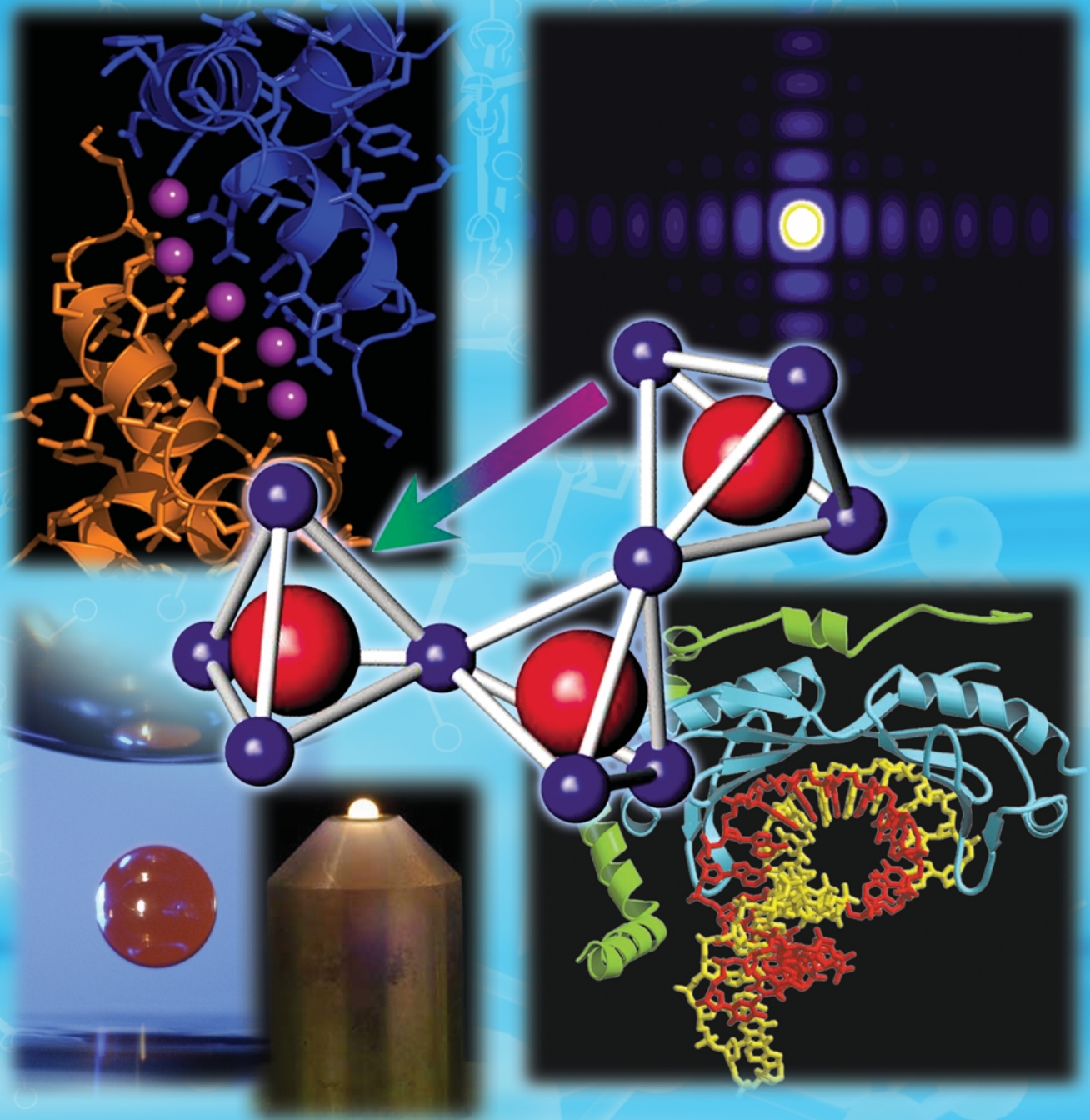


APS SCIENCE

The annual report of the
Advanced Photon Source at
Argonne National Laboratory

2003

May 2004 • ANL-04/07



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WELCOME

J. MURRAY GIBSON...

... is Associate Laboratory Director of Argonne National Laboratory and Director of the Advanced Photon Source.

