1108-92-337 **Kelin Xia***, 619 Rred Cedar Road, East Lansing, MI 48824. *Geometric modeling of biomolecules.*
Recently, the structure, function, stability, and dynamics of subcellular structures, organelles, and multiprotein complexes have emerged as a leading interest in structural biology. Geometric modeling not only provides visualizations of shapes for large biomolecular complexes but also fills the gap between structural information and theoretical modeling, and enables the understanding of function, stability, and dynamics. We introduce a suite of computational tools for volumetric data processing, information extraction, surface mesh rendering, geometric measurement, and curvature estimation of biomolecular complexes. Particular emphasis is given to the modeling of cryo-electron microscopy data. Analytical models are designed to test the computational accuracy and convergence of proposed algorithms. We finally demonstrate the efficacy of the proposed algorithms in handling biomolecular surfaces and explore the capability of geometric characterization of binding targets. We offer a comprehensive protocol for the geometric modeling of subcellular structures, organelles, and multiprotein complexes. (Received January 18, 2015)