Poster Presentation

Ten years of the CCP4/APS school in macromolecular crystallography

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Computational Collaborative Project #4 (CCP4) has a rich tradition of conducting computational workshops worldwide. Ten years ago the CCP4 joined forces with the GM/CA group at Argonne National Laboratory (ANL) to organize first such workshop in the US. Starting in 2009, a data collection component was added, transforming the computational workshop into a broad crystallographic school. The school is typically held in the second half of June at the Advanced Photon Source (APS) of ANL, near Chicago. Applications to the school are accepted from graduate students, postdocs and young independent scientists worldwide, and 20 are selected for participation. The school is designed for researchers with some expertise in crystallography; it is not an introductory course. The main focus is to address crystallographic problems in data collection, data processing, phasing and refinement.

The school comprises two workshops – data collection and computation. Data collection is carried out on the GM/CA@APS beamlines (https://www.gmca.aps.anl.gov), funded and operated by the National Institute of General Medical Sciences (GM) and the National Cancer Institute (NCI, CA) of the NIH. The 23ID-D and 23ID-B beamlines are equipped with Pilatus3 6M and EIGER 16M detectors, respectively. The photon flux and X-ray optics on the beamlines offer highly intense and stable beam in sizes from 5 to 100 micrometers, making them particularly well suited for data collection from technically challenging samples. Data are collected only from the participants' crystals under the supervision of GM/CA staff, data processing software developers and other experts.

The computational workshop is organized in three daily sessions with lectures in the morning followed by tutorials and hands-on problem solving in the afternoon and evening. Over the last ten years, many software programs and packages have been presented at the school by the developers and other premier experts, including ARCIMBOLDO (G. Shedrick), ARP/wARP (A. Perrakis, G. Langer, J. Perreira, C. Carolan, T. Wiegels), BALBES (G. Murshudov), BP3 (R. Pannu, I. Sikharulidze), Buccaneer (K. Cowtan), CCP4 (R. Keegan), CCP4mg (S. McNicholas), Coot (B. Lohkamp), Crank (R. Pannu), DIALS (G. Evans, R. Gildea, D. Waterman), HKL2000/3000 (D. Borek), JLigand (A. Lebedev), Molrep (A. Lebedev), MOSFLM (P. Evans, A. Leslie), MrBUMP (R. Keegan), Parrot (K. Cowtan), PDB_REDO (R. Joosten), Phaser (R. Read, G. Bunkozci, A. McCoy), Phenix (P. Adams, T. Terwilliger, P. Afonine, N. Echols, J. Headd), PISA (E. Krissinel), Refmac (G. Murshudov), SHELX (G. Sheldrick, T. Gruene), TLS (E. Merritt), Whatcheck (R. Joosten), and XDS (K. Diederichs, T. Gruene). Data abnormalities and data collection strategies have been also discussed by Z. Dauter of NCI and R. Sanishvili of GM/CA.

To date, nearly 50 publications acknowledged the contribution of the school: http://www.ccp4.ac.uk/schools/APS-school/publications.php. Details of the past and upcoming schools along with contact information can be found on the school web site http://www.ccp4.ac.uk/schools/APS-school/index.php.

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