**Identifying NCS in Electron Density Maps: A Pattern Recognition Approach**

Reetal Pai[a], James Sacchettini[b], Thomas Ioerger[a], [a]*Department of Computer Science, Texas A&M University, Texas, USA.* [b]*Department of Biophysics and Biochemistry, Texas A&M University, Texas, USA.*
E-mail: reetalp@cs.tamu.edu

The determination of the NCS operators between multiple copies of a protein in an asymmetric unit is essential to the process of density modification and phase improvement by NCS averaging. This process improves the quality of the electron density and aids structure determination. The real-space method presented here determines the NCS operators between related copies of a protein by recognizing structurally similar regions. The algorithm uses rotation invariant features (based on a preliminary backbone trace) to perform feature based matching between density patterns. These matches are then extended by fragment superposition. This algorithm allows for the NCS operators to be determined early on in the structure determination process and requires neither the location of heavy atoms nor any other sequence information.

The results of testing this algorithm on 20 representative proteins 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**