IUCr Crystallographic Computing School Melbourne 2023

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Saturday 19-Aug-2023

15:00-18:00h	Arrival
18:00h	Dinner
19:30h	School organizers
	Welcome/Introduction
20:00h	Harry Powell

Now you see it…
a short history of visualisation in (molecular) crystallography

How we view structures has changed dramatically over the course of the last 110 years since the first X-ray structures were published. In addition to the actual views that are presented, the way that the images are produced has also changed. All the early models were either drawn by hand or physically modelled in three dimensions, and it was only after about 50 years that computer systems were both advanced and available enough to allow structural scientists to start producing the views that we expect to see today.

Since my background is in molecular crystallography, I will concentrate on a few aspects of structure representation that are encountered in chemical and macromolecular crystallography and not on those with which materials scientists may be more familiar. In passing I may mention some historical aspects that I think might be illuminating.

21:00h	Drinks

Sunday 20-Aug-2023

9:00h   Christian Jelsch
Visualizing intermolecular interactions on the Hirshfeld surface
MoProSuite is a software for the charge density refinement using very high resolution X-ray data or modelling using ELMAM2 atomic database. It allows electrostatic energy computation between molecules/atoms in interaction.The Hirshfeld surface is the region of space where the electron density of a molecule is equal to that of its surroundings (when considering a crystal packing) or of an interacting molecule. The atomic contacts on the surface can be decomposed in terms of interacting chemical species X,Y with software MoProViewer (crm2.univ-lorraine.fr/en/software/mopro). The program computes the contacts enrichments Exy, which highlights the contacts types which are over-represented, given the chemical composition of the interacting molecules. The surface can colored according to molecular properties suchas the chemical species, electron density or electrostatic potential and the statistics numbers can be saved. Scatterplots of the electrostatic potential provide a fingerprint of intermolecular contacts and of the electrostatic complementarity.

10:00h   Christopher Gutiérrez
Creating dynamic figures and cover artwork using open- source Blender (Part 1)
In these two interactive workshops, I will give a real-time interactive introduction to making scientific figures and cover artwork using Blender, a powerful (and free!) open- source software for rendering 3D objects.

In Part 1, I will first discuss the importance of creating efficient figures and will provide tips on improving work- flow. Next, we will together run through simple interactive Blender exercises that will go over the basics of how to create and edit objects/structures, and how to light and render a scene.

11:00h   Coffee break
11:30h   Discussions/Projects
12:30h   Lunch
13:30h   Robert Hanson
Web-based visualization of crystal structure and symmetry
14:30h   Tutorials
16:30h   Coffee/Tea break

17:00h	Koichi Momma
	Visualizing magnetic structures and quasicrystals
18:00h	Dinner in nearby restaurants
20:00h	Simon Billinge
	Plotting data with Matplotlib: tips and tricks

This talk will be down in the trenches and aimed at a target audience of programmers. Those of us who use Python extensively for our data analysis and modeling find ourselves often making plots and figures using the ubiquitous matplotlib package. It is deliciously easy to use to make great exploratory graphics using its defaults and interactive plot interfaces. On the other hand, it gets tedious when we want to start making publication quality graphics for our papers. I will share a number of tips and tricks for making this part more straightforward and resulting in better looking figures more quickly, for example, the use of style sheets, and powerful gridding tools. I will share a few style tips about along the way, but mostly it will be about how to structure your code to make better matplotlib figures more easily.

21:00h	Drinks

Monday 21-Aug-2023

9:00h	Alan Coelho
	Programming visualization in TOPAS

TOPAS is an optimization/refinement program and the display of data whilst a refinement is running gives insight into the process. It incorporates the graphical display of X- ray powder diffraction data in terms of charts and 3D graphics for displaying atomic structures using OpenGL. Such dynamic display of data requires programming techniques that are robust and computationally fast. These techniques include the use of a DataTree for storing program data, computer algebra for allowing the User to communicate with the DataTree, and, keeping the DataTree 'Live'. A Live DataTree is simply the concept that items within the tree are always up-to-date and valid. Many algorithms are unique and rewriting already existing third-party algorithms have largely been avoided. Use of a single programming language, c++, has simplified the task of coding. TOPAS is also a large program and without the techniques described it would have probably died a long time ago.

10:00h	Christopher Gutiérrez
	Creating dynamic figures and cover artwork using open-source Blender (Part 2)
	In these two interactive workshops, I will give a real-time

interactive introduction to making scientific figures and cover artwork using Blender, a powerful (and free!) open- source software for rendering 3D objects.

In Part 2, we will go over more advanced skills such as importing and visualizing atomic structures (e.g. from PDB or protein data base files) and other 3D structures, such as CAD models and Fermi surfaces.

11:00h	Coffee break
11:30h	Discussions/Projects
12:30h	Lunch
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16:30h	Coffee/Tea break
17:00h	Gemma de la Flor

Visualizing symmetry

There are different ways to visualize symmetry and Python offers several interesting possibilities. This lecture is mainly focused on the use of the Python libraries matplotlib and graphviz for symmetry visualization. Different ways to visualize symmetry will be explored, such as the construction of stereographic projections for three-dimensional point groups or group-subgroup related graphs.

18:00h	Dinner in nearby restaurants
20:00h	Rita Giordano

Visualising statistics: The art of transforming scientific results into visual graphics

The use of data visualization enables readers to gain a more in-depth understanding of scientific findings presented by their peers.

Scientists rarely apply data visualisation principles.

In general, they give extra care in planning and conducting their research, but show less care for chart design.

The art of data visualization encompasses more than just charts. Charts alone are not enough if colours, annotations and accessibilities are not also considered and well-designed. If a chart is incapable of conveying a narrative, it indicates that something is absent.

In science, data visualisation is often seen as the cherry on the cake and therefore is not necessary.

This talk aims to show that using data visualization is more than just a pretty thing to look at. It's an important part of the whole picture.

21:00h	Drinks

Tuesday 22-Aug-2023

9:00h	**Martin Lutz**

Martin Lutz
Visualising X-ray intensities from single crystals
Currently, single-crystal X-ray reflections are usually recorded on a two-dimensional detector. The corresponding reflection profiles are three-dimensional. Methods for displaying the profiles and difference-profiles will be demonstrated.

10:00h   Professor Stephen K. Burley, M.D., D.Phil.
Protein Data Bank: Understanding and Visualizing 3D Biostructure Quality
Approximately 87% of the more than 200,000 atomic-level three-dimensional (3D) biostructures in the PDB were determined using macromolecular crystallography (MX). Agreement between 3D atomic coordinates and experimental data for >100 million individual amino acid residues occurring
within 150,000 PDB MX structures have been analyzed in detail. The real-space correlation coefficient (RSCC) calculated using the 3D atomic coordinates for each residue and experimental- data-derived electron density enables outlier detection of unreliable atomic coordinates (particularly important for poorly resolved sidechain atoms) and ready evaluation of local structure quality by PDB users.

Evaluation of MX structure quality will be discussed both in general and in detail, with emphasis on the content of the publicly-disseminated Worldwide Protein Data Bank (wwPDB) validation reports that accompanies each structure.

11:00h	Coffee break
11:30h	School organizers:
	Closing ceremony
12:00h	Lunch
13:00h	Departure to IUCr congress