5. ENABLING TECHNICAL CAPABILITIES

The scientific performance of users depends on an appropriate source of x-rays, and, as importantly, on many enabling technical capabilities. Detectors, for example, are recognized as the "weak link" in many third-generation x-ray experiments. We propose to provide, either by acquisition or development, the best detectors available for the renewed beamlines. The other technical systems described in this section are equally important in leveraging the science of our users.

Strong technical support is the backbone of a vibrant, state-of-the-art science program at a user facility. This includes support for areas that are typically too large or complex for individual users and staff members to undertake by themselves. Items that fall under this category include detector development, precision positioning capabilities, beamline controls, scientific software, data analysis, and general information technology (IT support). In many cases these support areas are intimately coupled; for instance, framing-rate area detectors often drive the needs for high-performance computing, massive data storage, and higher speed connections among the experiment, storage, and high-performance computers. During the renewal, we intend to strengthen not only the hardware and software that enable high-impact experiments, but also work to strengthen the human capital in support of these systems (section 7).

5.1 DETECTORS

The science underlying the two overarching themes of the APS renewal will require advanced detectors that are efficient for energies up to 100 keV and are capable of high data throughput; large solid angle coverage for imaging, diffraction, and spectroscopy; high contrast; and improved spatial and energy resolution. No single detector can satisfy all of these requirements; the task at hand is then to define performance goals and to identify paths to achieve them, setting priorities in harmony with the science goals of the APS renewal.

The renewal is an outstanding opportunity, not to be missed, to provide state-of-the-art detectors to the users of APS. The detector strategy for the renewal is to acquire state-of-the-art detectors through commercial procurement, collaboration with various partners, and in-house development, and to deploy the detectors to the beamlines with appropriate software. We note that in-house development is crucial for nurturing a solid and long-lasting detector program at the APS and for establishing external collaborations. A reasonable portfolio for in-house effort includes developing sensors for very high energies (E > 40 keV), picosecond electronics and detectors, and novel superconducting sensors.

COMMERCIAL DETECTORS

As with most new light sources, a significant fraction of the detector needs at APS beamlines in the next 2-5 years can be satisfied by purchasing commercial off-the-shelf equipment or by contracting with companies for the fabrication of custom detectors. Most of the commercial detectors to be procured are fast, large-area detectors, either amorphous silicon (a-Si) flat panels for E > 40 keV or Pilatus silicon pixel array detectors (PAD) for lower energies. Additional commercial detectors that are planned include charge-coupled device (CCD) cameras with varied specifications, silicon strip detectors, and assorted single-element photon counting detectors. There is also a strong science case for custom-designed energy dispersive silicon drift detector (SDD) arrays; these custom detectors, with a modest number of elements, can be purchased from commercial suppliers. For reference, table 5.1.1 shows the approximate number of commercial detectors requested by APS beamline advisory committees. (This does not reflect a detailed proposed list but is given as an indication of user needs).

Table 5.1.1. Detector types requested from beamlines

Detector type	Requests from beamlines
Si PAD (e.g. Pilatus, various sizes)	12-14
a-Si flat panel	12-14
CCD (varied specs)	8
Fluorescence SDD arrays	6
Si strip, single SDD, etc.	15

DETECTOR DEVELOPMENT

Expanded support for a strong detector development program must be an integral part of the APS renewal project. Some of the most challenging science being proposed requires novel detectors. A robust detector development program will include several avenues for collaboration, as well as in-house development.

The APS renewal vision has identified two overarching driving themes: *mastering hierarchical structures through x-ray imaging* and *real materials in real conditions and real time*. In the near future (3-7 years), detector technologies that can be implemented to support these themes include fast-framing area detectors (both photon counting and integrating), large solid angle spectroscopy detectors, and sensors efficient for "very hard x-rays" (E ~ 40-100 keV). Further in the future, improvements in energy and time resolution may be achieved with superconducting sensors and picosecond electronics.

