Correlating protein surface shape and hydrophobicity using spherical harmonical expansions

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In protein docking schemes it is often necessary to efficiently correlate certain properties of the potential partner molecules. Most often, the correlated property is surface shape, but other properties, like hydrophobicity, are queried as well.

One possible way to get correlation score (matching quality) is by representing protein surface (or protein skin which has a certain thickness) as a function of spherical polar coordinates and expanding it in a spherical harmonical series. Correlation is then done using the expansion coefficients, thus effectively reducing the computational cost.

Furthermore, molecule rotations, which are computationally very expensive part of analogous Cartesian (FFT) approach, are done via expansion coefficient manipulation. This is possible since spherical harmonics of a given order transform among themselves in a known way when rotated.

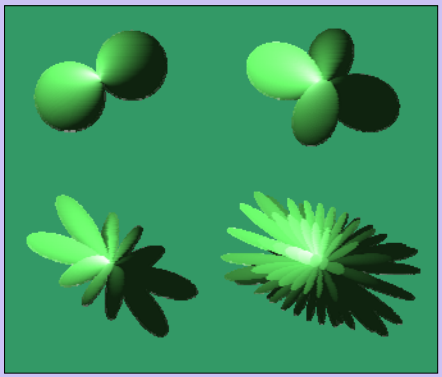

Figure 1. Several sample spherical harmonics.

Protein skin is defined as a volume between molecular surface and surface accessible area (exterior skin). Special radial functions are introduced to account for the skin thickness. These are unaffected by rotations. MATLAB routines are written for spherical harmonical expansion, reconstruction, rotation and translation of 3-D functions. Implementation is tested by reconstructing skin of a cube.

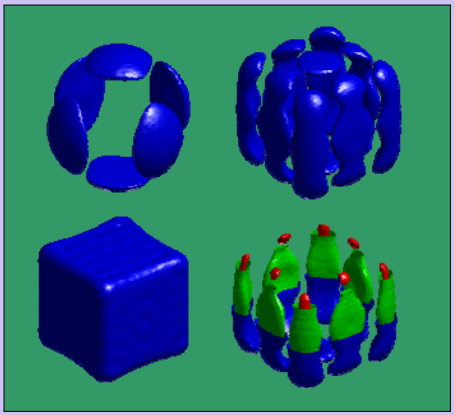

Figure 2. Reconstructed skin of a cube at different expansion orders and isosurface values.

Hydrophobicity is mapped onto the protein surface by assigning to the surface regions values 1 and zero, for those belonging to hydrophobic amino acids residues and otherwise, respectively. That way we get another surface property that is easily correlated using the implemented schema.

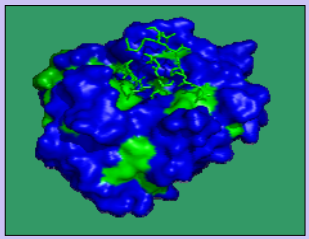

Figure 3. Protein complex. Hydrophobic areas on receptor are shown green, and hydrophobic residues of ligand are represented with green sticks.

Obtained results suggest that the method is feasible and that correlating hydrophobicity may be helpful in better ranking docked complexes, albeit more testing is needed, and some modules will have to be implemented with greater regard to numeric precision and stability.

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2. D.W. Ritchie, "Parametric Protein Shape Recognition", *Doctoral thesis*, University of Aberdeen, Departments of Computing Science & Molecular and Cell Biology, Aberdeen, 1998.
3. D.W. Ritchie, "High-order analytic translation matrix elements for real-space six-dimensional polar Fourier correlations", *Journal of Applied Crystallography*, (2005), 38, pp 808-818.