Intra-Laboratory Memo

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APS Renewal: Scientific Software in Five Years

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Each experiment performed at the APS requires three crucial ingredients: the powerful x-ray source, an optimized instrument to perform measurements, and computer software to acquire, visualize, and analyze the experimental observations. It is this combination that transforms a set of instruments into a research facility. Software underpins all aspects of the scientific output of the APS from data acquisition and reduction to real-time analysis, data visualization, modeling, and simulation software. As scientists attack problems of increasing sophistication and deal with larger and more complex data sets, the role of software expands. Demand for excellent and flexible scientific software can only be expected to increase as the upgrade of the APS facility and the implementation of advanced detectors and computational facilities create a host of new measurement capabilities. By taking a leading role in the development and maintenance of open-source software for the entire process of X-ray data analysis, and by partnering with APS users, scientists, and developers at universities, national laboratories, and other scientific facilities throughout the world, the APS has a unique opportunity to improve the state of the art of X-ray science.

High-performance computing capabilities, including computing clusters, high-speed/high-capacity file servers, and network access, are being delivered now to a few beam lines within XOR, providing dedicated access to real-time data processing and analysis. In the case of X-ray Photon Correlation Spectroscopy, access to HPC capabilities allows the instrument to exploit the 60 frame/second data acquisition on a continuous basis and provides real advancement in the XPCS facility. HPC advances the high throughput capability for X-ray tomography, providing APS users with both local and remote access to perform data reduction and analysis. New high frame-rate detectors for X-ray microdiffraction will rely on routine access to HPC resources as part of the routine data collection in addition to post-experiment support of users. Infrastructure is designed to support the expansion of HPC capabilities to other sectors as needs arise.

Data visualization tools are fundamental to the success of research investigations as they connect scientific data directly with scientific intuition. A finding from the 2006 XSD Scientific Software Workshop (ANL-APS-TB51) is emphasized as the APS assumes operating responsibility for a majority of the sectors that a facility-supported common tool set for viewing 1-D, 2-D, 3-D, and higher dimensional data is in strong demand.

APS users will rely on common software to support the flow of scientific data from experiment to HPC, data visualization, and through analysis. Upgrades in the small-angle facilities at sector 12, concentrating several SAXS instruments in one location, include the development of a common software tool set integrating data acquisition, reduction, analysis, visualization, modeling, and simulation. This tool set is expected to become the basis for a standard suite used at all APS small-angle instruments. Continued contributions to this tool suite are expected from the APS user community.

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APS Renewal: Beamline Controls Software in Five Years

Beamline controls software is vital to the efficient, flexible, and easy to use operation of all APS beamlines. This software is used to control the beamline optics, sample positioning, and detectors. The APS has standardized on EPICS as the underlying architecture for beamline controls on all facility beamlines, and most CAT beamlines. The choice of EPICS allows collaboration with the accelerator controls group, and indeed with many other groups around the world. That being said, improving the extent of interaction between the accelerator controls group and the beamline controls group should be a goal for the next five years. There are currently tools that could be better shared, and more importantly the development of new and better tools in the future should be coordinated with all of the controls personnel at the APS.

Some of the areas that should be targeted for improvement and development in the next 5 years are:

1) Development of higher level tools for managing IOCs. There are few common tools used by beamlines for managing EPICS devices on beamlines, such as motors, detectors, etc. Tools that make it easy to add new devices, including save/restore, change device configurations, etc. would be very helpful.
2) Better tools for logging and diagnostics. Too often when intermittent problems arise one finds that there is no useful data being logged, making the problems hard to diagnose.
3) Better tools for realtime display of data as it is being collected. The tools that exist are getting old and are no longer well supported. Modern tools are needed for this important task.
4) Continue the transition away from VME/vxWorks IOCs to IOCs running on higher-powered and more modern computer systems (e.g. Linux, Windows, RTEMs) where appropriate. Improve, standardize and deploy the tools to manage such soft IOCs, including logging, remote access, automatic startup, etc.
5) Develop more specialized data acquisition programs, and standardize them around the APS. There should probably only be one program for EXAFS data collection, one program for tomography, one program for diffractometer control, etc. It is a waste of resources for multiple applications to continue to be developed and supported for these relatively standard applications. The programs must have the flexibility to allow for the new types of experiments that will be done in the future.
6) Develop the infrastructure and a framework for high-performance data acquisition. Modern detectors and smart controllers are capable of rapid on-the-fly data collection. However, these capabilities are often not being appropriately used because there is no easy mechanism to incorporate them into the existing data acquisition and control systems.
7) Coordinate the beamline controls and data acquisition software with data reduction and analysis software to facilitate the real-time feedback into experiments.

