

Hierarchical Molecular Modelling with Ellipsoids

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The talk will be in three parts. In the first, protein and DNA structures are represented at varying levels of details using ellipsoidal RGBA textured splats. The splat texture at each level is generated by rendering its children in a hierarchical model, from a distribution of viewing directions, and averaging the result. For rendering, the ellipsoids to be used are chosen adaptively, depending on the distance to the viewpoint, with cross dissolves between the levels of detail. This technique is applied to visualize DNA coiling around nucleosomes in chromosomes.

The second part discusses the ProteinShop system, which is used by a group at Lawrence Berkeley Laboratory and the University of California, Davis, to generate initial structures for a local and global energy optimization search for predicting protein structure from sequence. It features interactive rigid body motion of beta strands and alpha helices, with inverse kinematics on selected flexible loop regions to maintain the correct covalent bond lengths and angles in the backbone.

The third part involves the production of a tilted hemisphere dome IMAX stereo film for the Fujitsu pavilion at Expo '90 in Osaka, Japan, showing photosynthesis and muscle motion. It was rendered on a vector supercomputer, using back to front compositing of subobjects, with 2D motion blur of each object before compositing. Ball and stick models were used for substrates, and stick models for enzymes. Larger assemblies were represented using "metaballs", as contour surfaces of sums of spherical or ellipsoidal gaussian-like densities.