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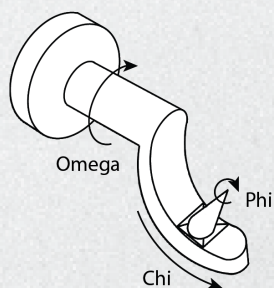
Workshop on Advanced Data Collection with Multi-Axis Goniometer and Single-Photon Counting Detector

06 - 08 November 2012
Swiss Light Source at Paul Scherrer Institute - Switzerland

http://indico.psi.ch/event/multiaxis2012

Book of Abstracts

PAUL SCHERRER INSTITUT
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Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
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BioStruct‑X

Workshop on Advanced Data Collection with Multi-Axis Goniometer and Single-Photon Counting Detector

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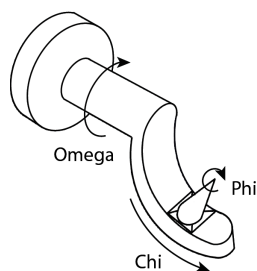*Swiss Light Source at Paul Scherrer Institute - Switzerland*

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Host Institution

PAUL SCHERRER INSTITUT
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Organisers

Meitian Wang, PSI
Andrew Thompson, SOLEIL
Vincent Olieric, PSI
Sandro Waltersperger, PSI

Secretariat

Sonia Reber, PSI
Charlotte Heer, PSI

Scope

This workshop will address multi-axis goniometers applications for difficult phasing experiments, data collection optimisation for single-photon counting detectors, as well as data processing. Hardware and software developments, as well as user applications will be covered with lectures and practicals.
Data collection practicals will be performed at beamline X06DA at the Swiss Light Source (http://www.psi.ch/sls/pxiii/) on a multi-axis goniometer PRIGo and a PILATUS 2M detector.
Data processing tutorials will be on AutoPROC, PROTEUM, and CrysAlisPro programs.

Speakers

Gerard Bricogne, Global Phasing Ltd.
Sandor Brockhauser, EMBL
Kay Diederichs, Uni. Konstanz
Gwyndaf Evans, Diamond Light Source
Zheng-Qing (Albert) Fu, SER-CAT APS
Pierre Legrand, SOLEIL
Timm Maier, Uni. Basel
Andrew McCarthy, EMBL
Marcus Mueller, Dectris Ltd.

Vincent Olieric, PSI
Michael Ruf, Bruker AXS
Thomas Schneider, PETRAIII
Clemens Schulze-Briese, Dectris Ltd.
Tadeusz Skarzynski, Agilent
Andrew Thompson, SOLEIL
Clemens Vonrhein, Global Phasing Ltd.
Sandro Waltersperger, PSI

Sponsors

BioStruct‑X   DECTRIS Next Generation X-Ray Detectors   MiTeGen

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Workshop on Advanced Diffraction Data Collection with Multi-Axis Goniometer and Single-Photon Counting Detector in Protein Crystallography

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16:00 - 18:00	**Session I: Introduction to multi-axis goniometry and single-photon counting detector** **Chair: Meitian Wang, PSI (WBGB/019)**
16:10 - 16:50	Andrew Thompson, SOLEIL *Crystallography and diffraction geometry*
16:50 - 17:30	Clemens Schulze-Briese, Dectris Ltd. *Pixel-array detectors for protein crystallography*
17:30 - 18:10	Kay Diederichs, University of Constance *Linking data and model quality*
18:30 - 20:00	Dinner (WBGB/Time-Out building)
20:00 - 21:00	**Keynote lecture - Gerard Bricogne, Global Phasing Ltd.** *Phasing with a Goniometer: the Anisotropy of Anomalous Scattering* **Chair: Andrew Thompson, SOLEIL (WBGB/019)**
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09:00 - 09:30	Pierre Legrand, SOLEIL *Kappa strategy and phasing at SOLEIL*
09:30 - 10:00	Marcus Mueller, Dectris Ltd. *Getting the best data using photon counting pixel detectors*
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10:30 - 11:00	Kay Diederichs, University of Constance *XDS and beyond*
11:00 - 11:30	Clemens Vonrhein, Global Phasing Ltd. *AutoPROC*
11:30 - 12:00	Michael Ruf, Bruker AXS *Automated Data Collection Strategy for Crystallographic Systems*
12:00 - 12:30	Tadeusz Skarzynski, Agilent Technologies *CrysAlisPro*
12:30 - 13:50	Lunch (WSLA/SLS entrance hall)
14:00 - 15:20	**Session IV: Multi-axis goniometry at synchrotron beamlines** **Chair: Andrew McCarthy, EMBL (WBGB/019)**
14:00 - 14:20	Sandor Brockhauser, EMBL *The ESRF/EMBL MiniKappa*
14:20 - 14:40	Thomas Schneider, PETRA III *Vertical MD3 at PETRA III*
14:40 - 15:00	Vincent Olieric, PSI *PRIGo: a new goniometer concept at beamline X06DA at SLS*
15:00 - 15:20	Zheng-Qing (Albert) Fu, SER-CAT APS *A Few Handy Tools to Help Monitoring Data Quality On-the-Fly*