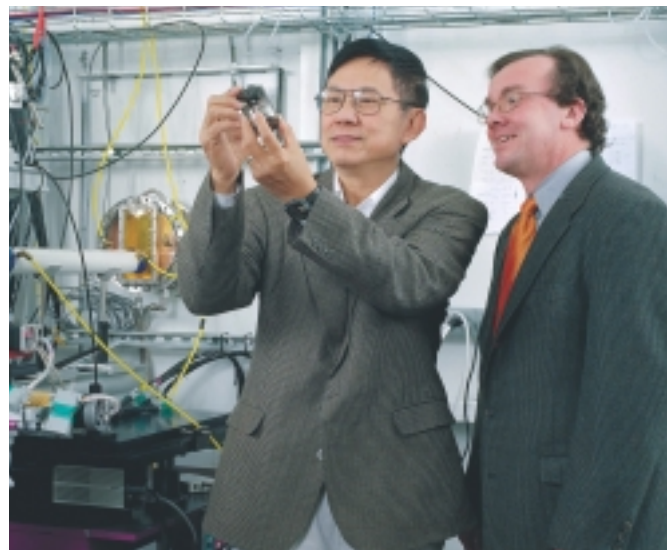
The year 2003 was a landmark for the Advanced Photon Source (APS). The number of users who did an APS experiment at least once in 2003 increased by 20% over 2002, to reach 2,747*. This made us, for the first time, the largest scientific user facility in the Western Hemisphere. And we're not done growing! Other metrics reflected the same trend; for example, the APS became the world's most prodigious depositor of structures into the Protein Data Bank. This annual report demonstrates the real product of our facility through a rich variety of scientific highlights in areas from soil science to condensed matter physics.

In 2003, we were reviewed by a committee, appointed by The University of Chicago and chaired by Yves Petroff, former Director of the European Synchrotron Radiation Facility. The review was very positive about the performance of the APS accelerator complex; the orbit stability was described as "state-of-the-art," and top-up mode as a "resounding success." We are also very proud of the level of availability and reliability, which we work very hard to attain—over 96% availability with over 42 h mean time between faults in calendar year 2003. It remains a significant challenge for us to sustain this level of performance in the years to come, as we deal with aging equipment and strive to make continuing performance improvements. Innovations in machine performance last year described in this report include implementation of real-time orbit feedback and the first light from hard x-ray canted undulator sources at sector 23.

It is exciting to see the many new beamlines being developed at the APS. Three new structural biology sectors are under construction—the General Medicine and Cancer Institutes Collaborative Access Team (CAT, sector 23), Northeastern CAT (24), and Life Sciences CAT (21). In the physical sciences, the Inelastic X-ray Scattering Collaborative Development Team (CDT, sector 30), the hard x-ray Nanoprobe-CDT (26), and a bending magnet powder diffraction beamline (11-BM) are all under development. The Nanoprobe beamline will be intimately coupled with the Center for Nanoscale Materials, which will sprout up at the south wall of the APS in the summer of 2004. The building was generously provided by the State of Illinois, and the equipment and operating budget will be funded by the Department of Energy (DOE).

In 2003 we submitted to the DOE Basic Energy Sciences Advisory Committee (BESAC) a four-phased plan for upgrades

*This was in part due to increases in the allocation of beam time on APS-operated sectors and to the increase in the number of beamlines accepting general users (22 vs. 25 insertion device beamlines and 8 vs. 10 bending magnet beamlines in 2002 and 2003, respectively).



David H. Mao (left, Director of the High Pressure Collaborative Access Team, or HP-CAT) showing a panoramic high-pressure diamond-anvil cell to Murray Gibson, inside the beamline 16-ID-D research station. The HP-CAT is one of the most recent APS sectors to pass through commissioning and into operations. The integrated high-pressure facility at HP-CAT is opening myriad new research frontiers in multidisciplinary physical sciences.

to the APS over the next 20 years, which would deliver over three orders of magnitude performance improvement to our users. The first two phases, constructing the remaining beamlines and tailoring insertion devices for the science of each sector, were strongly endorsed by BESAC. We are engaged in a study to identify "New Scientific Directions for the APS," sponsored by the APS Scientific Advisory Committee and co-chaired by Gopal Shenoy (Senior Scientific Advisor, Argonne National Laboratory) and Sunil Sinha (Professor, University of California, San Diego). The study has identified a number of key areas and will host workshops, culminating in a strategic planning meeting to be held August 29–September 1, 2004 (<http://www.dev.aps.anl.gov/News/Conferences/2004/apsspm/asfsd.htm>). From that meeting, we aim, among other things, to identify the strongest scientific proposals for the four uncommitted sectors.

