LOOS: A Tool for Analyzing Molecular Dynamics Simulations

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Analyzing Molecular Simulations

- Molecular simulations have unmatched resolution in time and space
- Need better analysis tools to extract maximum value
  - Most projects require custom code
  - Data analysis is an iterative process
  - Rapid development is key

LOOS Design Goals

- Package-agnostic
  - Read all common file formats
    - NAMD, Amber (netcdf and mdcrd), GROMACS, TINKER, OpenMM, LAMMPS
  - Programs don't care where files came from
  - Reduce duplicated effort
  - Improve reproducibility

- Easy to use
  - Powerful tools
  - Unique functionality
  - Convenient atom selection facility
  - Highly scriptable
  - Detailed documentation
  - High performance
    - 1-2 orders of magnitude faster than VMD, mdanalysis
    - Comparable to cpptraj

- Easy to develop
  - C++ core
    - Good object design makes code expressive
    - 4 key classes means easy to learn
    - No memory management
    - Atom selection identical to tool level
  - Python interface
    - Rapid application development
    - Easy code reuse
    - Interoperable with NumPy, SciPy, Scikit-learn
  - Extensive documentation
    - Code level via doxygen
    - Github wiki

- Available everywhere
  - Install via conda-forge or from source
  - Linux and Mac

Using LOOS

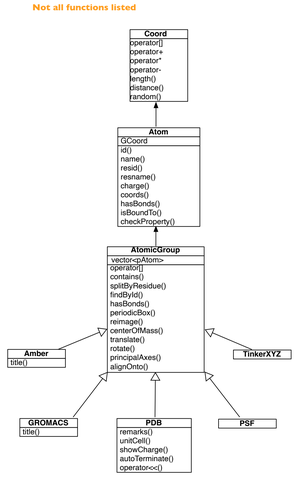
Example Tools

Macromolecules	
rmsds	All-to-all structure comparison
rmsf	Molecular fluctuations
svd	Principal component analysis
rdf	Radial distribution function
Membranes and membrane proteins	
order_parameters	Chain tilt in membranes
density-dist	Distribution along membrane normal
xy_rdf	Radial distribution in membrane plane
membrane_map	Lipid properties around membrane
mops	Molecular order parameters for chains
dibmops	mops vs. distance from macromolecule
Trajectory manipulation	
merge-traj	Rapidly merge trajectories
subsetter	Merge, reimage, and subset trajectories
Convergence Package	
block_average	Block average of time-series data
decorr_time	Decorrelation time of structural histograms
bcom, boot_bcom	Block covariance overlap method
Voronoi Package	
area_per_molecule.py	Area distribution for a membrane slice
area_profile.py	Voronoi area for protein along normal
Elastic Network Model Package	
anm	Anisotropic network model
enmovie	Visualize ENM modes via a trajectory
vsa	Vibrational subsystem analysis
Gridded Density Package	
water-hist	3D density histogram for atoms
near_blobs	Find residues near density peaks
grid2xplor	Convert density grid to X-plor format
Optimal Membrane Generator Package	
omg.py	Build membrane systems
solvate.py	Build water around soluble molecules

Developing with LOOS

Structure Classes

Not all functions listed

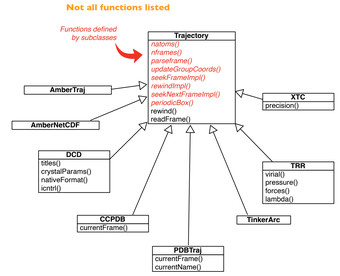


Classes map to key concepts

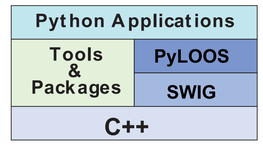
- Makes code expressive
- AtomicGroup is workhorse
  - File formats are subclasses
  - Common tasks are methods
- Trajectory formats are subclasses
- Code with parent classes is format-agnostic

Trajectories

Not all functions listed



Application Layers



Most new tools are python

- Easier development
- Great libraries
  - Interoperate via NumPy, SciPy, Scikit-learn
  - Voronoi package, clustering
- Performance gap is small as most work is done in the library

Example Code

Relative motion of domains

Read command line
Create system
Select "domains"
Loop over trajectory
Compute distance
Compute axis angle
Compute torsion

```
#!/usr/bin/env python3
import sys
import loos
import loos.pyloos
import math

system_file = sys.argv[1]
traj_file = sys.argv[2]
sel_string1 = sys.argv[3]
sel_string2 = sys.argv[4]

system = loos.createSystem(system_file)
traj = loos.pyloos.Trajectory(traj_file, system)

sel1 = loos.selectAtoms(system, sel_string1)
sel2 = loos.selectAtoms(system, sel_string2)

for frame in traj:

    # compute distance
    centroid1 = sel1.centroid()
    centroid2 = sel2.centroid()

    diff = centroid2 - centroid1
    distance = diff.length()

    # Compute angle between principal axes
    vectors1 = sel1.principalAxes()
    axis1 = vectors1[0]

    vectors2 = sel2.principalAxes()
    axis2 = vectors2[0]
    angle = math.acos(axis1 * axis2) * 180/math.pi

    # Compute torsion between principal axes
    p1 = centroid1 + axis1
    p2 = centroid2 + axis2

    tors = loos.torsion(p1, centroid1, centroid2, p2)

    # write output
    print(traj.index(), distance, angle, tors)
```

Future directions

- Built-in featurizers for MSMs
- Membrane curvature and entropy
- Better community engagement
- Take over the world

Getting Help

- Github
  - User and Developer docs
  - HowTo stories on GitHub wiki
  - Discussions
- loos.maintainer@gmail.com

New in LOOS 4.0

- Distributed via conda-forge
- Build with cmake
- New tools
  - Contact-based PCA and clustering
  - Nucleic acid stacking
  - Scattering

Getting LOOS

YouTube Tutorial | LOOS Paper | This poster | LOOS on GitHub

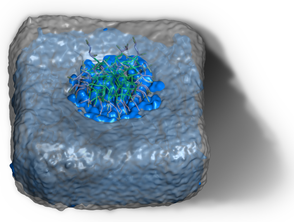
J. Comput. Chem., 2014, 35, 2305-2318

System Visualization

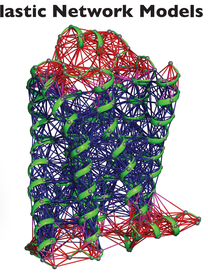
Made with LOOS

Water Density

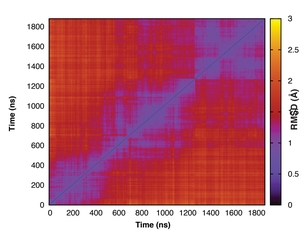
Lipid Density



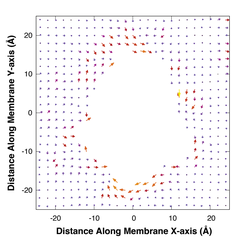
Elastic Network Models



All-to-All RMSD

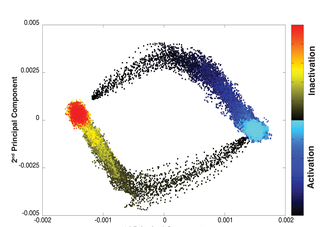


Membrane Properties



Principal Components

Structural Transitions



Tools:	custom software	water-hist	water-hist	ANM/VSA (rebond)	rmsds	membrane_map	svd & porcupine	transition_contacts & svd