15:20 - 15:40	Zvieri - Break
15:40 - 17:00	**Session V: Case studies and future** **Chair: Clemens Vonrhein, Global Phasing Ltd. (WBGB/019)**
15:40 - 16:00	Andrew McCarthy, EMBL *Experience using the mini-kappa goniometer head for diffraction experiments at the ESRF*
16:00 - 16:20	Sandro Waltersperger, PSI *Taking advantage of multi-axis goniometer and single-photon counting detector for S-SAD experiments*
16:20 - 16:40	Timm Maier, University of Basel *Data collection and processing for crystals of large macromolecular assemblies*
16:40 - 17:00	Gwyndaf Evans, DLS *The DIALS Collaboration*
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Day 3: Friday, November 8th, 2012

Practicals for data collection at beamline X06DA and data processing (autoPROC, PROTEUM, CrysAlisPro)

A - Data collection at beamline X06DA and processing with AutoPROC (beamline X06DA-PXIII)
     Vincent Olieric, Sandro Waltersperger, Clemens Vonrhein
B - Processing with PROTEUM (WSLA/108)
     Michael Ruf
C - Processing with CrysAlisPro (WSLA/008)
     Tadeusz Skarzynski
D - Free (Time-Out)

Groups
I   - Nikolaus Schmitz, Simone Pellegrino, Matthew Bennett, Raquel Arribas, Luisa Ströh, Ariel Mechaly
II - Brice Kauffmann, Shiyu Chen, Gerlind Sulzenbacher, Manuel Hilbert, Arjen Jakobi, Falk Syberg
III - Albert Fu, John Rose, Scott Classen, Andrea Prota, Ramona Duman, Ralf Flaig
IV - Guillermo Montoya, Jérôme Basquin, Richard Bunker, Alan Cheung, Heinz Gut, Tobias Krojer

	Group I (Large unit cell)	Group II (Native)	Group III (SAD phasing)	Group IV (MAD phasing)
08:30 - 10:00	A	B	C	D
10:30 - 12:00	B	A	D	C
12:00 - 13:20	Lunch (WSLA/entrance hall)			
13:30 - 15:00	C	D	A	B
15:30 - 17:00	D	C	B	A
18:00 - 21:00	Dinner (Metzgete buffet at restaurant OASE Villigen PSI)			

Abstracts

Crystallography and diffraction geometry

Andrew Thompson

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Abstract:

Macromolecular crystallography and "small molecule" crystallography have followed divergent paths in terms of data collection methods. In the former, the need to efficiently measure large numbers of densely spaced diffraction peaks drove data collection in the direction of oscillation geometry, high redundancy data collection with integrating area detectors, whereas in the latter precision "low redundancy" measurements with 0d photon counting detectors and multi axis goniometry.

More recently small molecule crystallographers have "discovered" the area detector (see, for example, Howard et al, Acta Cryst, 1999, B55, 861 - 881) whereas MXers have started to learn of the advantages of multi-circle goniometry and combining data collected around multiple rotation axes. The advent of large area photon counting pixel array detectors, such as the PILATUS, makes the "convergence of data collection methods" even greater.

At SOLEIL, the PROXIMA 1 beamline has, since 2007, been used to collect data using a 3 circle kappa goniostat, and   different data collection strategies evaluated. The beamline was upgraded with the installation of a PILATUS 6M detector on the beamline in 2011, and the combination of multi-circle goniometry and rapid, noiseless data collection has been very succesful in resolving many crystal structures with, in particular, a significant rise in successful S-SAD structure solution.

A brief introduction to multi circle goniometry for MX will be presented, with the intention of familiarising potential users with the range of different data collection possibilities offered. The availability of multi-circle goniometers at European synchrotron sources will be briefly discussed.

Pixel Array Detectors for Protein Crystallography

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on behalf of DECTRIS Ltd.