The later phases of our upgrade plan include rebuilding the storage ring to reduce the emittance by an order of magnitude. The upgrade, more than 10 years from today, would deliver improved beam to existing ports and might allow our users to access fourth-generation capabilities. The new super storage ring, which we are calling APS², was listed in the long-term priorities for new facilities by the DOE Office of Science (http://www.er.doe.gov/Sub/Facilities_for_future/facilities_future.htm). Dennis Mills (Deputy Associate Laboratory Director for the APS) and Kwang-Je Kim (Senior Accelerator Physicist) are in charge of strategic planning for APS², and they will be

Cont'd. on page 6

REPORT FROM THE APS USERS ORGANIZATION—2003

STEPHEN M. DURBIN...

... (Chair, APS Users Organization) is Professor of Physics at Purdue University and a user with X-ray Operations and Research.

The highlight of the year was the Twelfth Users Meeting for the Advanced Photon Source on April 19-May 1, where nearly 500 APS users set a new attendance record. They were rewarded with an outstanding collection of scientific talks and workshops that ranged from imaging insect respiration to the latest in nanoscience and proteomics. Special presentations were given by Paul Doucette, chief aide to U.S. Representative Judy Biggert (R-IL13), who represents the Argonne area in Congress and is a leader in promoting funding for the Department of Energy (DOE) Office of Science, and by Susan Ginsberg of the American Physical Society, who provided a Capitol Hill-view of the merits of user outreach to their elected representatives. The meeting itself generated over 100 letters sent by users to their senators and representatives, and clearly motivated the APS user community to be more active in educating our federal government about the value of synchrotron science at the APS.

Washington outreach was a recurring theme for the Advanced Photon Source Users Organization (APSUO) in 2003. In April, a team of user-group chairs from the APS as well as from our sister DOE labs, the National Synchrotron Light Source, the Advanced Light Source, and the Stanford Synchrotron Radiation Laboratory, traveled to Washington, D.C., to expound on the importance of the DOE investment in synchrotron science. In addition to meetings at the Office of Science & Technology Policy that included an unscheduled session with its director, Dr. Jack Marburger, we met with officials from the Office of Management and Budget (OMB) as well as staff of the House Science Committee, the House Appropriations Committee, the Senate Committee on Energy and Natural Resources, and the Senate Appropriations Committee.

In the fall of 2003, the users of the APS submitted electronic letters to Congress and OMB: nearly 400 APSUO members generated over 1,000 letters to Washington, a total nearly ten times higher than from any other DOE user group! The APSUO has set a standard for Washington outreach that is the envy of our colleagues, and one that we should strive to surpass in 2004. The APSUO also initiated the first joint letter to Congress from the "Consortium of Science User Groups," consisting of the elected chairs of 15 different user organizations associated with DOE Office of Science facilities.

At the quarterly meetings throughout the year, the APSUO Steering Committee has been called upon to advise APS management on issues including the University of Chicago Review of the APS in September, the APS 20-year plan, the centralized General User Proposal system, the call for partner user pro-



Erin Miller (left), a student from the University of Washington, chats with Steve Durbin, APSUO Chair, in front of the Advanced Photon Source exhibit at the 2004 American Physical Society March Meeting.