Projected status concerning x-ray detectors at the APS, 5 years out.

Written by Steve Ross ANL/APS/XSD/BTSG/skross@anl.gov, per instructions from Denny Mills, July 29, 2008.

This memo assumes people have access to a similar memo, March 14, 2008 Strengthening x-ray detector development and support efforts at the APS, from P. Fernandez given as input to APS Medium Term Proposal). That memo discusses more the "how to get there" aspects – strengthening APS detector development effort, expansion of detector test and modeling capabilities, expected user community, enabling technology and infrastructure. REF: http://www.aps.anl.gov/Renewal/Proposals/BTS_medium_term.pdf

This memo addresses the question of "Where could the APS be in x-ray detectors in five years?" and is thus more of a forecast of what detectors will be like in general in 5 years. For convenience I give [electronic response times] of the detector families.

These are simply my opinions.

In the past 5 years, we have seen:

- Successful commercialization of pixel array detectors (PAD's) from light sources such as Pilatus from SLS. [250 ns]
- Greater synchrotron use of detectors developed for medical imaging (amorphous silicon flat panels). [0.1 to 0.03 sec]
- Modest commercial expansion in the capabilities of energy dispersive detectors. For example companies that make silicon drift diodes now are a bit more flexible in what they offer, trying to produce modest arrays. [1us]
- The pushing to the limits of performance the venerable charge coupled device (CCD), with near column parallel readout and direct detection. [0.01 sec]
- At least at the APS, very modest use of application specific, customized detectors, such as strip detectors for arrays of energy dispersive elements, or counting. [microseconds]

One can make some predictions for 5 years from now (no particular order here….):

- Large format **CCD cameras** [1 sec] will continue in use, and will be sold almost entirely by commercial companies.
    - o Their size will not grow much past 30-40 cm active area linear dimension; past that point their maintenance cost becomes high. Such things will cost approximately $1M.
    - o Companies will seek to commercialize national lab progress in column parallel readout cameras, and in 5 years we might see 10 cm x 10 cm size 100 fps, direct detection cameras, for $1M.
- **CCD development** [0.1sec to 0.1ms] will focus on niche markets – small formats, customized pixel sizes, fast readout, and direct detection. Today it is not possible to buy a CCD, or a CCD camera with specifications, say, of pixel size 23 um x 180 um, array of 16 x 54, direct detection, frame rates of 300 frames per second. In 5 years

this arbitrary example CCD will like be more available “on-demand”. A CCD wafer run costs about $200K, and if enough small jobs join together, a variety can be made on a 4” or 6” silicon wafer. Such wafer runs will be paid for by coordinating multiple synchrotron’s needs and funds.