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Abstract:
High brightness undulator radiation beamlines had and still have a tremendous impact on the development of modern protein crystallography. Micro-crystallography, high resolution data collection on mega-dalton complexes as well as data collection from crystal sub-volumes were enabled by the extreme brightness of these beamlines and benefited from complementary developments of beamline optics, goniometry, robotics, detectors and software. The down side of the exceedingly high flux densities and very small beam cross-sections are severe radiation damage frequently impeding phasing experiments and high sensitivity to any instabilities of beam, goniometry or sample mounting. Filters are typically the only tool to adjust the flux density to levels suitable with the collection of complete data at oscillation speeds low enough to not compromise data quality. A more appropriate way to adjust the flux density is to reduce the angular divergence or to focus the beam on the detector or beam stop. Experimental results obtained with both strategies will be presented and the consequences for low resolution data collection will be discussed. On the other hand hybrid-pixel detectors such as the PILATUS are ideally suited to exploit the full potential of high brightness undulator radiation in the collection of optimal data from challenging crystals. Rapid diffraction based alignment of thin needles or plates as well as grid scans for the location of microcrystals rely on high frame rates. Shutter-free continuous data acquisition is the fastest way to collect data and hence optimizes the throughput. The combination of noise-free counting and high frame rates with a low divergence beam allows the data quality to be improved by optimal fine-phi-slicing. The absence of any detector noise enables the collection of high redundancy data at low dose rates, a data collection strategy which is of particular benefit in phasing experiments in combination with multi-axis goniometers. The excellent point-spread-function of the pixel detector gives rise to optimal signal-to-noise ratio resulting in highest resolution data, when the beam size is minimized on the detector surface. Examples of the various strategies and techniques will be presented.

Linking data and model quality

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Abstract:

In macromolecular X-ray crystallography, typical data sets have substantial multiplicity. This can be used to calculate the consistency of repeated measurements and thereby assess data quality. Recently, we characterized the properties of a correlation coefficient, $CC_{1/2}$, that can be used for this purpose, and showed that it has superior properties compared to 'merging' R values. A derived quantity, CC*, links data and model quality.

Using experimental datasets, we compare the behaviour of $CC_{1/2}$ and the more conventional indicators in three situations of practical importance: deciding about the high-resolution cutoff, merging datasets from different crystals; and selectively rejecting weak observations or (merged) unique reflections from a dataset. In these situations controlled 'paired-refinement' tests show that even though discarding the weaker data leads to improvements in merging R-values, the refined models based on these data are of lower quality. These results show the folly of data filtering practices aimed at improving merging R-values, and reveal rational ways to obtain the best possible data.

References:

[1] Karplus, P.A. and Diederichs, K. (2012) *Science* **336**, 1030-1033

KEYNOTE LECTURE

Phasing with a Goniometer: the Anisotropy of Anomalous Scattering

Marc Schiltz[1], Gerard Bricogne[2]

[1]*École Polytechnique Fédérale de Lausanne(EPFL), Laboratoire de Cristallographie, Lausanne, Switzerland*
[2]*Global Phasing Ltd., Cambridge, UK*

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Abstract:
The X-ray polarization anisotropy of anomalous scattering in crystals of brominated nucleic acids and selenated proteins has been shown to have significant effects on the diffraction data collected at an absorption edge. For conventionally collected single- or multi-wavelength anomalous diffraction data, the main manifestation of the anisotropy of anomalous scattering is the breaking of the equivalence between symmetry-related reflections, inducing intensity differences between them that can be exploited to yield extra phase information in the structure-solution process. A new formalism for describing the anisotropy of anomalous scattering which allows these effects to be incorporated into the general scheme of experimental phasing methods using an extended Harker construction is introduced. This requires a paradigm shift in the data processing strategy, since the usual separation of the data merging and phasing steps is abandoned. The data are kept unmerged down to the Harker construction, where the symmetry-breaking is explicitly modelled and refined and becomes a source of supplementary phase information. These ideas have been implemented in the phasing program SHARP. Refinements using actual data show that exploitation of the anisotropy of anomalous scattering can deliver substantial extra phasing power compared with conventional approaches using the same raw data. Examples are given that show improvements in the phases which are typically of the same order of magnitude as those obtained in a conventional approach by adding a second-wavelength data set to a SAD experiment. It is argued that such gains, which come essentially for free, i.e. without the collection of new data, are highly significant, since radiation damage can frequently preclude the collection of a second-wavelength data set. Finally, further developments in synchrotron instrumentation and in the design of data-collection strategies that could help to maximize these gains are outlined. The use of multi-axis goniometers is an important part of fully exploiting the experimental phasing potential of AAS [1].

References:

[1] M. Schiltz & G. Bricogne, Acta Crystallographica, D64 (711-729), 2008.

Back to the Future: Revisiting and Improving Experimental Phasing Protocols, from Design to Processing

Gerard Bricogne[1], Clemens Vonrhein[1], Andrew Thompson[2], Pierre Legrand[2], Vincent Olieric[3], Sandro Waltersperger[3], Ezequiel Panepucci[3], Meitian Wang[1]

[1]*Global Phasing Ltd, Cambridge, UK*
[2]*Synchrotron SOLEIL, Gif sur Yvette, France*
[3]*Swiss Light Source at Paul Scherrer Institute, Villigen PSI, Switzerland*

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Abstract:
In the early days of the MAD method, Hendrickson et al. (see e.g. [1]) used carefully designed protocols to maximise the signal-to-noise (S/N) ratio of anomalous and dispersive signals. Optimal anomalous S/N was achieved by re-orienting crystals on a multi-axis goniometer to record Bijvoet pairs on the same image, or by the interleaving of thin wedges (typically, 5 to 10 degrees) of data collected 180 degrees apart in rotation angle ("inverse-beam" method). High-S/N dispersive differences were obtained by similarly interleaving inflection point and remote wavelengths. The special accuracy of these phasing differences was then exploited via the MADSYS software suite [2].