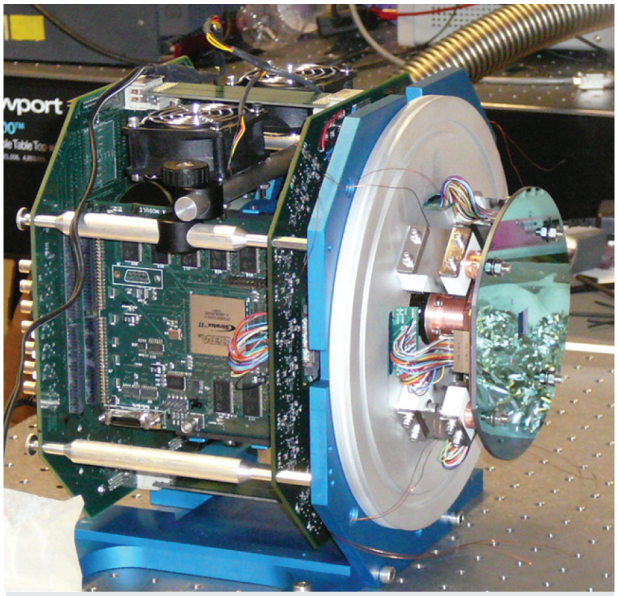

Fig. 5.1.1. *Prototype quasi-column parallel CCD detector for XPCS, developed by the APS Beamline Technical Support Group in collaboration with the Advanced Light Source (LBNL). This novel CCD detector can operate at 200 fps with full resolution.*

Area detectors capable of fast frames rates (100-1000 fps) with moderate pixel sizes (~ 50-100 μm) and large number of pixels (~ 2 k by 2 k) will be very effective for time-resolved diffraction, fast radiography, and time-resolved MX. For diffuse scattering applications (e.g., SAXS), single photon counting can be achieved, while radiography and MX need integrating pixel detectors due to the large instantaneous flux involved. Area detectors with smaller pixels (< 30 μm) and high frame rates, for example, parallel readout CCD cameras, will be appropriate for soft matter studies using XPCS and can also be used for time-resolved scattering. Avalanche photodiode (APD) arrays capable of nanosecond-time resolution are required for nuclear resonant scattering. These various types of area detectors can be developed through collaborating with other national laboratories, e.g., Lawrence Berkeley National Laboratory (LBNL) (fig. 5.1.1), Brookhaven National Laboratory (BNL), and Fermi National Accelerator Laboratory (FNAL), and universities such as Cornell (Vernon 2007); contracting industrial partners such as ADSC, Dectris, Voxtel, and RMD; or joining international collaborations with other facilities, such as SPring8 and ESRF, and the DESY collaboration on APD arrays. We also expect to benefit from the Linac Coherent Light Source (LCLS) development projects (Haller et al. 2007).

Spectroscopy detectors with large solid angle coverage, i.e., hundreds of detector elements, will allow for fluorescence microscopy imaging with greatly increased elemental sensitivity. A modular detector that can be easily configured into custom geometries for different sample environments can have many applications, for example, in condensed matter physics and environmental science. A possible path to large solid-angle spectroscopy arrays is to pursue energy-resolving pixel array detectors, evolved from the existing BNL spectroscopic PAD (Siddons et al. 2006); another avenue is to build SDD arrays. In all cases, these detectors can be developed in collaborations or through contracts with industrial partners. Developing better sensors for efficient detection of high-energy x-rays ($E > 40$ keV) will enable studies of real materials in real environments. These sensors could be used in pixelated area detectors and would be beneficial for diffraction and imaging studies at high energies, with applications in engineering and applied research. Development in this area would be pursued with industry, for example, in the case of cadmium-zinc-telluride sensors, and with other national laboratories (LBNL, BNL) in the case of germanium. Collaborations on structured scintillators with Risø (Olsen et al. 2008), for example, can be a path to high energy detection with good spatial resolution.

Picosecond electronics and detectors provide a complementary approach to the scientific challenges addressed by picosecond x-ray sources. We plan to expand work at the APS on streak cameras, on fast photodiodes, and on x-ray photo cathodes coupled to fast-readout multichannel plates, some of which have been seeded by Argonne Laboratory Directed R&D (LDRD) funds.

Superconducting sensors for very high energy resolution can be of several types [superconducting tunnel junctions, transition edge sensors, and kinetic inductance detectors (Mazin et al. 2006)] and are capable of a resolution of ≤ 10 eV at 6 keV. This energy resolution allows for increased element sensitivity in fluorescence measurements and makes spin-dependent XAFS possible, with application to environmental, biological, and materials science. Because high-resolution superconducting detectors are inherently slow, they must be arrayed to achieve the count-rate capabilities required for use on synchrotron radiation sources. We will pursue such development in collaboration with the Argonne Materials Science Division and Center of Nanoscale Materials (CNM), and with collaborators at the National Institute of Standards and Technology (NIST) and University of California at Santa Barbara.