- Similarly **photodiode arrays** [1ms – 0.1 us] will be more custom format. In this case a 4” wafer run costs about $30K, again opening things up for many custom jobs. Photodiode arrays will generally be faster frame rate than CCD arrays, essentially just a fact of physics. However they will require application specific integrated circuits as readout, they cost $20K - $50K now. An example “funny” shaped array might be an array with a hole in the center for the beam to pass thru. We might see some use of germanium, or of high resistivity silicon used in a CMOS-like process.
- **Silicon drift diode** [1 us] arrays will start to appear quasi-commercially. Perhaps we see an 8 x 8 array of 300 um size diodes, each with 250 eV energy resolutions in a few microseconds. It seems that arrays larger than this may suffer from yield problems, but if people can live with this, then array size can grow much more. Why not a 100 x 100 SDD array, where 90% of them function? The cost will drop to the range of <$1K per channel, with pro-rated economies of scale.
- Improvements will be made to **PAD detectors**. [1us to 1ns] They will become the dominant detector architecture for high end applications.
  - They will become faster (dropping from 200 ns/ sample to perhaps 10 ns/sample. Their readout time will fall by a factor of 5 – 10 (from several milliseconds to several hundred microseconds).
  - There will be increased circuitry or logic under each pixel, perhaps by use of so-called 3-D CMOS, essentially layers of planar CMOS stacked, currently the stack height is 3.
  - There will be more complex counters, some polling of adjacent pixels to try to account for split-pixel events, some forms of MCA (energy resolving, multi-channel analyzer) functionality pixel-by-pixel.
  - There will be variations of analog and digital storage of information inside the PAD. The circuits are so similar at times that words fail to distinguish.
  - Larger arrays will be made mostly by silicon-on-insulator processes.
  - It is interesting to note that a complete, small PAD array, say 32 x 32, 1 mm area, might cost about $130K for a prototype development today. Again one can forecast the coming of niche chips.
  - It is also interesting to note that ASIC amplifiers have noise 10-100 times lower than printed circuit board based ones – lower capacitance, better packing, the future belongs to the IC.
  - PAD arrays will be tried with “time slicing” protein crystallography – no shutter, fast motor rotation. Crystallographers will also be brought on board by expanded digital logic / pixel.
- **Avalanche Photodiode Arrays** [50 ns to 500 ps]
  - An ESRF, DESY development of arrays for timing applications will become available. An emphasis here is on in-elastic scattering applications, measuring the time duration between x-rays.
  - There can be avalanche photo diode arrays responding in the100-500 ps range.
- **Picosecond level detectors** [500 ps to 5 ps] will start to appear in research format.

    - It is straight forward to see a path to 500-100 ps count times, and it is conceivable to see 10 ps count times.
    - Propagation delay thru a logic gate, 0.11 um, (110 nm) feature size is 25 ps [Ref: foundry], and this number scales linearly with feature size reduction. Hence 45 nm features, about 12 ps delay.
    - There will be niche applications of fast response photoconductors, perhaps modified by neutron damage, or by insertion of spoiler dopants such as gold.
    - There will intense interaction in this area with other technology areas, for example microwave engineering. We will see a shortage of microwave engineers.
    - There will be research into <10ps count times by groups that can work directly with modern foundries.
    - There will continue to be research in ballistic (no scattering by carriers) transport inside nano-sized devices. These can be ps-fast.
    - There will be growing connection with nano-technologies in general.
- **Amorphous silicon** array [0.1 sec to 0.01 sec] performance will improve very modestly or perhaps not at all.
    - The charge trapping, image lag issue is inherent in the material. Perhaps there will be some push for direct detection. On the other hand, they will be more commercially available, and thus exist, and serve needs on beamlines.
    - Organic film transistor arrays will begin to appear at the research level, competing for the same niche. They are slow, and noisy, but cheap and will be sprayed on like ink. Detectors can ride the wave of electronic-folding-paper.
    - Somebody might produce a detector that conforms to the inside of a 2 m sphere.
- There will be increased integration of detector technology **with x-ray optics** (multi-layers, energy dispersive gratings, etc). Fast detectors are electronically noisy detectors, so cannot have good energy resolution.
- **Micro channel plate** detectors [1us] will continue to have niches in fast framing. It seems that image intensifiers are pretty much gone the way of film.
- There will be modest pushes for **signal processing –** FPGA's to compress the data and so-forth. In general however, beamlines seem to like to have the "raw" data. This will be seen to be more and more impractical.
    - Programming an FPGA is about 1/10 as efficient (time-wise) as programming in C-code.
    - Software tools and libraries are expensive, but synergistic with demands of controls groups.
- I doubt much will be done **with superconducting detectors**, [1ms to 10 us] transition edge sensors etc, applied to the APS in next 5 years. Their count rates are very low, and they only exist in specialized labs (and at the ALS).