The advent of third-generation synchrotron sources and of CCD detectors created strong pressure towards data collection strategies that would be devoid of the complications of inverse-beam and wavelength-interleaving protocols, after it was shown that simpler strategies involving the collection of full datasets, for one wavelength at a time, around a single axis, were capable of yielding MAD-phased structures in remarkably short times [3]. From that point on, although many beamline still offered options to do inverse-beam and/or wavelength-interleaved experiments, these protocols rapidly fell into disuse except in the hands of a few devotees.

We have revisited the original complex protocols with modern approaches to data processing, substructure solution and phasing and assessed the gains in substructure solution rates and in phasing power provided by these protocols over the conventional ones.

Besides presenting our specific results, we will discuss prospects for implementing these protocols and the associated processing and phasing procedures in the form of integrated workflows suitable for the modern context of high-speed beamline operation and requiring little or no expertise from the users.

References:
[1] HENDRICKSON, W.A., PAHLER, A., SMITH, J.L., SATOW, Y., MERRITT, E.A. & PHIZACKERLEY, R.P. (1989). "Crystal structure of core streptavidin determined from multiwavelength anomalous diffraction of synchrotron radiation." *Proc. Natl. Acad. Sci. USA* **86**, 2190-2194.
[2] HENDRICKSON, W. A. (1991). "Determination of macromolecular structures from anomalous diffraction of synchrotron radiation." *Science* **254**, 51-58.
[3] WALSH, M.A., DEMENTIEVA, I., EVANS, G, SANISHVILI, R & JOACHIMIAK, A. (1999). "Taking MAD to the extreme: ultrafast protein structure determination." Acta Cryst. D**55**, 1168-1173.

Kappa strategy and phasing at SOLEIL

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Getting the best data using photon counting pixel detectors

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Abstract:
Hybrid pixel detectors have fundamentally different characteristics and offer various advantages over CCD detectors [1,2]: (i) No readout noise and no dark current. (ii) A sharp point spread function of one pixel. (iii) Millisecond readout times and high frame rates. (iv) A high dynamic range of 20 bits. To fully exploit the advantages of hybrid pixel detectors, different data collection strategies than those established for CCD detectors have to be applied because of the different characteristics of the two types of detectors.

Fine-slicing is a strategy particularly well suited for hybrid pixel detectors because of the fast readout time and the absence of readout noise. This strategy was systematically investigated collecting a large number of data sets from crystals of four different proteins to investigate the benefit of fine φ-slicing on data quality with a noise-free detector in practice. The results show that fine φ-slicing can substantially improve scaling statistics and anomalous signal [3]. Furthermore, unpublished results on the influence of the detector readout time on data quality will be presented.

References:
[1] Hülsen, G., Broennimann, C., Eikenberry, E.F., Wagner, A. (2006). *J. Appl. Crystallogr.* **39**, 550-557.
[2] Tate, M.W., Eikenberry, E.F., Gruner, S.M. (2006). In *International Tables for Crystallography, Vol. F.* Edited by Rossmann MG, Arnold E. 148-153.
[3] Mueller, M., Wang, M., Schulze-Briese, C. (2012) *Acta Cryst.* D**68**, 42-56.

XDS and beyond

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Abstract:
Principles of data processing with XDS will be presented. New developments include a version for processing of "serial crystallography" data from a Free Electron Laser, and a stand-alone graphics program that will facilitate data processing for novice users.

autoPROC

Clemens Vonrhein, Claus Flensburg, Peter Keller, Woldek Paciorek, Andrew Sharff, Oliver Smart, Thomas Womack, Gerard Bricogne

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Abstract:
The autoPROC toolbox [1] has been designed to help both novice and expert users to handle a diversity of datasets, from the simple and straightforward to the complex and challenging. Particular emphasis is placed on the correct integration and combination of multi-sweep datasets, eg. multi- wavelength MAD experiments, high- and low-resolution passes, helical data collection, inverse- beam experiments or collection on different crystals. autoPROC allows a detailed and general description of the underlying hardware, including more common multi-axis goniostats like Kappa or Eulerian systems.

The system makes use of some very sophisticated programs like XDS [2], POINTLESS or SCALA/AIMLESS [3], concentrates on the optimal usage of these and adds additional functionality, tools and diagnostics to these.

