Sandia workshop draws top theoretical thinkers in bid to improve understanding of materials behavior

Nobel laureate Walter Kohn, father of density functional theory, speaks at Labs-sponsored event

By Bill Murphy

In understanding the structure and properties of solids and molecules and their chemical reactivity at the most basic level, sometimes less is more and more is less.

That insight lies at the heart of quantum-level Density Functional Theory (DFT), for which Prof. Walter Kohn of UC/Santa Barbara shared the 1998 Nobel Prize in chemistry (see "Kohn's insight" below). Conventional calculation of the properties of solids and molecules is based on a simultaneous description of the collective behavior of all electrons in the molecule or unit cell of a solid. Such methods are mathematically very complicated and become intractable even for a modest number of atoms. Kohn showed that it is not necessary to consider the detailed collective behavior of all the electrons: it suffices to know the average number of electrons located at each point in space.

Now, DFT — which in many cases offers a practical research alternative to the proven, but often unwieldy, Schrödinger equation in describing the properties of materials — is assuming a key role in, for instance, developing better materials descriptions in computational-based modeling and simulation, an area in which Sandia has obvious and urgent interest.

Kohn, as the father and leading light of the field, was the honored guest and first speaker at a Sandia-sponsored workshop last week in Albuquerque to explore new avenues in DFT. Other speakers and presenters at the workshop constituted a who's who of the international DFT community. Sandian Ann Mattsson (1114), who did postdoctoral work with Kohn on DFT, organized the workshop and presented, with colleagues, two papers to the proceedings.

Sandia VP Al Romig, whose Physical and Chemical Sciences Center 1100 co-sponsored the workshop, noted that "something as focused and collegial as this [workshop] is really quite special; it's really a way to let us get at some fundamental problems we can grapple with . . . . It's a wonderful way to advance the state-of-the-art."

Al noted that to fulfill its mission, Sandia must invest substantially in a science and technology underpinning. DFT, he said, is a valuable — and likely to be an increasingly valuable — tool in helping the Labs advance the state of knowledge in areas of computationally enabled nanosystems, high-energy physics, and materials science. As such, he said, "We thought that getting people [of your expertise] together would provide us a real opportunity to get some cross-fertilization, to solve problems and discuss important issues in the field."

NOBEL LAUREATE WALTER KOHN and Ann Mattsson (1114), orgaganizer of a Sandia-sponored workshop on density functional theory, discuss Kohn's latest ideas on the subject for which he won the 1998 Nobel Prize in chemistry.

Solving real problems

Al offered a personal anecdote about his early experiences in modeling and simulation at Sandia in the early- to mid-1980s. Although his team succeeded in their efforts, Al says he would have loved to have DFT-based tools available at the time for the challenges he worked on.

"It's exciting," he said, "to see that the theory [DFT] has progressed to the point where it's being used to solve real problems."

Senior VP Tom Hunter — his division includes the Computer Science Research Institute (CSRI), the other cosponsor of the workshop — noted that the Labs has "an awesome responsibility" to certify the safety, security, and reliability of the nation's nuclear weapons. As such, he said, there is a profound sense of obligation for Sandia management to "invest in understanding at the fundamental level and the application level." That sense alone would justify the Labs' interest in further refinement and advancement of DFT. But the Labs' interest goes further: "We want to be leaders in the revolution in engineering," Tom said. And that means a heavy reliance on advanced modeling and simulation, and thus on tools — such as DFT — that make modeling and simulation more effective.

Tom cited a well-known quote variously attributed to Yogi Berra, Casey Stengel, Freeman Dyson, and even Niels Bohr: "Making predictions is hard — especially about the future." To emphasize the remaining challenge, Tom advanced the corollary, "Simulation is hard, especially when it is dealing with reality."

Tom offered a long list of issues for which more effective modeling and simulation would be indispensable:

"We worry about a lot of things. Like, how do things age? Materials and desiccants; chemical reactions and their influence on corrosion; response to adverse environments.

"We worry about radiation effects, all the way from global effects to single-point events in silicon in integrated circuits. And we worry about very small devices. Sandia's largest investment for the future is about small, smart things — and they don't always lend themselves to macroscopic understanding. So we have to worry about how small machines work, and particularly about how integrated systems work that combine optical systems, chemical sensors, processors, and tiny machines. We care about those things; and we intend to invest in [gaining an understanding of] those things."

At the core of all these concerns, Tom said, is an underpinning of quantum mechanics.

"So now," he said, "the challenge is to explore what knowledge we have and ask how it can open up new frontiers for us in better understanding materials and their interactions."

Kohn's insight

(Adapted from the official 1998 Nobel Prize press release announcing that Walter Kohn and John Pople would share the Chemistry prize for their related, but autonomous work in quantum chemistry.)

The laws of quantum mechanics as formulated more than 70 years ago make it theoretically possible to understand and calculate how electrons and atomic nuclei interact to build up matter in all its forms. The task of quantum chemistry is to exploit this knowledge to describe the molecular system. This has proved easier said than done. It was not until the beginning of the 1960s that development really started, when two events became decisive. One was the development of an entirely new theory for describing the spatial distribution of electrons. . . . **Walter Kohn** showed in 1964 that the total energy for a system described by the laws of quantum mechanics can be theoretically calculated if the electrons' spatial distribution (electron density) is known. The question is only how the energy depends on the density. Kohn gave important clues based on what this dependence looked like in an imaginary system with free electrons. It was to take several decades and contributions from many researchers, however, before the equation for determining the energy was sufficiently accurately mapped to permit large-scale studies of molecular systems. This has taken place partly through the adaptation of a small number of variables to experimental data. The method Kohn introduced came to be known as the density-functional theory. It is now used in studies of numerous chemical and material problem areas, from calculating the geometrical structure and properties of solids and molecules to mapping chemical reactions.

Sen. Bingaman views homeland security work

SEN. JEFF BINGAMAN, D-N.M., asks Ruth Boyd (12345) about details of the Weapon Recovery Decision Support System, a tool used by DOE's Accident Response Group. Bingaman visited the Labs' new International Programs Building earlier this month to receive briefings and demonstrations of Sandia-developed technologies with homeland security applications. During the visit, Bingaman discussed with local news media his views on the proposed Homeland Security Department and about the roles the national labs may play in counterterrorism efforts. (Photo by Randy Montoya)