abnormally large errors in the phase of systematically weak reflections. To avoid this, special treatment is needed. Direct methods have been developed to solve the phase problem for small structures having pseudo-translational symmetry. The method can be used to obtain the actual heavy-atom substructures from the Bijvoet differences in the presence of pseudo-translational symmetry. Various phasing procedures have been tested and compared using a set of artificial protein SAD data.

Keywords: SAD phasing, pseudo symmetry, proteins

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Automated Web- and Grid-Based Protein Phasing with *BnP*

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BnP is a protein structure-determination package that couples the direct-methods program *SnB*, used to locate heavy-atom substructures, with parts of the protein-phasing suite *PHASES* [1]. Thus, *BnP* provides an automated pathway from intensity data to an unambiguous protein electron-density map. In large or difficult cases, substructure determination can be a bottleneck. However, the *Shake-and-Bake* algorithm that is used to phase substructures can be readily adapted to a parallel computing environment and throughput increased in direct proportion to the number of available nodes.

Versions of *BnP* with a Java interface are currently available from http://www.hwi.buffalo.edu/BnP/. In addition, a new interface has been developed in PHP, a general-purpose scripting language that is especially suited for web development and allows users to run *BnP* from a browser displaying dynamically created web pages. It supports remote computation and has the capability of distributing multiple parallel jobs over a computational grid. The PHP version has been implemented on a stable prototype grid that was developed at SUNY Buffalo's Center for Computational Research and includes hardware at several different locations. An elegant backfill facility provides access to idle CPU time on many machines and makes it available for *BnP* calculations without disturbing other jobs. This work was supported by NIH grant EB002057 & NSF ACI-0204918.

[1] Weeks C. M., *et. al*., *Z. Kristallogr*., 2002, **217**, 686-693.

Keywords: shake-and-bake, parallel computing, automation

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A Deterministic Algorithm for Phasing Using Triplet and Quartet Invariants

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Traditional approaches to the crystallographic phase problem minimize merit functions of structural geometry to determine the missing phases [1]. To accurately model the diffraction physics, these merit functions are highly nonlinear and multimodal. As a result, phasing requires the solution of challenging global optimization problems. Trial-and-error, in combination with local search, has been used extensively to solve these optimization problems but is a tedious and difficult process, even for small molecules.

For centric structures, the phase problem has recently been approached via combinatorial optimization techniques that are guaranteed to find a global optimum of a minimal principle formulation of the phase problem [2]. This methodology leaves no ambiguity regarding the correctness of the phases thus derived.

We study how the addition of quartet invariants to the phasing model affects the resolution limits of the previous work [2], which only included triplet invariants. Phasing is accomplished with a polynomial-time binary Gaussian elimination algorithm. For a collection of structures, our methodology leads to considerably improved solutions at lower resolutions.

[1] Debaerdemaeker T., Woolfson M. M., *Acta Crystallographica A*, 1983, **39**,193-196. [2] Vaia A., Sahinidis N. V., *Acta Crystallographica A*, 2003, **59**(5), 452-458.

Keywords: direct methods, low-resolution phasing, optimization

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Neutron Structure Determination via Macromolecular H/D Derivatives

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The principle of H_2O/D_2O solvent variation (Schoenborn, 1976) in neutron diffraction has long been used as a tool for structural phasing. The first crystal structure application of this procedure gave a 5Å map for the peptide antibiotic gramicidin A that was originally crystallized from ethanol (Koeppe & Schoenborn, 1984). A gramicidin derivative was synthesized for which the two methyl groups of Val^1 had been deuterated, to be contrasted with the native wild-type hydrogenated structure. Unfortunately crystals of sufficient size could not be obtained to help extend the initial 5Å model to the 2.5Å limit of the native data.

A problem arises when multiple H/D replacement sites are covalently bound to the same atom, in that these atoms will be only 1.7Å apart: the substructure can not be easily determined by conventional ΔE direct methods unless data are measured to better than 1.2Å. This is highly unlikely due to the weak flux rates at most neutron scattering facilities.

We have devised a new structure determination method for such H/D derivative applications which allows one to obtain the macromolecular phases directly without first having to solve the substructure, such that lower resolution neutron data sets can be successfully utilized. Support from NIH grant EB002057 is gratefully acknowledged.

[1] Schoenborn B. P., *Biochim. Biophys. Acta*, 1976, **457**, 41-55. [2] Koeppe R. E. , Schoenborn B. P., *Biophys. J*., 1984, **45**, 503-507.

Keywords: neutron diffraction, direct methods, macromolecular phase determination

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A Modified ACORN to Solve Protein Structures at Resolutions of 1.7 Å or Better

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The first development of ACORN provided an efficient density modification procedure for the *ab initio* solution of protein structures with diffraction data to better than 1.3 Å starting with poor phases. An initial phase set could be obtained from a variety of sources such as the position of a heavy atom, a set of scatterers such as Sulphur atoms that had been positioned from anomalous dispersion measurements, a fragment or a very low homology model placed from a molecular replacement search. New procedures have been developed that yield good quality maps with data sets of resolution down to 1.7 Å. These new developments involve the artificial extension of data to atomic resolution and novel density-modification processes that develop density at atomic positions that was previously suppressed. The several known protein structures have been tested starting from a heavy atom, small α-helix and a model from molecular replacement search. The F-map from ACORN can be trace easily and the E-map can show most atom positions with the data extended to atomic resolution.

Keywords: data extension, density modification, Sayre equation refinement

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Electron Density of $ScRh_3B_x$: Relation of the Electron Density to the Hardness

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