of liquid crystals on several types of alignment layers.

The results provide direct evidence for the structural dynamics responsible for laser-induced anisotropy as observed by polarisation holography [1], and gives an intriguing insight into the interaction of forces acting on liquid crystal molecular arrangements.

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Keywords: liquid crystals, laser-induced alignment, grazing incidence X-ray diffraction

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MS90 APPLYING NON-CRYSTALLOGRAPHIC ALGORITHMS TO CRYSTALLOGRAPHY

Chairpersons: Ralf W. Grosse-Kunstleve, Maryjane Tremayne

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Cluster Analysis in Crystallography

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Cluster analysis is a well established tool in statistics, but one that is used surprisingly little in crystallography despite its considerable potential. We have established its use in several diverse areas of crystallography, in particular:

1. Pattern matching in powder X-ray diffraction: High throughput screening experiments designed to search for polymorphs and salts of drug candidates use PXRD to characterize the results, and this produces large quantities of data. We show how pattern matching methods based on appropriate correlation coefficients can be used in conjunction with clustering calculations to classify patterns automatically [1,2].
2. Databases: Database searching using the Cambridge Structural Database (CSD) [3] can produce thousands of 'hits' if a simple fragment is used, and as a result processing and interpreting the results becomes a considerable task. Cluster analysis using dendrograms, metric multidimensional scaling and suitable visualization tools can reduce the workload to a few hours of computer time with minimal user intervention.
3. Indexing powder patterns: In difficult indexing problems, it is possible to produce a large number of potential unit cells with figures of merit that are only marginally useful. Cluster analysis can be useful here, especially when self-organizing maps are utilised.

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Keywords: cluster analysis, pattern matching, databases

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Crystal Structures from Powder X-ray Diffraction using Genetic Algorithms

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Contemporary advances of direct space strategies in solving crystal structures directly from powder X-ray diffraction data [1,2], and in particular, the success of the Genetic Algorithm method [3], have opened up a whole area of research which has hitherto been inaccessible even as recent as fifteen years ago. Applications to the study of synthetic products *in situ*, as well as the tackling of structural problems which have the complexity of more than one molecule in the asymmetric unit, are now at the forefront of these techniques. In addition to tackling such new challenges, structure solution strategies employing other analytical or computational methods have become a natural complement alongside the X-ray diffraction data. For example, multi-component molecular co-crystals have been prepared by an *in situ* solid state grinding process, yet have been solved using a combination of powder X-ray diffraction and solid state NMR techniques [4]. Moreover, the collection and assessment of reliable powder diffraction intensity prior to structure solution calculations is an avenue of study that shows considerable promise [5].

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Keywords: diffraction data, powder diffraction, X-ray crystallography of organic compounds

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Powders, Prediction and Epitaxy: Applications of Differential Evolution

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Differential evolution (DE) is a robust and efficient global optimization algorithm based on evolutionary principles, which has been applied to a wide range of problems [1]. It shares the attractive features of other evolutionary algorithms but has a simpler implementation and fewer user defined control parameters enabling a greater insight into the control of the optimization process to be achieved.

Direct space methods of structure determination from powder diffraction is a field of rapid growth due to a number of computational and experimental developments [2, 3]. DE has been successfully applied to the determination of a number of organic and inorganic molecular structures from laboratory powder data.

The DE algorithm has also been applied to the prediction of crystal structures and epitaxial interfaces of organic crystals. In both cases, the lattice energy of the trial packing is calculated by an appropriate force field and then minimized by the DE algorithm. Utilization of a Beowulf cluster enables optimization of the DE algorithm control parameter to be performed in parallel.

In this talk, I will discuss these applications of DE with particular attention to the optimization of the performance of the algorithm, while highlighting areas of potential improvement and future developments.

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Keywords: optimization algorithms, ab-initio powder structure determination, epitaxy

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Refinement when Amplitudes aren't enough: Real-Space, H-Bonding & Electrostatics

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Methodological improvements have reduced, but not eliminated over-fitting in macromolecular structure refinement. It is well known that over-fitting depends on freedom in the atomic model compared to the quality and quantity of the experimental data. The latter depends on resolution – 3 Å usually being considered the minimum.

Our goal is to improve the robustness of refinements at resolutions that are at best marginal, by using fully the available data, or by adding stereochemical restraints to the model freedom. Real-space refinement is most advantageous when model-independent phases can be used as additional data. The local nature of the refinement eliminates the over-fitting due to compensating errors that occurs in reciprocal-space where all atoms depend on all data points. Atomic density functions that rigorously incorporate resolution limits allow