This not only allows the detection of multiple lattices and ice-rings, but some initial treatment of those rather common artefacts at the stage of indexing, integration and scaling/merging (to avoid contamination of the final dataset). Automatic decision making, regarding the high-resolution limit of the data, uses a combination of common criteria such as I/sigI, Rmerge, Rpim, Rmeas or completeness and includes the handling of loss of diffraction, problematic centering or very anisotropic diffraction limits.

Recent developments include global dose stamps to measurements when data is collected with interleaving or inverse-beam strategy as well as composite scaling of data with AIMLESS and 0-dose extrapolation in XSCALE.

References:
[1] Vonrhein C, Flensburg C, Keller P, Sharff A, Smart O, Paciorek W, Womack T, Bricogne G. (2011). Acta Cryst. D67, 293-302.
[2] Kabsch W (2010). Acta Cryst. D66, 125-132.
[3] Evans P (2006). Acta Cryst. D62, 72-82.

Automated Data Collection Strategy for Crystallographic Systems

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Abstract:

Best structure quality requires collection of complete and sufficiently redundant data. Modern area detector systems combined with multi-axis goniometers are most effective to acquire both highly redundant and accurate data sets in an efficient manner.

Planning the optimum diffraction experiment with an area detector on a state of the art 4-circle goniometer is more complex than on simple single circle instruments, especially if the particular crystal possesses low symmetry or is oriented unfavorably on the goniometer.

This presentation will focus on how to best determine data collection strategies using PROTEUM2. The program takes general criteria into account such as the availability of time, the desired redundancy, or collision restrictions on the goniometer and low temperature device. PROTEUM2 provides an intuitive graphical user interface and is fully integrated in the comprehensive programs for structure determination for macro and small molecules.

PROTEUM2 makes it easy to design an individual and efficient data collection strategy for every single crystal and to acquire better data than a generic standard strategy will generally provide.

CrysAlisPro

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Abstract:
CrysAlisPro is a data collection and processing program supplied by Agilent with its range of X-ray diffractometers for chemical and macromolecular crystallography applications. The software, when installed on the Agilent diffractometer, is used to control all aspects of hardware operation, including automatic power management of the X-ray generator, control of cryo-devices attached to the system and complete control of the 4-circle goniometer and CCD detector during data collection. The program offers sophisticated strategy calculation making full use of the 4-circle goniometer capabilities and a fully automatic workflow for crystal unit cell determination and subsequent data collection, processing and scaling. In addition to automatic protocols, CrysAlisPro includes a collection of a large number of manual tools for experts. It allows successful indexing and processing of non-merohedral twin crystals. Images can be exported to other data processing programs like Mosflm, XDS and HKL2000. The off-line version of the program allows processing and scaling of data from Agilent X-ray systems and from a number of third-party detectors including Dectris Pilatus 6M. At the meeting we will demonstrate capabilities and functionality of CrysAlisPro with a live demo of the whole data collection and processing process and we will show specific unique features of the program. Processing of data from Pilatus 6M will be also demonstrated.

The ESRF/EMBL MiniKappa

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Abstract:

A main design goal of The EMBL/ESRF MiniKappa was to minimize one of the major risk of traditional multi-axis goniometers: collisions. Compromising, but keeping the rotational freedom as high as practically possible, allowed the integration of this device to the crowded sample environments of highly automated modern synchrotron beamlines. Being available in more than 25 beamlines around the world, it brought the breakthrough of re-enabling automated sample reorientation in macromolecular crystallography practices. Software components were written for helping the integration into beamline control system[1,2] as well as into sample characterisation and data collection strategy pipelines (STAC, EDNA, DAWN)[3]. Practical issues on how to use the minikappa most efficiently is discussed. Also the possibility of using the same software environment and smart multi-orientation experimental protocols with different multi-axis goniometers is highlighted.

References:

[1] McCarthy, A. A., Brockhauser, S., Nurizzo, D., Theveneau, P., Mairs, T., Spruce, D., Guijarro, M., Lesourd, M., Ravelli, R. B. G. & McSweeney, S. J. Synchrotron Rad. 16, 803-812 (2009).
[2] Brockhauser, S., White, K. I., McCarthy, A. A. & Ravelli, R. B. G. (2011). Acta Cryst. A67, 219-228 (2011).
[3] Brockhauser, S., Svensson, O., Bowler, M. W., Nanao, M., Gordon, E., Leal, R. M. F., Popov, A., Gerring, M., McCarthy, A. A. & Gotz, A. (2012). Acta Crystallogr. D Biol. Crystallogr. 68, 975-984 (2012).

Vertical MD3 at PETRA III

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Abstract:
EMBL is currently commissioning a micro-focus beamline P14 at the high-brilliance synchrotron radiation source PETRA III (Hamburg, Germany). In order to fully exploit the small focal size of less than 5 micron in both vertical and horizontal beam direction, a new diffractometer was developed in collaboration between EMBL-Hamburg and EMBL-Grenoble.

