EUROGRAPHICS 2003 / P. Brunet and D. Fellner
(Guest Editors)

Volume 22 (2003), Number 3

Volumetric Filtering, Modeling and Visualization for Nano-Medicine

Chandrajit Bajaj

Center for Computational Visualization
University of Texas at Austin, Texas, USA

Abstract

The 3D structures of individual proteins or small complexes, such as most of the Protein Data Bank entries, are still unable to yield the "full picture" of a functional biological complex. The study of large macromolecular complexes, such as viruses, ion channels, the ribosome and other macromolecular machines of various types, offer more complete structural and functional description of the nano-machinery of life.

In addition to x-ray crystallography, NMR spectroscopy, electron cryomicroscopy (cryoEM) imaging of single particles, and in-vivo molecular tomographic imaging has become indispensable at revealing the structures of large macromolecular complexes at subnanometer resolutions.

In this talk, I shall describe some of the recent computational advances in filtering, modeling, analysis and visualization, that have propelled structure determination by cryoEM and tomographic imaging, to steadily increasing accuracy.