One can predict how the work will be done:

- Most successful projects will involve industry. We will feel the need to train people to work as contracts managers.
- Synergy with x-ray medical imaging will remain a hoped for, but never-quite-realized goal, as has been the case for the past 15 years.
- Collaborations with other national labs will be advocated, but will generally fail because we see each other as competitors for scarce DOE funds.

- The main source of original information will be semiconductor foundries.
- Given funding, detector development will continue to ride the wave of the semiconductor industry, the largest and most vibrant industry on earth, which has produced almost miraculous improvements. If you want to understand detectors, understand as well this foundation technology.
  - For example, I now have a 32 GB memory stick – 2 years ago it was 64 MB. Some interesting scaling:
  - Per the textbooks, the power of an IC scales with the cube of the feature size, so dropping the size of a transistor by ½ reduces the power to 1/8. Power is typically a worry, or a limit, with dense, fast circuitry.
  - The scale size of transistors drops by ½ every 18 months, and is now at 45 nm for commercial IC's at, say IBM. To keep this scaling law going, people will turn to 3-D CMOS. Google 3-D CMOS.
  - Transistors must be modeled to be used:
    - Transistors larger than 2 um conform to simple parameterization, called SPICE level 3, about 20 free parameters.
    - Smaller than 0.5 um, the transistor must be treated as a 2 or 3-D structure. But typically this is fudged, and the empirical models for transistors now have some 150 free parameters. Obviously there is an intense push to get the models correct, but analog lags digital.
    - With digital electronics, speed is the most important, with analog electronics predictability is the most important, even if speed is lowered. (Ref: IBM foundry person, at HEP conference.)
  - The scale size of the transistor seems to be the largest determinant of the cost of the wafer run, the mask set, etc.
    - Currently this cost rises quickly below 0.25 um. (Ref: MOSIS)
    - There will come a day when mask sets are not required, and the semiconductor pattern is raster scanned on. The mask cost will disappear. (Ref: work at Bell Labs etc….)
  - The unity gain frequency of transistors is expected to approach 1 THz in coming years. This is the frequency up to which a transistor can provide gain. (Ref Stanford SOI short course) Germanium doped silicon bipolar transistors are in this range, I am not that knowledgeable about III-V transistors, but obviously GaAs or InP are fast.
  - The HEP community is very interested in fast electronics, for example Analog to Digital conversion at speeds > 5 GSamp / sec. The aerospace community is also, but has a bigger budget. One sees them working with III-V compounds such as InP, with perhaps 10 GSamp/sec. (Ref: NGC Corp)
  - CERN people know a lot more about radiation damage; I am pretty ignorant here other than to know that oxide charging damage rates drop as feature sizes drop below 0.25 um.
  - Per foundry people, there is no substitute for prototyping, and trying it out.
- Most of the development work will be done in Europe.
  - The delay time before the instrumentation comes to the APS will be inversely proportional to the detector's speed. (Faster detectors are harder to integrate into beamlines.)

Nanopositioning instrumentation in 2013

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Since nanopositioning is a relatively young technique, it is very hard to predict the future performances of the nanopositioning instruments five years from now. This brief writing is based on today's technical challenges and tries to project the future performances and capabilities of the nanopositioning instrumentation for synchrotron radiation applications in 2013. For the APS synchrotron radiation instrumentation development, if there are no commercial products available, a customized device will be developed with modular design consideration to improve cost effectiveness and cross application compatibility.

- Advanced linear encoders and angular encoders

  Performances of optical linear encoders will continue to improve with finer grating scales and advanced readout electronics. Nanometer resolution will be a standard for many products, and sub-nanometer resolution will be possible for grating encoders, but their accuracy can not compete with that of laser-interferometric encoders. Laser-based encoders with integrated multi-reflection optics will reach picometer level resolution for linear encoder and sub-nanoradian level resolution for angular measurement.