The prototype-instrument - name HPGonioV - was based on the construction principles of the well-known MD2 diffractometer (marketed by MAATEL). To achieve a sub-micron sphere of confusion (SOC), the rotation axis was arranged vertical and 'hanging'. The observed SOC with a mini-kappa goniometer mounted was less than 100 nm and the instrument has been used successfully in test and user data collections since the summer of 2011. The delivery of the first production version MD3 as manufactured by MAATEL is expected for October 2012.

We will discuss the rational behind the vertical spindle arrangement and implications of beam polarization for crystallographic data collection. Results of measurements of the mechanical precision the and quality of crystallographic data collected with the device will be presented.

PRIGo: a new goniometer concept at beamline X06DA at SLS

Vincent Olieric[1], Sandro Waltersperger[1], Marco Salathe[1], Wayne Glettig[2], Ezequiel Panepucci[1], Claude Pradervand[1], Clemens Schulze-Briese[3], Meitian Wang[1]

[1]*Swiss Light Source at Paul Scherrer Institute, Villigen PSI, Switzerland*
[2]*Centre Suisse d'Electronique et de Microtechnique, CSEM SA, Neuchâtel, Switzerland*
[3]*DECTRIS Ltd., Baden, Switzerland*

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Abstract:

The **P**arallel **R**obotics **I**nspired **Go**niometer (PRIGo) is a novel and compact goniometer which provides an alternative for kappa goniometers used at synchrotron macromolecular crystallography beamlines. Based upon a combination of serial and parallel kinematics, PRIGo consists of the usual Omega ω rotation performed by an Aerotech, followed by four linear stages working synchronously to allow the three translations (X,Y,Z), the Chi χ rotation (0-90º), and finally the Phi φ rotation (0-360º) around the sample holder axis. Spheres of confusion of <1 μm, <7 μm and <10 μm were obtained for ω, χ and φ respectively, thanks to the use of SmarAct linear positioners replacing conventional linear spindle stages.

Installed at beamline X06DA at the Swiss Light Source in January 2012, the PRIGo offers new data collection opportunities. It allows to precisely reorient crystals and to better exploit anomalous signals in SAD and MAD phasing experiments.

A Few Handy Tools to Help Monitoring Data Quality On-the-Fly

Zheng-Qing Fu, John Rose, Bi-Cheng Wang

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Abstract:
The bright 3rd-generation synchrotron X-ray source combined with shutter-less high-speed detecting systems has reduced the time from hours to minutes in collecting a typical full data set. The high-speed data acquisition makes data quality control very challenging. A few handy tools utilizing powerful and/or parallel computers were developed to quickly evaluate data quality during data collection. These tools can assess the data at different stages from data reduction, heavy-atom sites searching to experimental phasing of the structure-solving process. Details and live demos will be presented. Work supported by the SER-CAT Member Institutions.

Experience using the mini-kappa goniometer head for diffraction experiments at the ESRF

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[2]Leiden University Medical Center (LUMC), Leiden, The Netherlands

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Abstract:

Most macromolecular crystallography (MX) synchrotron based diffraction experiments use single-axis diffractometers. This markedly contrasts with small molecule crystallography, where the majority of diffraction data are collected using multi-axis goniometers. A novel miniaturised κ-goniometer head, the MK3, has been developed by the EMBL/ESRF in Grenoble to allow the reorientation of macromolecular crystals. It is now available on the majority of the structural biology beamlines at the ESRF [1], as well as elsewhere. In addition, a Strategy for the Alignment of Crystals (STAC) software package, including automatic translational correction protocols [2], has been developed to facilitate the use of the MK3 and other similar devices. Use of the MK3 and STAC has recently been streamlined by their incorporation with online analysis tools such as EDNA and MX controls software such as MxCuBE using our recently developed workflows [3]. The current use of this user friendly software and the MK3 on the MX-beamlines at the ESRF is briefly discussed. We also present some of our recent results, which show that the alignment of macromolecular crystals can result in improved diffraction data compared to data obtained from randomly aligned crystals.

References:

[1] McCarthy, A. A., Brockhauser, S., Nurizzo, D., Theveneau, P., Mairs, T., Spruce, D., Guijarro, M., Lesourd, M., Ravelli, R. B. G. & McSweeney, S. *J. Synchrotron Rad.* **16**, 803-812 (2009).
[2] Brockhauser, S., White, K. I., McCarthy, A. A. & Ravelli, R. B. G. (2011). *Acta Cryst.* A**67**, 219-228 (2011).
[3] Brockhauser, S., Svensson, O., Bowler, M. W., Nanao, M., Gordon, E., Leal, R. M. F., Popov, A., Gerring, M., McCarthy, A. A. & Gotz, A. (2012). *Acta Crystallogr. D Biol. Crystallogr.* **68**, 975-984 (2012).