The APS renewal project also must include the implementation of detector development infrastructure (test facilities, simulation software, etc.) necessary to carry out the planned detector program. Access to beamlines to evaluate, debug, and calibrate detectors is difficult to obtain given the user demand for beamtime at the APS. We plan to mitigate this access problem by partnering with the optics group in their proposed development of a bend magnet beamline for at-wavelength metrology. (See section 6.3 for more details on the proposed metrology beamline.) Another fundamental component of our development plan is access to application specific integrated circuit (ASIC) technologies. Basic detector physics implies that faster, lower noise (from lower input capacitance) detectors must be realized at the integrated circuit level. We have recently strengthened our ASIC design capabilities by establishing a formal collaboration with the FNAL ASIC Design Group.

5.2 NANOPOSITIONING

Two areas of nanopositioning development are needed in support of the key APS renewal science drivers. In short, these areas are *more* and *better*. More positioning systems are needed to enable more users to employ optics with 100- to 30-nm spatial resolution. Better positioning systems need to be developed to keep the APS at the forefront of hard x-ray microscopy and imaging by enabling users to exploit the next generation of x-ray optics with 30- to sub-10-nm spatial resolution. A new paradigm in the design of x-ray nanopositioning systems is required. The domains of mechanics, sensing, actuation, controls, and environment must be considered as a coupled systems problem.

NEW POSITIONING SYSTEMS

Expanded engineering developments are necessary to underwrite the proposed APS renewal capabilities, especially to support the nanoprobe and nanoimaging applications. While the APS with its partner the Argonne CNM is currently a leader in hard x-ray nanofocusing and nanoimaging, additional engineering infrastructure is required to meet these needs, regardless of whether new instruments are designed and built in-house or conceptualized in-house and contractor built.

The demands on the positioning system are reduced when the operational environment is quiet. Passive isolation is insufficient to ensure sub-10-nm performance. New instruments will require active isolation to minimize the environmental disturbances. Active isolation systems create the quietest conditions for nanopositioning devices and have high stiffness and low drift. These characteristics are needed to maintain position relative to the x-ray beam.

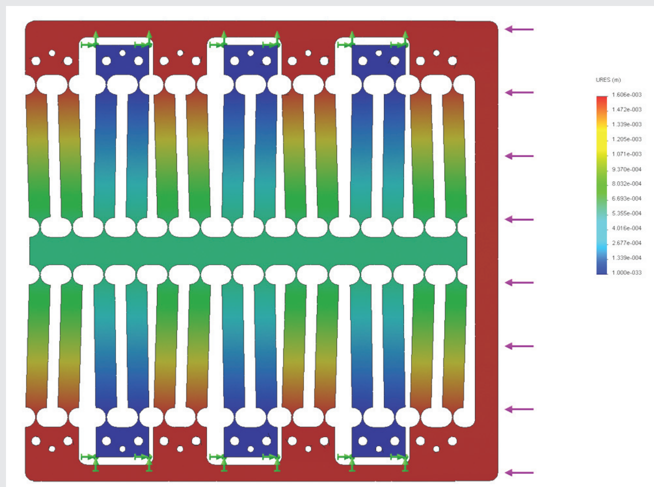

Fig. 5.2.1. *A finite element analysis result for displacement of the multiple parallelogram weak-link structure. Sub-nanometer positioning resolution could be achieved within a sub-centimeter level travel range.*

We will set up test facilities in the APS experimental hall associated with the proposed bending magnet optics metrology beamline to 1) evaluate dynamic performance of nanopositioning instruments to be used in the APS beamlines with the same floor vibration environment, 2) characterize instrument supporting structure vibration response to the APS floor environment, and 3) carry out R&D programs to develop new passive and active vibration isolation and damping mechanisms.

