MS46-T01

Crystallography Hic et Nunc (Quo Vadis revisited).
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There is growing concern, particularly in the United States, that education in general is neither training adequate numbers of students for careers in science and technology, nor developing broad scientific and technological literacy that is necessary for full participation in society. In our own field of crystallographic science, recently we have seen high profile and embarrassing retractions in the peer reviewed literature, often the result of pathological science or inadequate review. Academic crystallography has largely migrated from a research specialty to a technique employed by a wide community of users. Few university departments hire faculty capable of teaching crystallography, and formal courses have all but disappeared from course catalogs. Yet, increasingly large numbers of "naïve" users, who require more assistance than the experienced user, work in academia and industry. This has led to the growth of and dependence on independently funded workshops and summer schools in crystallography, aimed at different audiences, as well as an increasing dependence on other, non-traditional curricular resources for instruction that allow crystallography to be self-taught. If crystallographic science is to remain vibrant, and the results of its analyses reliable, how will we instruct and train in ways that attract and retain a broad pool of talented people in the next decade? This talk will explore the current state of affairs in crystallographic science, particularly macromolecular crystallography, and survey the ways that crystallographers are pushing the boundaries of technology to educate and train the next generation of scientists.

Keywords: crystallographic education, macromolecular crystallography, World Wide Web

MS46-T02

***RapiData*: A practical course in macromolecular x-ray diffraction data measurement and structure solving at the NSLS**. R.M. Sweet, A. Soares, *Biology Department, Brookhaven National Laboratory, Upton, NY, USA.*

Synchrotron radiation is an indispensable tool for many macromolecular crystallography groups. Some synchrotron-specific skills are learn best in an intensive hands-on training program. To provide such an educational experience, we have designed a course in Rapid Data Collection and Structure Solving, which we have presented twelve times.
The course accommodates nearly 50 students. All students are encouraged to **bring their own specimens** for data collection, and to bring old data for the data-reduction and structure-solving tutorials. The course includes an optional five-hour lecture course on the fundamentals of crystallography, then two days of lectures on detailed aspects of data collection and structure solving. Then for two more days we move to the NSLS for data collection, and concurrent tutorials on the contents of the lectures.
Students are divided into 10 sections. Each section gets a total of about 20 hours on a beamline, including undulator beamlines if appropriate. A crystal-preparation lab is available for all students, with crystals supplied for those without crystals, and a beamline is available for these students to try their hand at diffraction measurements on sample specimens they will have mounted themselves. The course is sponsored by grants from the US National Institutes of Health, and Department of Energy, and by donations and in-kind assistance from pharmaceutical and equipment companies.

MS46-T03

Update on the Tutorial for Learning and Teaching Macromolecular Crystallography.
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The previously described macromolecular crystallography tutorial [1] has been significantly revised and expanded. Two new experiments (SIRAS and RIP) have been designed to complement the five experiments (S-SAD, MAD, MR, ion binding and ligand binding) of the first edition of the tutorial for learning and teaching macromolecular crystallography. Furthermore, the tutorial has been re-organized and in part re-written to reflect the comments and suggestions of the users. The most significant overhaul was applied to the data processing part of the tutorial. A major design feature of the tutorial is that all of the utilized proteins used are commercially available; they can be easily and reproducibly crystallized and mounted for diffraction data collection. For each of the seven experiments the raw images and the processed data are provided for learning or teaching the steps of data processing and structure determination.

[1] Faust *et al.* (2008). *J. Appl. Cryst.* 41, 1161-1172.

Keywords: teaching of crystallography, training, X-ray crystallography of biological macromolecules

MS46-T04

Applications of the Cambridge Structural Database in Chemical Education.
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The Cambridge Structural Database (CSD) represents a vast and ever growing compendium of accurate 3D structures that has massive chemical diversity across organic and metal-organic compounds. For these reasons, the CSD is finding increasing application in chemical education. This talk will introduce a teaching subset of more than 500

CSD structures created specifically to illustrate key chemical concepts, and a number of teaching modules that make use of this subset in a teaching environment. All of this material is freely available from the CCDC website, and the subset can be freely viewed and interrogated using WebCSD, an internet application for searching and displaying CSD information content. Examples of more extensive educational applications that utilise the complete CSD System will also be reviewed.
The educational value of visualising real 3D structures, and of handling real experimental results, will be stressed throughout.