Taking advantage of multi-axis goniometer and single-photon counting detector for S-SAD experiments

<u>Sandro Waltersperger</u>[1], Vincent Olieric[1], Marco Salathe[1], Claude Pradervand[1], Ezequiel Panepucci[1], Wayne Glettig[2], Lirong Chen[3], B.C. Wang[3], Clemens Schulze-Briese[4], Meitian Wang[1]

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Abstract:
The anomalous differences from sulphur and phosphor are very weak if the diffraction data is collected in the regular energy range provided by most beamlines and home sources today. Therefore, it is crucial to reduce any source of error to improve the signal-to-noise ratio for successful S(P)-SAD experiments. Using multi-axis data collection in combination with a noise free single photon counting detector, like PILATUS, allows to better exploit the weak signal from the intrinsic sulphur and phosphor in protein and RNA/DNA crystals, respectively.

The beamline X06DA at the Swiss Light Source is a very stable bending magnet source and offers a broad energy range from is 5 to 18 keV with decent photon flux throughout the whole energy spectrum. Furthermore, the beamline is equipped with the multi-axis goniometer PRIGo and a PILATUS 2M-F detector. The combination of a noise-free single photon counting detector and the possibility to collect diffraction data around several axes is advantageous for many types of experiments. High redundancy low dose data collection together with precisely reoriented crystals enables the user to better exploit the weak anomalous signals in S(P)-SAD phasing experiments, by capturing Bijvoet pairs on the same image or by collecting multi-orientation diffraction datasets. Strategies and examples of usage will be presented to state the potential of this specific beamline setup for S(P)-SAD data collection.

Data collection and processing for crystals of large macromolecular assemblies

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Biozentrum, University of Basel, Switzerland

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Abstract:

Large proteins, protein-protein or protein-nucleic acid complexes are a particular challenge for crystallographic structure determination. Such large macromolecular assemblies are often difficult to prepare in large quantities. They are more likely affected by compositional or conformational heterogeneity than average-sized proteins and obtaining high-quality well-diffracting crystals of large assemblies is a challenge. Also at the level of data collection and processing, huge macromolecular complexes cause specific problems: (i) Their crystals have large unit cell volumes causing weaker diffraction for a given crystal size (ii) Unit cell dimensions are often variable between or sometimes even within crystals (iii) Parts of the assemblies may be heterogeneous or disordered and diffraction is often anisotropic (iv) Long unit cell axes may cause overlaps between reflections depending on crystal orientation.

This talk focuses on procedures for crystal preparation to minimize problems during data collection as well as data collection strategies for large unit cell crystals, in particular multi-position and multi-crystal data collection approaches. Past and present methods for data collection of crystals with large unit cell axes are reviewed. Strategies for data processing and quality control for datasets from multiple crystals of large macromolecular assemblies are discussed with practical examples.

The DIALS Collaboration

Gwyndaf Evans

Diamond Light Source, UK

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Abstract:
The DIALS (Diffraction Integration for Advanced Light Sources) collaboration is developing new macromolecular crystallography (MX) diffraction data integration software that is compatible with both synchrotron and FEL MX data collection methods. Funded by the BioStruct-X grant within the EU FP7 scheme DIALS will produce a modular and 'future proof' software framework and associated algorithms that will be optimised for the latest PAD detector technology. The talk will describe the collaboration and the progress made to date in sketching the program framework and prototyping the key integration and refinement modules.

General Information

Internet Access

There is free and open WiFi (public) at PSI.

Meeting Phone Numbers

In case of problems, please call:

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Vincent Olieric	+41(0)56 310 5233
Sandro Waltersperger	+41(0)56 310 5617
Sonia Reber	+41(0)56 310 3759

Useful Links

Transportation	http://www.sbb.ch
Paul Scherrer Institute	http://www.psi.ch
Beamline X06DA - PXIII	http://www.psi.ch/sls/pxiii
Biostruct-X	http://www.biostruct-x.eu/

Situation Plan

Accommodation & Bus

Hotel Terminus in Brugg

Bahnhofplatz 1–5
CH-5200 Brugg
phone: +41 (0)56 460 25 25
email: info@terminus-brugg.ch
http://www.terminus-brugg.ch/

To arrange check-in after 22.00 please contact the hotel in advance.

Bus	Brugg, Train Station	Villigen PSI West
376	07:35	07:49
direct	08:04	08:15
376	08:05	08:19

Hotel Rotes Haus in Brugg

Hauptstrasse 7
CH-5200 Brugg
phone: +41 (0)56 441 08 08
email: info@roteshausbrugg.ch
http://www.roteshausbrugg.ch/

Check-in after 23.00: pick up your key from the keysafe (code: 1122A) which is at the entrance of the hotel on the right side on the wall. The rooms are at the second floor.