LINEAR WEAK-LINK STAGES WITH LARGE TRAVEL RANGE

X-ray scanning microscope scientists always dream of having a compact single stage to cover large travel range with very high positioning resolution and stability. Drawing upon a fishbone-shaped laminar weak-link structure design (Shu et al. 2009), we are exploring the feasibility of building a weak-link-based precision linear guiding system with sub-nanometer resolution and sub-centimeter travel range in a reasonably compact size. (See fig. 5.2.1.) Based on this novel design, a test bed will be built to support the APS renewal project. The test bed includes a 3-D high-resolution, high-stiffness nanopositioning system with six laser interferometric encoders with 30-pm spatial resolution. A sub-nanometer closed-loop resolution is expected for this 3-D flexure nanopositioning system with a 3 mm x 3 mm x 3 mm travel range.

NANOPOSITIONING WITH CRYOGENIC SAMPLE CONDITIONS

Samples preserved at cryogenic temperatures are substantially more resistant to radiation damage than at room temperature. For the proposed bionanoprobe, and the CNM nanoprobe, a nanopositioning system must be compatible with cryogenic sample conditions and robotic sample exchange (Maser et al. 2006). To complete this challenging task, a nanopositioning test bed for cryogenic sample conditions will be employed.

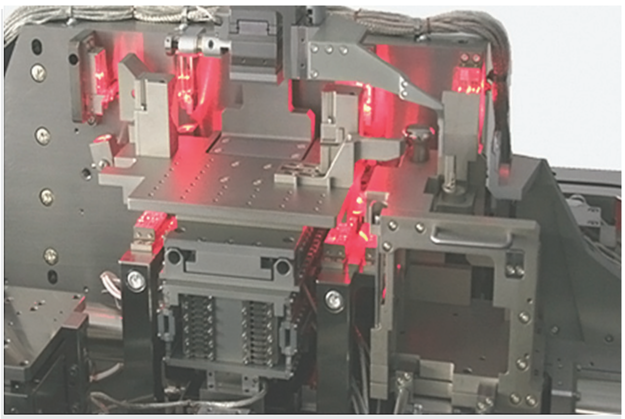

Fig. 5.2.2. *A photograph of the x-ray nanoprobe scanning stage system using seven laser interferometric encoders for nanometer-scale closed-loop resolution. Developed by Argonne, and manufactured by Xradia, Inc.*

Figure 5.2.2 shows a photograph of the CNM x-ray nanoprobe (APS designed and Xradia, Inc., manufactured) at APS/CNM sector 26. The ultimate performance of nanopositioning systems is limited by the ability of the control system to account for the system dynamics, environmental disturbances, sensor noise, and actuator authority. The bandwidth of the system is limited not only by control hardware, but also by the dynamics of the whole system. This holistic approach to x-ray nanopositioning designs will leverage advancements in fields such as scanning probe microscopy where CNM has excellent experience. An accurate model of the mechanism dynamics will be included in the control algorithm. Feed forward control will increase the operational bandwidth, while robust control techniques will balance resolution with environmental and sensor noise rejection. We propose applying these techniques first to a design based upon current positioning mechanics to meet the *more* need—that is, additional robust 30-nm resolution instruments. Then, the same techniques can be combined with the proposed new long-travel flexure systems to meet the *better* need—that is, systems with sub-10-nm resolution.

5.3 COMPUTING AND SOFTWARE

The summary report of the 2006 APS User Workshop on Scientific Software states, "New software analysis tools must be developed to take full advantage of these capabilities. It is critical that the APS take the lead in software development and the implementation of theory to software to ensure the continued success of this facility." Strong coupling is required between teams that implement scientific ideas in software and teams that establish and maintain the computing infrastructure.

DATA ANALYSIS SOFTWARE

Developments in software capabilities will play a key role in realizing the two overarching scientific themes: *mastering hierarchical structures through x-ray imaging* and understanding *real materials in real conditions in real time*. Clearly stated in one of the science cases (APS 2009), "Software is the key to widening the experimental community and is a ***deciding factor in facility productivity***."

Software development is a collaborative process, and our goal is to *enable partnerships*. Our partnerships across the APS user community and beyond will continue to evolve with our science objectives. The Argonne Mathematics and Computer Science Division is ready to help us with key technologies for exploiting IT-secure high-performance computing technologies and data visualization. Other facilities have been partnering with APS for years on the development and maintenance of the experimental physics and industrial control system (EPICS), especially through components that support beamline science. Our collaborations also engage similar groups at other x-ray and neutron sources. Further, we must remain aware of and involved with international standardization efforts such as NeXus (data storage) and DANSE (data analysis).