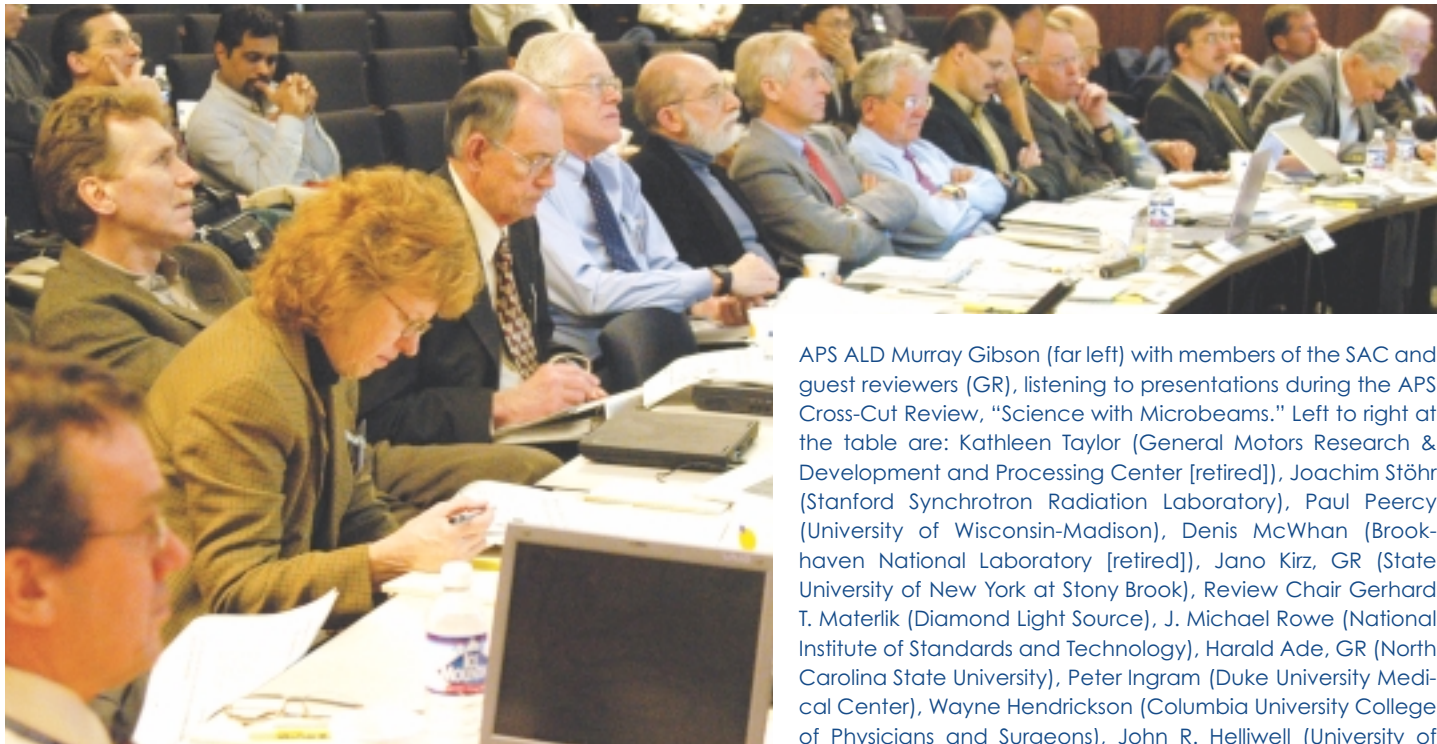
posals, non-resident user access issues, and the transfer of Office of Basic Energy Sciences (BES) sectors to APS operations support. A new policy was implemented to help keep the Steering Committee up to date on new developments among users. This was accomplished by inviting user group representatives to join the Committee for lunch and give short presentations. In the course of the year, all APS user groups have this opportunity to share issues and concerns with the Steering Committee.

Finally, the Steering Committee initiated a special workshop to focus attention on an area of importance to a large fraction of the users, the "Technical Workshop for Protein Crystallography CATs" held on January 13, 2004. Presentations were made by representatives from nearly all of the life-science CATs on three critical subjects: future developments in common user interfaces, implementation and development of robotics, and the future of telepresence. Consensus was achieved that telepresence in particular is an especially promising area in which to invest now, in order to achieve the highest level of productivity and standardization. These issues are being pursued further at workshops associated with the 2004 Users Meeting for the Advanced Photon Source, sponsored as always by the APSUO. ○

APS SCIENTIFIC ADVISORY COMMITTEE MEETING, JANUARY 20-22, 2004

J. MICHAEL ROWE...

... (Chair, APS Scientific Advisory Committee) is the Director of the Center for Neutron Research at the National Institute of Standards and Technology.



