
Tod D. Romo and Alan Grossfield
University of Rochester Medical Center, Rochester, NY, USA

http://loos.sourceforge.net

We have developed LOOS (Lightweight Object Oriented Structure-analysis) as a tool for making new tools to analyze molecular simulations. LOOS is an object-oriented library designed to facilitate the rapid development of new methods for structural analysis. LOOS is written in C++ and is easily extensible, only requiring knowledge of 4 core classes. A Python interface is also available, further facilitating rapid development of analysis tools and broadening the LOOS community. LOOS supports reading the native file formats of most common simulation packages and can write NAMD formats (PDB and DCD) and Gromacs XTC. A dynamic atom selection language, based on C expression syntax, is included and is easily accessible via a single function call. LOOS includes over 140 pre-built tools for common structural analysis tasks, including analyzing simulation convergence, D3 histograms, and elastic network models. Python-based packages include the OptimizedMembraneGenerator and tools for the Voronoi tessellation of membranes. In addition, tool templates for common analysis work-flows are included to facilitate the development of new tools. LOOS is available for download at github.com/GrossfieldLab/loos or can be cloned from github.com/GrossfieldLab/loos. LOOS is available for convergence, 3D histograms, and elastic network models.