For the APS to take a more concerted and focused approach to the development of real-time analysis and data visualization software, we must enrich the suite of software tools. The goal is that users can input changes to their experiments based on real-time feedback from the data visualization, modeling, and visualization (fig. 5.3.1).

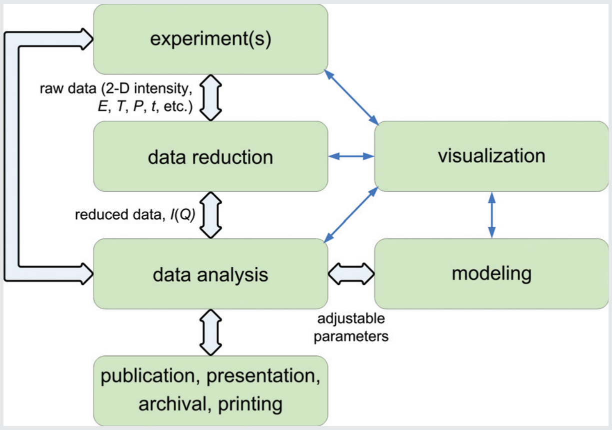

Fig. 5.3.1. *Scientific work flow diagram*

To illustrate, the experimental techniques of x-ray tomography and XPCS differ in their experimental protocols, yet both techniques share the need for high-performance computing (HPC) to reduce the experimental data in real time and provide indications about the outcome of the data just collected and feedback on how best to proceed. Once the experimental data are reduced, 3D x-ray diffraction (3DXRD) microscopy also requires HPC resources to visualize and render the 3D structures. Application of HPC resources to scientific investigations such as these requires specialized expertise that is beyond the scope and capability of an individual user or even group of users, yet common to many APS instruments. During the renewal, we intend to develop staff expertise that is ready to apply HPC and visualization to user's scientific investigations.

Increasingly, the APS will rely on remote (i.e., off-site) collaboration for routine data analyses and, in some cases, even experiments. Often automation is required to reach real-time scientific goals or for mastering one's understanding of the data. Strong, standardized information security protocols must underpin the software to enable remote access by our user community.

To realize the proposed science objectives of the renewal, we plan to expand in concert significantly the number of APS staff supporting the software and controls at each APS beamline. The software staff should work at the beamline *with* beamline staff as *application specialists*, where they will be able to identify and execute the specific software needs of the science program, whether that involves hardware-specific controls such as advanced detectors, application-specific user interfaces, or even implementation of high-performance computing technologies. Furthermore, we need to build and support the user interface software that joins controls together with data analysis and visualization.

During the renewal, APS will develop a central group, separate from the beamline support noted above, to coordinate the scientific software for data reduction, analysis, modeling, and simulation used throughout the APS user community. Only by integrating that software with beamline data acquisition will the APS be able to fully support the theme of *real materials in real conditions in real time*. The Scientific Software Group will rely on high-speed data networks, abundant data storage, and a fast computation server, all of which must be able to provide service to both on-site and off-site users.

COMPUTING INFRASTRUCTURE

High-quality information technology resources and infrastructure, along with experienced, well-qualified personnel, are essential to the success of the APS. Information technology is our prime communication device internally and externally, our most widely used research tool, an essential resource for our programs, and an indispensable tool for administration. Our ability to accomplish our mission as a Laboratory and our ability to attract and retain the best employees are increasingly dependent on our information technology assets. Thus, it is critical that we provide well-coordinated, high-quality, cost-effective information technology services to all APS users.

The march of technology: Detector technology increases in resolution and acquisition rates every year. Most important, APS is committed to pursuing leading-edge science, and APS scientists are constantly pushing the envelope of available and upcoming technologies. This environment creates a huge challenge for APS IT Support to keep the APS technological infrastructure for data transmission, security, and storage up to date and able to meet the ever-changing needs of beamline users. We must respond to that challenge with innovative computer hardware, expertise in interfacing, and responsive support.

Future growth of APS beamlines: After the renewal is complete we will have ~10 to 12 additional operating beamlines (through build-out of the remaining sectors and canting of IDs in existing sectors) that will require additional support from APS IT. Cyber security is a growing challenge for all user facilities, and we will work to support this need while opening as efficiently as possible a gateway for legitimate data flow.