- Novel linear stages and angular stages

  New type of weak-link stages will provide precise and vibration-free motion guiding systems for linear stages and angular stages. PZT-based motion driver will provide sub-nanometer level motion control with centimeter level travel range.

- Multidimensional positioning with sub-nanometer resolution

  FPGA-based controller will provide multidimensional positioning control in sub-nanometer level with centimeter travel range.

- New concepts for six degree-of-freedom positioning and measuring

  Direct positioning and measuring a target with six degree-of-freedom might be improved to the sub-micron level.

- Nanopositioning with extreme environmental conditions

  More nanopositioning devices will be compatible with extreme environmental conditions, such as ultra-high-vacuum, cryo-temperature, high-magnetic field etc.

X-ray Optics Considerations for Enhancing Beamline Performance

The quality of X-ray optics has an enormous impact on the performance of synchrotron radiation (SR) beamlines in terms of resolution, data collection rates, and ease of operation. There are many different optical components and all affect the productivity of a beamline. Some elements might seem innocuous like windows, filters, and slit systems, but in practice can have a significant impact on beamline performance and thus require careful consideration. To make the point, many beamlines currently operate with many windows and if the window material, or even its necessity, is not considered carefully, one may suffer significant and unnecessary cumulative losses that deteriorate beamline performance. These cumulative losses can be surprisingly large and one should consider limiting the number of windows wherever possible. Beryllium is the most common material for X-ray windows and even with the highest purity of beryllium that is commercially available (99.8% pure), the absorption due to the impurities is equal to the absorption due to the beryllium at approximately 18 keV. For lower energies, the absorption due to the impurities will dominate – at 10 keV, 2.3 mm will result in a factor of two loss. For lower grades of beryllium, the situation is significantly worse. For many beamlines, significant gains may be made simply by improving, or better, removing windows even if it comes at additional cost.

Apart from windows, filters, and slit systems, 90% of the remaining SR beamline optics involve monochromators and focusing elements. Other optics such as X-ray polarizers, phase retarders, flat mirrors, beam-expanders, beam-splitters, interferometers, et cetera are also needed for certain measurements, but may be considered specialty optics that have seen only sporadic development over the years. Monochromatization and focusing have experienced significant advances in the past 15 years and it is worth outlining some of the current directions of research that are affecting available resolutions and efficiencies. In the next five years, there is an opportunity for further advancement in these areas if appropriate resources for doing so are allocated now.

Monochromatization

Currently, cryogenically-cooled silicon and water-cooled diamond monochromators are performing reasonably well at energies where most measurements are performed. Amidst possible source upgrades, the question of continued good performance needs to be examined. Heat-load issues remain an uncertain area without knowing the degree to which power loads may increase due to the possibility of higher stored current and/or improved insertion devices that produce greater radiative power. Well-engineered versions of the two designs above should perform well for modest increases in power load.

Primary monochromators typically produce energy resolutions ($E/\Delta E$) of 10^4. To achieve higher resolutions, a secondary monochromator is needed. In the 5-40 keV energy range, resolutions are readily achievable that can produce bandwidths down to 10 meV with good spectral efficiency (50%-90%). Producing 1 meV bandwidths can be done with approximately 50% spectral efficiency using cryogenic technology. Producing a 0.1 meV bandwidth has been demonstrated, but building an instrument suitable for a user community would require development. Provided with adequate resources, such an instrument can be produced within five years.

For X-ray energies 40-80 keV, there has been little development to date with regard to high resolution. If high energy-resolution were needed, moderate development should be able to realize energy bandwidths as low as 5 meV with spectral efficiencies of 50%. This level of spectral filtering at high energies has yet to be demonstrated, but would be a reasonable goal given adequate resources.

Energy analysis of large, divergent, X-ray beams is generally needed for spectroscopy to analyze the energy spectrum of scattered radiation. Currently, near-back-reflection analyzers can achieve energy acceptances around 1 meV, but suffer from low efficiency. The low efficiency is not intrinsic, but is related to the fabrication process. With allocation of appropriate resources, this could be improved significantly by developing a reliable procedure to manufacture highly efficient analyzers. As for improving the energy resolution of analyzers, there is currently no practical way to efficiently filter a large, divergent, X-ray beam with an energy bandwidth in the range of 0.1 to 0.5 meV.