Bus	Brugg, Train Station	Villigen PSI West
376	07:35	07:49
direct	08:04	08:15
376	08:05	08:19

Hotel Hirschen in Villigen

Hauptstrasse 42
CH-5234 Villigen
phone: +41(0)56 284 11 81
email: mail@hirschen-villigen.ch
http://www.hirschen-villigen.ch/

Check in from 09.00-13.30 and 17.00-23.30. If you are not able to check in during this time frame you can go in via the main entrance of the hotel and pick up an envelope from a littel table at the right which is labeled with your name. The envelope contains your room key and a form that you would need to fill out and give it to the hotel staff.

Bus	Villigen, Vor Tor	Villigen PSI West
376	07:47	07:49
376	08:17	08:19

Gasthof Schlossberg in Villigen

Hauptstrasse 32
CH-5234 Villigen
phone: +41(0)56 284 11 78
email: info@gasthof-schlossberg.ch
http://www.gasthof-schlossberg.ch/

Check in up until 24.00 via the restaurant staff.

Bus	Villigen, Vor Tor	Villigen PSI West
376	07:47	07:49
376	08:17	08:19

Hotel zum Sternen in Würenlingen

Endingerstrasse 7
CH-5303 Würenlingen
phone: +41(0)56 297 40 00
email: office@sternen-wuerenlingen.ch
http://www.sternen-wuerenlingen.ch/home/

You can check in up until 23.00 via the restaurant staff. After 23.00 and for guest who will arrive on Monday you need to walk around the hotel to the courtyard and enter via the official hotel entrance (unlocked glass door) in this room you can pick up your key. If you have problems to find it call +41 (0)79 756 9917.

Bus	Würenlingen, Post	Villigen PSI West
570	08:10	08:15

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Programme

Workshop on Advanced Diffraction Data Collection With Multi-Axis Goniometer and Single-Photon Counting Detector in Protein Crystallography

Day 1: Wednesday, November 6th, 2012

Time	Event
15:00 - 15:50	Registration (WBGB/Time-Out building)
16:00 - 16:10	Welcome - Friso van der Veen, Director of SLS
16:00 - 18:00	**Session I: Introduction to multi-axis goniometry and single-photon counting detector**
16:10 - 16:50	Andrew Thompson, SOLEIL
16:50 - 17:30	Clemens Schulze-Briese, Dectris Ltd.
17:30 - 18:10	Kay Diederichs, University of Constance
18:30 - 20:00	Dinner (WBGB/Time Out building)
20:00 - 21:00	**Keynote lecture - Gerard Bricogne, Global Phasing Ltd.**
21:00 - 22:30	Networking (WBGB/Time Out building)

Day 2: Thursday, November 7th, 2012

Time	Event
08:30 - 10:00	**Session II: Strategies for better data**
08:30 - 09:00	Gerard Bricogne, Global Phasing Ltd.
09:00 - 09:30	Pierre Legrand, SOLEIL
09:30 - 10:00	Marcus Mueller, Dectris Ltd
10:00 - 10:30	Znüni - Break
10:30 - 12:30	**Session III: Optimized data processing for complex data collection protocols**
10:30 - 11:00	Kay Diederichs, University of Constance
11:00 - 11:30	Clemens Vonrhein, Global Phasing Ltd.
11:30 - 12:00	Michael Ruf, Bruker AXS
12:00 - 12:30	Tadeusz Skarzynski, Agilent Technologies
12:30 - 13:50	Lunch (WSLA/SLS entrance hall)
14:00 - 15:20	**Session IV: Multi-axis goniometry at synchrotron beamlines**
14:00 - 14:20	Sandor Brockhauser, EMBL
14:20 - 14:40	Thomas Schneider, PETRA III
14:40 - 15:00	Vincent Olieric, PSI
15:00 - 15:20	Zheng-Qing (Albert) Fu, SER-CAT APS
15:20 - 15:40	Zvieri - Break
15:40 - 17:00	**Session V: Case studies and future**
15:40 - 16:00	Andrew McCarthy, EMBL
16:00 - 16:20	Sandro Waltersperger, PSI
16:20 - 16:40	Timm Maier, University of Basel
16:40 - 17:00	Gwyndaf Evans, DLS
18:00 - 22:30	Conference dinner (Swiss Fondue at Trotte Villigen)

Day 3: Friday, November 8th, 2012

Time	Event
08:30 - 17:00	**Practical for data collection at beamline X06DA and data processing**
12:00 - 13:20	Lunch (WSLA/SLS entrance hall)
18:00 - 21:00	Dinner (Metzgete buffet at restaurant OASE Villigen PSI)