Keywords: Teaching, Cambridge Structural Database, WebCSD

MS46-T05

Teaching Protein Crystallography using Interactive Whiteboard Technology. Ehmke Pohl, *Department of Chemistry, School of Biological and Biomedical Sciences, Biophysical Sciences Institute, Durham University.*
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Today's modern pedagogical concepts all recognize that learning experience and outcome is optimal when teaching is an active process with frequent interactions between teacher and students. It is widely accepted that understanding of the subject is best achieved through discovery, collaboration and dialogue.
Interactive whiteboards (IWB) allow the use of various electronic devices to draw on projections based for example on Powerpoint presentations. Teacher and students can directly annotate figures, drag-and-drop text and illustrations from one application to another and save all actions in electronic form. This material can then be evaluated and corrected before being distributed to all students. Furthermore, IWBs offer the advantage that the mouse control can be replaced by hand movements, which allows students to interact intuitively with the material displayed. Direct engagement is clearly motivating for all students but it also encourages lecturers to adopt innovative teaching methods and hence go beyond the safety of their regular powerpoint presentations.
IWB technology has been adopted for the protein crystallography course, which is one module in the newly established MSc in Biomathematics postgraduate program led by the Mathematics Department at Durham University. The PX course covers a wide range of topics from basic structural biology concept to mathematical crystallography and protein structure determination. Here, we will present general ideas and specific examples how IWB are utilized to enhance student's learning experience and outcome.

Keywords: interactive whiteboard, crystallography, structural biology

MS46-T06

Interactive 3D Visualization of Plane Groups and Layer Groups Using the SGV. Eckhard Hitzer[a], Christian Perwass[b]. [a]*Applied Physics, University of Fukui, Japan.* [b]*Raytrix GmbH, Kiel, Germany.*
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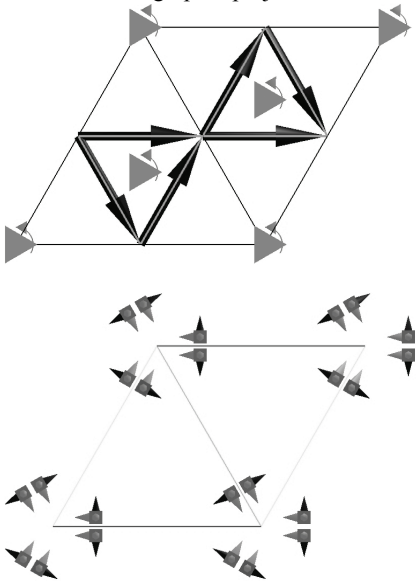
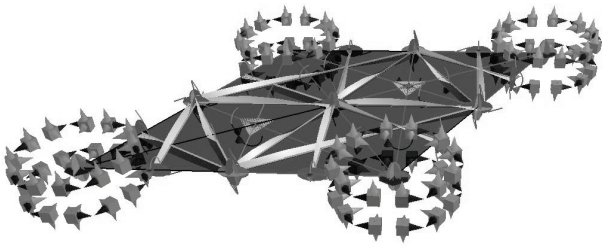
In this presentation we will show how the Space Group Visualizer (www.spacegroup.info) interactively visualizes two-dimensional (2D) plane groups [1], and layer groups [2]. We demonstrate how to successfully display the 17 plane 2D space groups in the interactive crystal symmetry software Space Group Visualizer (SGV). The SGV is based on a new type of powerful geometric algebra visualization platform CLUCalc.
The principle is to select in the SGV a three-dimensional super space group and by orthogonal projection produce a view of the desired *plane 2D space group*. The choice of 3D super space group is conveniently summarized in a lookup table. The direction of view for the orthographic projection needs to be adapted only for displaying the plane 2D space groups Nos. 3, 4 and 5. In all other cases space group selection followed by orthographic projection immediately displays one cell of the desired plane 2D space group, see e.g. the plane space group *p31m* in the Figure.



The full symmetry selection, interactivity and animation features for 3D space groups offered by the SGV software become thus also available for plane 2D space groups. A special feature is, that by canceling the orthographic pro-jection every plane 2D space group is seen to be a *subgroup* of a corresponding 3D super space group.
The visualization of *all* 80 *layer groups* relies on the SGV features of view reduction to 3D cells with 2D translations. It will be explained how to visualize layer groups, together with concrete examples. See e.g. *p6mmm* in the Figure below.



[1] Hahn, T. (ed.), *Int. Tables for Crystallography, Vol. A*, 5th ed., Springer, 2005. [2] Kopsky, V., Litvin, D.B. (eds.), *Int. Tables for Crystallography, Vol. E*, 1st ed., Kluwer, 2002.

Keywords: interactive 3D visualization, plane groups, layer groups