New servers will be needed to support new and upgraded beamlines. High-data-rate sectors will necessitate local storage systems for spooling real-time data. A data storage capacity of the order of petabytes will be required. Both high data-rate detectors and HPC demand large volumes of resident storage, but the additional needs of backup and archive of scientific data are significant. Remote collaboration and use of national HPC resources demand that such storage capacity is available to members of the APS user community whether they are on the APS campus or off-site.

5.4 LABORATORY FACILITIES

To make the best use of the new and refurbished beamlines that will result from completion of the renewal project, supporting facilities must be adequate. Perhaps most obvious is the need to provide ample laboratory and office space for scientific staff and visiting users. Not as visible to most, but just as vital is the need for sufficient space for other infrastructure components. We have identified the need for increased space for the data center and for more space for on-site early assembly and staging of components.

Fig. 5.4.1. Exterior of a lab-office module

LABORATORY AND OFFICE SPACE

The majority of beamline staff are housed in eight laboratory office modules (LOMs – see fig. 5.4.1) that are located on the outer side of the storage ring hall. As the name suggests, these modules provide laboratories and office space for scientific staff. The laboratories are essential for staff and users; they are used to prepare samples and beamline equipment for experiments.

The space currently available is barely sufficient for the current number of beamlines, staff, and users. The introduction of new beamlines and higher staffing levels at beamlines make it important to plan for provision of adequate accommodations. One of the existing LOMs (437) is currently only a building shell. We would like to build out the interior of LOM 437, providing 8,000 ft^2 of office and laboratory space, similar to that found in the other LOMs. Extending out at least one, preferably two (resources permitting), other existing LOM(s) will be needed to accommodate the anticipated increase in beamline staff population. Each extended LOM will provide an additional 8,000-14,000 ft^2 of space.

DATA CENTER

The current APS data center was designed over fifteen years ago. It has served well over the life of the facility, but the ever-increasing demands for computing capacity mean that it is ever more cramped. The vastly increased power density of today's servers and other computing equipment also makes it increasingly difficult to provide sufficient power and cooling for the data center. Today's data center design requirements are much different from those of 15 years ago. We include expansion of the data center to approximately double the size of the existing facility. It would be refurbished to modern standards and have sufficient power and cooling capability for anticipated future needs.

ASSEMBLY AND STAGING AREA

It is our plan to implement the accelerator, front-end, and insertion device enhancements within our present operations schedule. This means that tunnel installations will have to be all done in the three 3-week access periods each year. To accomplish this, an assembly and staging area must be available in close proximity to the facility to assemble, test, and partially commission the systems before installation in the tunnel. Up until now, the unoccupied sectors of the experiment hall (those sectors not yet containing beamlines) have served that purpose and, in fact, proved very useful to the everyday functioning of the APS. This area has been used for early assembly of large components and for storage of spare parts that need to be stored close to the accelerator for rapid access. Over the past few years, as we have built out the remaining sectors, we have been able to relocate spare parts stored in those sectors in the LOM 437 building shell. However, as the remaining unoccupied sectors and LOM 437 are being developed, this space will no longer be available for storage. Hence, we have a need for a general purpose facility that will be used for early assembly and staging during the renewal project and can later be repurposed as a “high bay” storage area to make up for the loss of space from the experiment hall.

IMAGING INSTITUTE

The APS is involved in negotiations with the State of Illinois for funding of what is known as the “Imaging Institute.” In concept, this building would be two stories high and modeled on the footprint of the main APS office building (401). It would have a floor area in the region of 85,000 ft^2. The ground floor would house clean rooms dedicated to optics and detector research and would accommodate the end stations of the proposed long beamlines. The second floor would be outfitted with offices that could house up to 50 people. No DOE funding is sought for this building, but it may liberate pressure on the expansion needs for LOMs. This Institute is not in the scope of the proposed renewal project however ANL has approached the State of Illinois seeking it as matching support similar to the successful partnering in the CNM project.

UTILITIES

We expect that a modest increased capacity will be needed in the APS utility infrastructure system. Initial estimates are modest, but as part of the process in preparing conceptual design reports, we will evaluate in more detail to determine if expansions are required in systems for power demand, chilled water, compressed air, nitrogen storage, etc.