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CCP4 Cloud: Potential for a European-Wide Resource in Computational Crystallography

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Collaborative Computational Project Number 4 in Protein Crystallography (CCP4 UK), founded in 1979, has a mission to produce, maintain and distribute a world-leading, integrated suite of programs for the determination of biological macromolecular structures in 3d by means of X-ray crystallography and other biophysical techniques. Today, CCP4 Software Suite, used by estimated 25,000 researchers worldwide, represents an enabling technology and underpins academic and industrial research in structural biology on world-wide scale.

Nowadays, experimental part of structural studies is represented by high-throughput lines at synchrotrons, producing tens of TBs of data on daily basis. The data are usually utilised in local research labs with own computational resources and software setups.

Following general trends in modern computing, CCP4 have developed a framework for distributed data processing and structure solution in crystallography, the CCP4 Cloud. The development was released in 2019, and since that adopted by several crystallography centres in the UK and continental Europe. An instance of CCP4 Cloud, capable of satisfying UK's needs in crystallographic computing, is maintained by CCP4 at STFC UK.

The many advantages of online computing: centrally maintained software, databases and project data, geographically agnostic access to considerable computational resources, became particularly obvious during the COVID-19 pandemic. In this presentation, I will reflect on the advantages, desirability and feasibility of making a global, cloud-based resource for computational macromolecular crystallography in Europe, which could combine data streams from experimental facilities, software and computing services, and a uniform user experience based on an interactive, graphical, online access from all modern client platforms.

Speaker bio:
Dr Krissinel leads the Core Group of CCP4, which is responsible for the maintenance, development and distribution of the CCP4 Software Suite in protein crystallography. In 2000-2009, Dr Krissinel worked in the PDBe (former Macromolecular Structure Database, MSD) at the European Bioinformatics Institute, UK, where he became known to the structural biology community for his works in the field of protein-protein interactions (PPI) and protein structure analysis. His software for the PPI and oligomeric state analysis and prediction (PISA), and protein structure alignment (SSM/Gesamt) are widely used and regarded as de-facto standard tools in the field. Before his career in structural bioinformatics and crystallography, Dr Krissinel worked on the theory of time-resolved diffusion and spin control in radical reactions, quantum kinetics (1997-2000 Humboldt Fellow, University of Konstanz, Germany, 1989-1995 Russian Academy of Sciences), and molecular dynamics of metallic alloy microclusters (1995-1997 Argonne National Laboratory, USA).
Weblinks: https://www.scd.stfc.ac.uk/Pages/Eugene-Krissinel.aspx

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