Experimental phasing

In its 25 years, CCP4 has become the most successful of the many collaborative computing projects by a considerable margin. Part of this success is because of the study weekends, which are now a well known and well attended part of the crystallographic calendar. This year there were 400 participants, including many people who were present at CCP4’s inception and who are still vital to the development of CCP4. For the last nine years, CCP4 has been chaired by Neil Isaacs. In this time CCP4 has met the challenges presented by changes in technology and initiated major changes in crystallographic software, a legacy that will inspire those looking to the future of CCP4. Neil’s retirement from the chairmanship was marked at the meeting by many tributes, including the presentation by the incoming chairman, Jim Naismith, of an engraved quaich (a traditional whisky drinking cup, for the non-Scottish amongst you) and a little tipple to test it with.

The CCP4 study weekend has a history of teaching those new to crystallography while at the same time presenting recent advances and providing a relaxed and small forum for specialists to come together and share ideas. In the teaching tradition, each session at this year’s meeting started with a talk giving an overview of the session. This set the scene for each session and allowed subsequent speakers more freedom to delve into the details of their particular topic. Garry Taylor and Randy Read started the meeting by introducing the phase problem, giving a rapid tour through the current methods of solving it; Elspeth Garman gave a vibrant talk on heavy-atom preparation; Ana Gonzalez rated data-collection methods and introduced a ‘Michelin Star Guide’ to synchrotrons; Ralf Grosse-Kunstleve described the different methods for finding heavy-atom sites with a special emphasis on the challenges of symmetry and special positions; Simon Parsons explained twinning with the humble London brick; and Gerard Brion and Clemens Vonrhein doubled up to present the theory and some impressive results from the latest version of the experimental phasing program SHARP.

Many talks at the meeting illustrated how different limitations on experimental phasing are still being overcome by a combination of new approaches, new software and new derivatization methods. Frank von Delft, Phil Evans and Ditlev Brodersen provided examples of difficult phasing problems either involving a very large substructure or a very large macromolecule or both. Results from recent experiments using sulfur anomalous dispersion or in-house phasing methods with chromium radiation also looked promising. For some, radiation damage was a problem to be avoided but for others it promises to be a tool to exploit for phasing. Raimond Ravelli and Domenika Borek in particular presented the case for the latter. A session on twinning gave inspiration to those struggling with twinned data, as Zbignew Dauter, Anke Terwisscha van Scheltinga and Dimitry Alexeev showed that twinned structures can be solved by MIR and MAD methods.

The meeting seemed to be enjoyed at many levels, by speakers and participants alike and conveyed some of the excitement of the many new developments in experimental phasing. We would like to thank all our speakers for the excellent contribution they made and for recording their research in these proceedings.