APS ALD Murray Gibson (far left) with members of the SAC and guest reviewers (GR), listening to presentations during the APS Cross-Cut Review, "Science with Microbeams." Left to right at the table are: Kathleen Taylor (General Motors Research & Development and Processing Center [retired]), Joachim Stöhr (Stanford Synchrotron Radiation Laboratory), Paul Peercy (University of Wisconsin-Madison), Denis McWhan (Brookhaven National Laboratory [retired]), Jano Kirz, GR (State University of New York at Stony Brook), Review Chair Gerhard T. Materlik (Diamond Light Source), J. Michael Rowe (National Institute of Standards and Technology), Harald Ade, GR (North Carolina State University), Peter Ingram (Duke University Medical Center), Wayne Hendrickson (Columbia University College of Physicians and Surgeons), John R. Helliwell (University of Manchester), Stephen Durbin, *ex officio* SAC member (Purdue University), Howard Birnbaum (University of Illinois at Urbana-Champaign [retired]), Paul Bertsch (Savannah River Ecological Laboratory), and William Bassett (Cornell University). A complete list of SAC members can be found in the appendices to this report.

The second meeting of the APS Scientific Advisory Committee (SAC) was held on January 20-22, 2003, at Argonne. Once again, the SAC spent much time on the reports of the sector review panels (SRPs) that met in 2003 to review APS sectors 8, 10, 14, 15, 17, 19, 20, and 22. The SRP membership included SAC members in every case, and in every case, a SAC member was chair. The chair of each SRP delivered an oral report in addition to the written reports, and the full committee discussed each report and formulated recommendations. We thank all of you for your cooperation in this process, which we understand is burdensome. However, it is a critical part of the never-ending assessment of the performance of the APS, which in turn is the key to continuing and increasing funding for operations. In addition, the SAC reviewed the responses to the prior round of sector reviews and developed additional requests for actions where appropriate.

Another task before the APS and the SAC is determination of optimal staffing levels for different sectors, and Gabrielle Long (Experimental Facilities Division) presented the results of her preliminary analysis of this problem. The SAC encourages the Partner User Council, the APS Users' Organization, and other interested parties to send us their thoughts, as this is a difficult area and additional input will be helpful. Finally, Partner User Proposals were reviewed, and recommendations given to the Director.

As a way of developing a broader view of the APS, the SAC has decided to perform cross-cutting reviews during its meetings. The first such review was a one-day review of microbeam capabilities and plans around the ring. This was a success in many ways, not only for the committee, but also for the APS staff and users (who were welcomed to the talks). It provided a snapshot of activities at a much broader scale than we normally can get from sector reviews, which is a necessary part of optimizing utilization of the country's brightest x-ray source. We intend to continue with these reviews and have tentatively agreed that the next such review will be centered on science that requires and exploits the time structure of the ring.

Among many other topics, the SAC also discussed metrics for industrial users, the "20-Year Plan for the APS," The University of Chicago review of the APS, and the Department of Energy roadmap for future facilities. In all, it was a very full meeting, and the committee ended exhausted but confident that the APS is doing great science. ○

THE APS PARTNER USER COUNCIL

P. JAMES VICCARO...

... (Chair, APS Partner User Council) is the Executive Director of the Consortium for Advanced Radiation Sources (CARS) at The University of Chicago and ChemMatCARS Principal Investigator.

The formation of the APS Partner User Council (PUC) was one of the last acts of the APS Research Directorate (RD), which had been the forum for discussion of management issues involving the APS and the collaborative access teams (CATs). In the last meeting of the RD and the first meeting of the PUC, the Chair, Jim Viccaro, was elected. His first act was to request that John Quintana, Director of DND-CAT, become the Deputy Chair. Quintana accepted, and the new forum was initiated.

