweight materials and materials that can operate in extreme conditions. There is tremendous growth potential in applying high-performance computing to climate modeling and monitoring, and in development of alternative sources of energy, such as advanced biofuels and nuclear power generation.

Biography in Brief

Dr. Steven E. Koonin was previously Chief Scientist for BP, where he was responsible for guiding the company's long-range technology strategy, particularly in alternative and renewable energy sources. Dr. Koonin joined BP in 2004 following a 29-year career at the California Institute of Technology (Caltech) as a Professor of Theoretical Physics, including a nine-year term as the Institute's Provost. He has served on numerous advisory bodies for the National Science Foundation, the Department of Defense, and the Department of Energy and its various national laboratories. Dr. Koonin's research interests have included theoretical and computational physics, as well as global environmental science. He did his undergraduate work at Caltech and has a Ph.D. from MIT.

How will you connect basic and applied sciences and create an effective mechanism to integrate national laboratory, university, and industry activities? Are the Innovation Hubs—Bell Lablets, as the Secretary has characterized it—the first instantiation of this model?
The Energy Hub concept is a funding model designed to support a coordinated R&D effort that leads to solutions of important national problems. Hubs allow new collaborations beyond existing department definitions and institutional scope, removing organizational barriers to solutions. We hope to put the tactical research management in the hands of the best scientists with substantial and sustained funding. Research across the whole technology chain of a given area, from basic science to commercial applications, is another important feature, as is the involvement of for-profit organizations, for these latter are the means by which the energy system is changed.

What is the role of Advanced Research Projects Agency-Energy (ARPA-E) in the DOE, and how will it act as an integrating mechanism between Office of Science and Energy Programs?
ARPA-E will focus on opportunities where tight coupling of a scientific discipline, basic research, and technological innovation will produce short-term results. The intent of ARPA-E is to support programs that are fast, nimble, and quick. The urgency of the energy challenge creates a need for near-term solutions while longer-term solutions are still in development in the existing programs.

As I scan the description of each of the eight Innovation Hubs, modeling and simulation is explicitly mentioned. We applaud DOE's commitment to modeling and simulation as the third leg of scientific discovery, along with theory and experiment. How do you see the Advanced Scientific Computing Research (ASCR) program working with these Innovation Hubs that are distributed across the various program offices in DOE?
ASCR currently supports several programs that span multiple disciplines, such as SciDAC. I hope to draw upon ASCR's experience to understand how computing capabilities are best integrated with theory, laboratory work,

and large-scale demonstrations or experiments. Another instance where such activities occur is the extensive work within the National Nuclear Security Administration (NNSA), less well-known or recognized outside of that community. I hope to make those achievements and capabilities more prominent, and to apply the underlying computer science to solutions of problems normally outside of NNSA's purview.

DOE's Office of Science is the largest supporter of physical sciences and the steward of major User Facilities for the nation. Each of the Offices (BES, BER, HEP, NP, FES, and ASCR) has accomplished this goal by supporting not only the user facilities but also a balanced portfolio of science. Historically, the ASCR program has stopped short of funding the science needed to effectively utilize the user facilities it manages for the nation, focusing on math, computer science, algorithms, and tools. SciDAC is the first departure from this model, where the office has partnered with other offices to enable science. Do you see an expansion of this model both within Office of Science and beyond to include the applied programs?

Integration of computing with domain knowledge is extraordinarily important if we are to have any impact. One of my goals is to increase communication and collaboration within the DOE, as we are underutilizing many existing strengths. Nearly a decade of experience with SciDAC demonstrates that well-designed programs help people understand the scientific and technical challenges a field faces. A compelling case and solid plan for execution attracts financial and intellectual resources and delivers research that matters. We hope to expand upon and improve the multidisciplinary approach it has pioneered.

The President and the Secretary have articulated the impact of climate change and the need to study and understand climate change. What is the role of computing in ascertaining climate mitigation and adaptation strategies? What science prospects will be enabled by exascale computing? In what science and/or technology area does computing have the best chance of delivering a game-changer? Now that we have reached the petascale, the next step would be exascale. What doors might that open? The scientific community developed through town hall meetings a prospectus for exascale computing, in particular for applications in energy and the environment. What are, in your opinion, the biggest scientific opportunities for computing in the age of petascale and beyond?

I think the Department and the various scientific communities will need to identify where the forefront of scientific simulation will contribute centrally to solving major problems in scientific and technical areas supported by the Department. Once those scientific drivers are clear, we will be able to design specific paths for hardware development, create codes for the community that take full advantage of the highest-end machines, and begin applied mathematics research for development of new algorithms. A broad research program is needed to address software considerations and the many interesting hardware problems, such as power consumption, memory bandwidth, and data storage and retrieval.

There are several areas that I expect would benefit tremendously from the continued increase in computing capabilities. The previous advance to petascale was a game-changer in our understanding and maintenance of the nuclear stockpile, and I fully expect similarly significant impacts from exascale.

Nearly a decade of experience with SciDAC demonstrates that well-designed programs help people understand the scientific and technical challenges a field faces.

Such computing capability can drive many energy and climate related simulations. I look forward to useful regional climate prediction and the validation of climate models against data from the entire observational network. There is also opportunity for systems-level simulations that look at, for example, the national electricity infrastructure, including integration of solar and wind power coupled to weather modeling. It will be a great day when we have a flexible energy infrastructure that allows a grid operator to access accurate weather predictions to decide when to turn on a backup generator for a wind farm; this cannot be achieved without high-performance computing.

In your experiences as a physicist, you have seen computers play an ever-increasing role in how scientists approach theoretical problems. Would you please describe how high-performance computing has advanced your own research?

I started using what was, at the time, large-scale computing in about 1975 for time-dependent Hartree–Fock simulations of nuclear collisions. At the Bohr Institute in Copenhagen—where we did some of this work on machines that charged users for any job that ran longer than a minute—we managed to chain together many calculations in just under a minute and so got the entire calculation done without charge. I suspect that the facility managers knew what was going on, but turned a blind eye.

Fifteen years later, I led the development of Shell Model Monte Carlo methods, which was one of the more productive embarrassingly parallel calculations. In reflection, I have computed on machines all over the world, and my best work required large-scale computing. My experiences have shown me how high-performance computing can take a theoretical idea that was solvable in very simple cases and apply it to solve complex problems in the real world. This is why I believe high-performance computing will play a large role in addressing energy challenges, just as it has in nuclear security.

Thank you for taking the time to answer our questions.