

KN09

The charge flipping method: a new approach to solve periodic and aperiodic structures Gábor Oszlányi, András Sütő, Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, H-1525 Budapest, POB. 49, Hungary. E-mail: go@szfki.hu

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The talk summarizes the current state of charge flipping, a recently developed and deceptively simple algorithm of ab initio structure determination [1,2]. This algorithm is iterative and works in dual spaces. Its operation is based on the presence and perturbation of large plateaus of low electron density, but not directly on atomicity or statistical phase relations. Such a working principle radically differs from that of classical direct methods, and offers complementary applications. Charge flipping can be used at different stages of the structure solution process. It can either operate in a truly ab initio manner, without utilizing any preliminary structural information (atom types, chemical composition or space group symmetry), or can be applied to complete a partially known structure or phase set, it can check the stability of a solution, but it can also be adapted to work as an ingredient of other dual-space schemes.

The list of already successful structure solution cases includes periodic and aperiodic crystals using single crystal and powder diffraction data measured with X-ray and neutron radiation [3-12]. Apart from counting applications, the talk mainly deals with algorithmic issues: it describes the basic algorithm and its properties, introduces and compares new improvements of the iteration scheme in real and reciprocal space, helps to identify convergence by new figures of merit, defines the computational cost of a single solution and helps to find parameters that maximize the efficiency of the algorithm. It also discusses the present limitations of structure size, data completeness and of utilizing known information. Finally, we try to foretell what is the future of such an alternative among well-established direct methods.

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KN10

Combining Electron Microscopy and X-Ray techniques Jorge Navaza, Laboratoire de Microscopie Electronique Structurale.IBS, Grenoble, France.

Transmission Electron Microscopy (TEM) and X-Ray crystallography are two complementary techniques used in structural biology. TEM fascinates by its apparent simplicity to visualize isolated biological systems in almost "in vitro" conditions. The observed systems are, in

general, large assemblies of macromolecular structures, for example virus and viral particles. The main limitation of the technique is the rather low resolution of the produced images, usually in the nanometer range.

On the other hand, X-Ray crystallography routinely determines the structures at atomic resolution of individual proteins or complexes involving a limited number of proteins. In most cases the phase problem is solved either experimentally (isomorphous replacement and related techniques) or by numerical methods where the information coming from previously determined molecular structures is efficiently used (molecular replacement). However, in the case of the very large complexes that are now crystallized, phasing by isomorphous replacement is often difficult and atomic models do not exist, in general. In these cases, EM and X-Ray data may be combined to start the process of crystal structure determination. Indeed, an initial phasing model may be a low resolution EM reconstruction of the complex used as a probe in the molecular replacement method. Phases are then extended by density modification, i.e. solvent flattening and non-crystallographic symmetry averaging.

This has been done in the case of big icosahedral particles(virus) where the high symmetry is a guarantee of success in the phase extension process. Moreover, the model is usually obtained by cryo-TEM, a technique that already provides a good representation of the particle in the crystal.

More recently we have applied the technique to multimeric proteins, a classic protein crystallography problem. The particles sizes were too small to use cryo-TEM so that the 3D reconstructions were performed using negatively stained samples. The main problems to solve are linked to the solvent contribution to the observed structure factors at low resolution, which is the range of resolution at which EM and X-Ray data overlap.

But EM and X-Ray data may also be combined the other way: very often X-Ray crystallography determines the structures of the individual proteins that constitute the assemblies whose low resolution reconstructions were determined by TEM. It is then possible to interpret the EM image in terms of atomic models, which brings considerable complementary information to molecular biologists.

This is achieved by docking individual molecules into the EM image, a technique related to molecular replacement, though a simpler one, as the role of observed structure factors is now played by the Fourier coefficients of the EM map, which provides both moduli and phases.

The combined use of EM and X-Ray data will be illustrated with some applications to viral and sub-viral particles, and some multimeric proteins.

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Most of materials exhibits pressure induced phase transformations which can induce strong modification of their properties (electronic, magnetic...). These properties are often related to the interaction between the neighboring atoms and therefore the knowledge of the