Abstract: Macromolecular Assemblies Visualization, Modelling and Analysis with UCSF Chimera, Y1

Macromolecular assemblies are molecular structures that are too big to be visualized and analyzed with a regular computer like entire viruses, viral infections or even bacteria therefore supercomputers are necessary for these structures to be analyzed in a computer screen at atomic level where many interactions can be studied which are not possible with electron microscopes. For these purposes dedicated software have been developed that can handle X-rays structures and cryoEM densities stored in databanks like the rcsb (for structures) and emdb (for cryoEM densities). One of them, UCSF Chimera (2004) from University of California San Francisco has proven very useful and versatile for more than a decade for analysis where the software has many capabilities including structural analysis, sequence alignments, molecular dynamics and many representations and visualizations, as well as tools for measurements including a command line interface very useful for the professional user. I have been using Chimera since 2007 in Catholic University of America for molecular modelling along with other online tools and standalone software leading to many publications as author or collaboration. Chimera made possible the modelling of portal protein gp20 of bacteriophage t4 when there was no available structure, modelling the complete bacteriophage t4 which is a full organism and is letting to achieve further goals like the modelling of entire biological processes like a bacteriophage infection or hiv-1 infection.