Focusing

There has been significant developments in focusing in the last 10-15 years. As a result, there are many focusing techniques and each has its respective advantages. Kirkpatrick-Baez (K-B) mirror systems, zone plates, and refractive lenses are the leading focusing technologies that are currently experiencing the most interest. All three of these technologies have demonstrated focal spot sizes that are well below 100 nm. Resolutions for all three device types are limited currently by fabrication difficulties that may be overcome in the near future.

K-B mirror systems are very versatile with a large parameter space of acceptable efficiency versus focal spot size. One can achieve few micron focal spots with full beam acceptance and good overall efficiency. Focal spot sizes as small as 25 nm have been reported. In the near term, focal spot sizes may be decreased further (say to 10 nm). If one may forgo the achromatic nature of total external reflection, it is possible to fabricate the reflecting mirrors as multi-layers and use a multi-layer Bragg reflection to increase the incident angle, which reduces the beam footprint and would allow the size of the optic to be reduced. K-B mirror systems should be considered for focusing x-rays with energies below say 70 keV. This approximate upper limit is due primarily to the low critical angle for total external reflection or low reflectivity in the case of a multilayer. Their advantages include good efficiency over a wide energy range and an achromatic response when using total external reflection.

Zone plates currently achieve few tens-of-nanometers sized focal spots. Again the limiting issue is related to fabrication. A number of alternative methods of fabrication and operation have been reported and steady progress may allow one to achieve 5-10 nm focal spots in the not so distant future. Zone plates should be considered for energies below 30 keV. At higher energies the thickness of the zone plate has to become large to achieve the requisite phase shift and the zone width of the outermost zone determines the focal spot size. This leads to aspect ratios and geometrical tolerances that are difficult to achieve without sacrificing overall efficiency. Their advantages include relatively good efficiency for sub-micron focusing, an in-line geometry, relatively easy operation, and relatively low cost.

Refractive lenses have also seen significant advances in recent years and have demonstrated focal spot sizes that are as small as a few tens of nanometers. Employing evermore sophisticated fabrication techniques may allow even smaller focal spot sizes in the future. They are usable over a very wide energy range; from 6 keV at the low end to many hundreds of keV at the high end. Their advantages include a wide range of focal spot sizes, an in-line geometry, relatively easy operation, and relatively low cost.

It is difficult to compare the three main focusing techniques without having a specific application in mind. This is because the optimal choice depends on many things such as energy, energy range, cost, beamline layout, needed working distances, and the inevitable trade-off between focal spot size and overall efficiency. With regard to overall efficiency, focusing to 30nm can be done today, but any technique for doing so results in overall efficiencies that are well below 1%. In the next five years, it may be possible to reduce focal spot sizes to 10nm, or even smaller. Perhaps a question more relevant to the majority of beamlines would be how much can efficiencies be improved. As this would make nano-focusing more accessible to a wider range of X-ray scattering techniques, as well as, improve data collection rates for existing techniques. Improving efficiencies will require greater control over the optic fabrication process and perhaps modifying source properties, but the possibility of employing multiple focusing systems to achieve larger acceptance of the SR phase space needs to be explored.

Shaped mirrors that produce 2-dimensional focusing in a single reflection are employed at many beamlines for full-beam focusing. The manufacturing and bending of such mirrors requires figure error tolerances that are exceedingly difficult to achieve. Alternative focusing schemes should be at least considered. K-B mirror systems tackle the problem of 2-dimensional focusing in two steps. As a result, the tolerances for fabrication and operation are more relaxed. This makes small focal spots more readily attainable with greater efficiency resulting in superior performance even though there is an additional reflection. Also, refractive lens technology is improving steadily and one should consider this for full-beam focusing. For beamline applications that use different energies, this may require multiple refractive lens configurations to accommodate their chromatic behavior.