From the outset, the PUC was not intended to be the Research Directorate with only a change in name. There are substantial differences in the way business is now conducted. The PUC is composed of a member representative from each APS sector; the representative is appointed by the partner user management responsible for the development and operation of the sector. These PUC members are non-APS employees; however the APS may also appoint *ex-officio* members, who may be APS employees at sectors not otherwise represented. Additional standing members of the Council include the chairs of the Technical Working Group (TWG), Reinhard Pahl (The University of Chicago/CARS) and Eric Dufresne (APS/MHATT/XOR); and a representative of the APSUO, Mark Rivers (The University of Chicago/CARS).

The PUC sets the agenda with input from the members and in consultation with APS management. The principal thrust of the meetings is to discuss issues related to current and future beamline operations, APS facility development, and APS/partner user relationships. The main objective is to provide advice and recommendations to the APS management. Towards this end, the Council may appoint *ad hoc* committees to focus on specific issues.

Three meetings were held in 2003, including the inaugural one. The meetings, which are preceded by an executive session, have been well attended with lively discussion. APS management has readily adopted the new format and been forthcoming and responsive to issues raised by Council members.

As a result of the change in operational paradigm, the partner users have quite a bit more responsibility as participants in APS committees related to operations and user issues. For example, John Quintana regularly attends the weekly APS Operations Meeting as the Council representative. The Council Chair is an *ex officio* member of the APS Scientific Advisory Committee (SAC), and the Council also has representation on



Jim Viccaro (third from right) with some of the advanced placement physics students from Riverside-Brookfield High School, in Illinois, who spent a day at the ChemMatCARS sector 15 beamlines in the APS experiment hall (see Murray Gibson's "Welcome"). ChemMatCARS and APS staff members guided the students through an intensive curriculum that ranged from basic scientific principles to the finer points of experimentation.

the SAC panels that review APS sectors. The PUC Chair and Deputy Chair also participate in setting the agenda for the monthly APS/User Operations Meetings.

In addition to these standing responsibilities, input on several issues has been requested by the APS. In some cases, the Council has formed *ad hoc* committees to meet the APS operations and CAT/partner user issues. In others, the requests have been forwarded to the TWG for discussion. In order to provide user input on current and future operational modes of the APS storage ring, a standing committee has been formed. Discussion is ongoing in an attempt to mitigate the apparently conflicting operational requirements of different user groups. Representation in this group will be expanded in 2004, and an impact statement to the APS is planned.

The Council has proven to be an effective forum for focusing on user concerns related to operations, etc. The initial Partner User Council forum to discuss user questions about a new insertion device front end developed by the APS helped clarify the relevant issues for both the user community and APS management. Subsequent mitigation by the APS was effective, and Council input was included during the process.

The year 2003 has been a learning experience for the user groups that participate in the Council. The new responsibility placed on the users to define and pursue to closure issues that are relevant to effective scientific productivity at the sectors is sometimes a daunting challenge. We look forward to an even more effective forum in 2004. ○

Cont'd. from page 2



Fig. 1. Participants in the fifth year of the highly successful National School on Neutron and X-ray Scattering (NSNXS). This year's NSNXS, whose Scientific Directors were Dean Haefner (XFD) and Raymond Osborn (MSD), welcomed 60 graduate students pursuing doctorate degrees at U.S. universities while majoring in physics, chemistry, materials science, or related fields. The school gives students tutorial lectures on scattering theory, neutron and synchrotron x-ray source characteristics, and scattering methods for condensed matter research; lectures by prominent scientists; and hands-on experiments at both the IPNS and APS.

organizing seminars, workshops, and feasibility studies over the next couple of years to narrow the design choices for this exciting upgrade.

The APS is a key partner in the major DOE project to construct the first x-ray laser (the fourth-generation x-ray facility) at the Stanford Linear Accelerator Center (see p. 160). We are also seeking external funding to develop our own fourth-generation free-electron laser into a source for vacuum ultraviolet radiation (see p. 159).

