MEMSURFER: A TOOL FOR ROBUST COMPUTATION AND CHARACTERIZATION OF BILAYER MEMBRANES

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BACKGROUND

- Advances in simulation methods and computing power enable larger, longer, more complex biological membrane simulations.
- Such membranes can be highly complex, and have curved geometries that greatly deviate from simple planar states.
- Analyzing such membranes requires appropriate characterization of geometric and topological properties of the membrane surface.

We present MemSurfer - a versatile tool to compute membrane surfaces for a variety of molecular simulations.
MemSurfer works directly on 3D coordinates, it can handle a variety of membranes, simulation resolutions, or trajectory types.
MemSurfer uses Delaunay triangulations and surface parameterizations to compute surface approximations.
MemSurfer provides common lipid properties of interest, e.g., areas and curvatures; MemSurfer also provides direct access to the membrane surface itself, allowing users to conceive and compute a variety of nonstandard properties.
The software is written in C++ with a simple-to-use Python interface, and is released open source under GPL license.
https://github.com/LLNL/MemSurfer

THEORY AND METHOD

INPUT

- A set of 3D coordinates (such as MDAnalysis array)

STEP 1

- Estimate normal vectors on the point set

STEP 2

- Compute approximate surface by Poisson Reconstruction

STEP 3

- Parameterize the approximate surface (and the projected points along with) onto a 2D plane
- The connectivity obtained in Step 3 is lifted on to original 3D points to give an "exact" membrane surface
- Projected points form the vertices of the approximate surface (allows per-vertex, i.e., per lipid properties)
- Parameterization done to compute connectivity graph between lipids, i.e., triangulation. This is done via 2D periodic Delaunay triangulation
- Smoothing - The final "smoothed" surface created by lifting triangulation onto the projected points (using connectivity from Step 3 to connect projected points)

OUTPUT

- Exact
- The connectivity obtained in Step 3 is lifted on to original 3D points to give an "exact" membrane surface

EXAMPLES

3-COMPONENT PHASE-SEPARATION

MEMBRANE OF BIOLOGICAL COMPLEXITY

MEMBRANE TETHER

REFERENCES