show that it is able to accurately identify the NCS operators between the various copies and superpose the structures to within 3Å of each other. This algorithm has proven to be rapid, robust and accurate. The performance of the algorithm is as good as or better than previous methods using refined models, despite the fact that this approach uses only a rough approximation of the backbone.

[1] Pai R., Sacchettini J.C., Ioerger T.R., I*dentification of NCS: A Feature Based Approach*, *Bioinformatics*, 2005, *submitted*.

Keywords: non-crystallographic symmetry, pattern recognition, averaging

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Structural Classification and Analysis of Homo Oligomer Interfaces of Proteins

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We tried to classify and analyze all the protein-protein interfaces to further understand the protein-protein interactions, paying attention to the interface of homo oligomer (homo-interface) and the molecular surface of proteins with physicochemical properties on the surfaces.

First, 374 homo-interfaces assumed to be biological interactions were selected for the analyses from 867 SCOP-fold representatives. Then they are classified into *dimer-type*, *cyclic-oligomer-type* and *twisted-type* interfaces according to the rotational symmetry of the interfaces, and the dimmer-type interfaces are further classified into *parallel, perpendicular* and *circular* classes according to the direction of spreads of interfaces against the crystallographic two-fold axis. In addition, we have analyzed the correlation between the classification and physicochemical properties such as hydrophobic interactions, electrostatic interactions and the shape complementarities of the molecular surface at the interaction sites.

As the results, we have found some strong tendencies between the classification and the physicochemical properties. For examples, (1) for the twisted-type interface, hydrophobic interactions and shape complementarities are preferably used, and (2) the parallel dimer-type interfaces tend to use hydrophobic interactions, but the perpendicular dimer-type interfaces are usually used electrostatic interactions.

Keywords: structure-function relationships, protein-protein interactions, interface surface

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Monte-Carlo Simulations of Radiation Damage Produced in Protein Crystals

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The data quality and the achievable resolution in X-ray structure analysis of protein crystals is limited by radiation damage. The aim of this investigation is a better quantitative understanding of the damage produced by the absorption of photons and the subsequent processes in protein crystals by Monte-Carlo approach.

The dominating inelastic interaction for X-ray photons with an atom in a protein crystal is the photo-effect, in which high energy photo-electrons and low energy Auger-electrons are created. At higher X-ray energies Compton scattering becomes dominant. In this case most of the energy is kept by the scattered photon, which interacts for normal protein crystal sizes usually once. The produced electrons have a high inelastic cross-section, so the resulting electron cascade has a high damage-potential.

By means of the simulation the electron cascade and the spatial distribution of ions and excited atoms produced by inelastic interactions are analyzed in order to obtain more quantitative information on the damage. Also, the average time for a cascade is evaluated. One of the aims of these investigations is to find the optimum data collection energy for a given chemical composition.

Keywords: radiation damage, protein crystals, synchrotron radiation

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Visualization of Structural Information with xPSSS

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A new molecular graphics viewer, jV [1], has been extended to display structural volume data, like electron densities. Display of these data is possible either as contour line grids or as isosurfaces. xPSSS, found at http://www.pdbj.org/xpsss/, uses an applet version of the viewer to display such volume information. Electron density maps are available for about 15,000 structures of the PDB and were calculated from deposited X-ray structures refined against deposited structure factor data. The visualization capabilities have been further extended to display other grid-based information such as molecular orbital data generated by the program AMOSS, stored in XML-format.

The software for most of the calculations is written in Python and Fortran-95 modules for computationally intensive operations. These modules are used as Python extensions. The volume data are stored in a binary byte-map format. Contour and isosurface data are stored as XML files.

[1] Kinoshita K., Nakamura H., *Bioinformatics*, 2004, **20**, 1329.

Keywords: databases, data representation, visualization

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Monte-Carlo Simulation of the Incommensurate Structure of 4,4'-Diethoxyazoxybenzene

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The aim of this work is to describe the behavior of an incommensurate molecular crystal using molecular dynamics simulations (MD). Incommensurate crystals are part of the more general class of aperiodic material. In addition to diffraction methods, molecular dynamical methods can be applied in order to give some information on the mechanisms leading to the aperiodicity of crystalline structures. Incommensurate crystals exhibit sometimes characteristics of disorder which should also be included in the modelling. The calculations are performed with the parallel code *ddgmq* [1]. The compound is 4,4 -diethoxyazoxybenzene (PAP) [2]. This compound exhibits two distinct crystalline phases from melting down to 100K. Phase II, stable above 356 K is described by a triclinic space group. Phase I is incommensurately modulated. The disorder is due to the distribution of the oxygen of the azoxy group on two possible sites.

Currently a model has been investigated in order to determine the correct sequence of the oxygen position with the development of a code based on the metropolis algorithm. Our aim is to find the configuration with the lowest energy. This structure will be used to initiate the molecular dynamic simulations.

[1] Brown D., Minoux H., Maigret B., *Comp. Phys. Comm.*, 1997, **103**, 170-186. [2] Pinheiro C.B., Gardon M., Pattison P., Chapuis G., *Ferroelectrics*, 2004, **305**, 83-87.

Keywords: disordered incommensurate, molecular dynamics, computational methods