MS47 New horizons in teaching crystallography in the 21st century

MS47-04
CCP4 Cloud as a system for crystallography teaching
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Abstract
The impressive progress in macromolecular crystallography is owed in considerable part to advances in structure solution software. While this simplifies the structure determination process, the structure determination becomes more accessible to the newcomers. Today, in many cases, structures can be solved without understanding the theoretical underpinnings or an understanding of the methods and algorithms used. However, this creates a risk of diminishing expertise in both theoretical background and efficient use of new tools in software packages, such as CCP4.
CCP4 therefore invests considerable effort into educational programs and software documentation. The educational capabilities of the CCP4 Cloud [1], a new front-end for the CCP4 Software Suite [2], are presented here. CCP4 Cloud has attractive new features, which make it particularly suitable for teaching MX to a range of audience, from undergraduate students to experienced post-doctoral researchers:
1) Web interface, i.e no need for dedicated software installation or specialised computing facilities for most task;
2) Possibility of sharing structure solution projects with teachers and other students, and working on them simultaneously in real-time, irrespectively of geographic location;
3) Provision of CPU power for experimenting with complex automatic software and difficult data on a reasonable time scale;
4) Highly systematic approach to the development of structure solution projects with an ergonomic interface;
5) Developed documentation for individual structure solution tasks, MX methods, and techniques;
6) Availability of specific tutorials that include data, demo projects, as well as seed projects for guided training and self-education;
7) Open architecture for contributing to the documentation, tutorials;
8) Provision of mechanisms that allow creating setups for own crystallography courses and sharing them with colleague teachers.
Since its first release, CCP4 Cloud is routinely used for teaching crystallography at International Schools and Workshops (e.g. CCP4/DLS Virtual Workshop, South American School, IUCr CCP4/CCP-EM Workshop) as well as university courses. As a community-driven project CCP4 welcomes contributions to software documentation and educational materials from users of these teaching resources and the structural biology community.

References
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