We have moved forward significantly in our efforts to support user sectors that were previously receiving operational support from the DOE Office of Basic Energy Sciences. Sectors 1, 2, 3, 4, 11, and 12 are now fully supported by the APS; sectors 7, 8, and 20 receive significant support; and sector 9 receives some support. Today we have 25 more beamline scientific staff within the X-ray Operations and Research (XOR) group than we had three years ago. We are delighted that Gabrielle Long has joined us as the Associate Division Director in the Experimental Facilities Division. She is responsible for all our beamline operations and research. Gabrielle will have the primary role of attracting outstanding new beamline staff as we expand in the future and of overseeing the evolution of focused, dedicated capabilities amongst our beamlines. The latter was identified by The University of Chicago review committee as the most significant challenge for APS to address in increasing the scientific impact of our users.

The APS Operations Division (AOD) has also increased support to users, in areas such as beamline controls and data acquisition, computer support, experimental safety review, and the detector pool. We were very pleased in 2003 to welcome Bill Ruzicka as Division Director for AOD. The University of Chicago review of the APS was very supportive of the changes we are making in XOR and AOD to maximize the scientific impact of users, and identified some areas where we could further leverage success, especially in the structural biology area.

Of course, the future of x-ray science is really in the hands of the next generation of x-ray scientists. The APS is committed to providing the opportunities and environment for young people who are interested in an up-close encounter with this excit-

ing field of research. The National School on Neutron and X-ray Scattering, organized each year by Argonne's (ANL's) Intense Pulsed Neutron Source (IPNS), the APS, and the ANL divisions of Materials Science and Education (Fig. 1); the program for advanced placement high school students hosted by the Chemistry and Materials beamlines of the Consortium for Advanced Radiation Sources Collaborative Access Team (ChemMatCARS-CAT) at APS sector 15; the group of undergraduate engineering students participating in a National Science Foundation Research Experience for Undergraduates program, who performed a series of synchrotron x-ray tomography experiments at GeoSoilEnviroCARS-CAT (GSECARS, APS sector 13) (Fig. 2); and the American Crystallographic Association Summer School in Crystallography, which brings students to the Industrial Macromolecular Crystallography Association (sector 17) and BiologyCARS-CAT (sector 14) beamlines, are a few examples of the community's commitment to science education.

I hope that you enjoy the information in this annual report. We at the APS are proud of the success of our users. Whether you are a present or prospective user, we hope that you will be a satisfied user in the future. The outlook for APS science is bright, although we face the challenge of securing the resources needed to achieve our vision. We are grateful to the DOE for its continuing support of our facility. ○



Fig. 2. Amy Grove, a senior Civil Engineering major at Cornell University, shown in the GSECARS 13-BM tomography station aligning a sediment/barrier core prior to collecting images of several sediment/reactive barrier systems. Her work is part of a pilot-scale study conducted at the University of New Hampshire and funded by the Cooperative Institute for Coastal and Estuarine Environmental Technology and the Hazardous Substance Research Center South/Southwest.



The APS facility occupies an 80-acre site on the Argonne National Laboratory campus, about 25 miles from downtown Chicago, Illinois.

For maps of the Argonne/Chicago area, see <http://www.aps.anl.gov/user/maps/maps.html>.

For directions to Argonne, see <http://www.anl.gov/OPA/anlil.html>.

ACCESS TO BEAM TIME AT THE APS

There are two ways to obtain beam time at the APS: as a general user (a researcher not associated with a particular beamline) or as a partner user, e.g., a member of a collaborative access team (CAT). If you are a CAT member, contact your CAT for instructions on applying for CAT beam time. All operating beamlines at the APS reserve at least 25% of their available beam time for general users.beam time.

How general users can apply for beam time at the APS:

- 1) New users should read the information for new users found on our Web site at http://www.aps.anl.gov/user/new_users.html before applying for beam time. Also, certain administrative requirements must be completed. In particular, a user agreement between the APS and each research-sponsoring institution must be in place.
- 2) To choose the appropriate beamlines, consult the APS techniques directory (http://beam.aps.anl.gov/pls/apsweb/bd_display_pkg.technique_dir). Detailed beamline specifications (<http://www.aps.anl.gov/aps/beamtime-nav.html>) are also available.
- 3) Submit a proposal via the Web-based system. Proposals are evaluated before each user run. For more information and the current proposal schedule, see the proposal system overview (http://www.aps.anl.gov/user/beamtime/prop_submission.html).