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Analytical symmetry detection in protein assemblies. II. Dihedral and Cubic symmetries

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Abstract

Protein assemblies are often symmetric, as this organization has many advantages compared to individual proteins. Complex protein structures thus very often possess high-order symmetries. Detection and analysis of these symmetries has been a challenging problem and no efficient algorithms have been developed so far. This paper presents the extension of our cyclic symmetry detection method for higher-order symmetries with multiple symmetry axes. These include dihedral and cubic, i.e., tetrahedral, octahedral, and icosahedral, groups. Our method assesses the quality of a particular symmetry group and also determines all of its symmetry axes with a machine precision. The method comprises discrete and continuous optimization steps and is applicable to assemblies with multiple chains in the asymmetric subunits or to those with pseudo-symmetry.

We implemented the method in C++ and exhaustively tested it on all 51,358 symmetric assemblies from the Protein Data Bank (PDB). It allowed us to study structural organization of symmetric assemblies solved by X-ray crystallography, and also to assess the symmetry annotation in the PDB. For example, in 1.6% of the cases we detected a higher symmetry group compared to the PDB annotation, and we also detected several cases with incorrect annotation. The method is available at http://team.inria.fr/nano-d/software/ananas. The graphical user interface of the method built for the SAMSON platform is available at http://samson-connect.net.

Keywords: Point-Group Symmetry, Cubic Groups, Group Theory, Discrete Optimization, Protein Structure, Continuous Optimization

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