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Building 25F, Seminar Room 456

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Integrative modelling platform for structural biology

We are fascinated by complex computational methods in information processing that can address data interpretation problems as we encounter them in structural biology. Indeed, recognising patterns in experimental data that describe macromolecules is itself an application of artificial intelligence.

Structure determination provides essential data for integrative modelling of the basis of life: DNA, RNA, proteins, macromolecular complexes and assemblies. Current approaches, largely based on macromolecular X-ray crystallography, concentrate on a reductionist view of a single structure from a single method or experiment. Future applications (e.g. a quantitative description of the living cell) will necessitate radically different approaches where a wider context of information, using data from complementary tools, is implemented in computational methods serving as an integrated platform for a model of life.

Some of aspects of integrative modelling will be discussed in the context of one of the group's main foci - the ARP/wARP software project for protein/DNA/ligand crystal structure determination. The comprehensive nature of its automated computational methodologies makes ARP/wARP applicable to the examination of protein assemblies and complexes at both high and low resolution. One of our emerging methods aims at combining X-ray diffraction with low-resolution methods such as electron microscopy, where recognising structural motifs and fold patterns at resolution as low as 20 Å greatly aids investigation of large macromolecular complexes.

Host: F. Stellato & H. Chapman, CFEL Coherent Imaging Division