

What's new in CCP4 and developments in the automation of the protein structure solution process

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CCP4, the Collaborative Computational Project Number 4, was set up in 1979 to support collaboration between researchers working on software for protein X-ray crystallography in the UK, and to assemble a comprehensive collection of software to satisfy the computational requirements of the relevant UK groups. The results of this effort gave rise to the CCP4 program suite, which is now distributed to academic and commercial users world-wide.

The program suite is constantly being updated with the latest contributions from developers in the UK and beyond. New releases (currently CCP4 6.0) are made on average once every two years and contain updates to the current programs and the latest contributed packages. Efforts are also being undertaken, in the form of the CCP4 Automation project, to take advantage of the latest developments in computational tools and infrastructure to help automate and speed up the various stages involved in solving protein structures from X-ray image data.

The CCP4 Automation project was set up to produce new software tools to be made available to users via the familiar interface of CCP4 but also to be deployed on automated synchrotron beam-lines. Developments have been made in the areas of image data processing (XIA2), molecular replacement (MrBUMP and BALBES) and experimental phasing (HAPPy). Some of these developments, such as MrBUMP, have been designed to take advantage of computational resources such as on-beam-line or Grid enabled compute clusters to speed up their processing.