Methodologies for the Analysis of Instantaneous Lipid Diffusion in MD Simulations of Large Membrane Systems

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Supplementary Material:

10 Spherical coordinates:

A spherical coordinates system is defined by 3 parameters: r, θ and φ.
- r is the radial distance from the center of the vesicle.
- φ is the azimuthal angle in the x-y plane, $0 \leq \varphi < 2\pi$
- θ is the polar angle on the z axis, $0 \leq \theta \leq \pi$

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Here, we used the relation to pass from spherical coordinates to Cartesian coordinates:

$$x = r \sin \theta \cos \varphi$$
$$y = r \sin \theta \sin \varphi$$
$$z = r \cos \theta$$

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Sup. Table 1: Benchmark of the different implementations for 1 frame. Values are averaged on 10 repeats. In the table, the planar membrane system is noted 2D while the 25 vesicle is noted 3D.

|		Tcl code	Python code (1 thread)	Python code (12 threads)
Lipid path calculation and visualization	2D	7.9 s.	--	--
	3D	17.6 s.	--	--
Vector field/ Streamlines calculation and Vector field visualization[a]	2D	35.4 s.	8.4 s.	7.8 s.
	3D	224.5 s.	25.4 s.	13.3 s.
Streamlines Visualization[b]	2D	~2 s.	21.6 s.	--
	3D	~2 s.	17.6 s.	--

[a]: streamlines are based on the same calculation as vector field. The time to render the vectors is too small in comparison of calculation to be quoted.

[b]: For the Python code, the visualization of Streamlines is performed only on a single thread.

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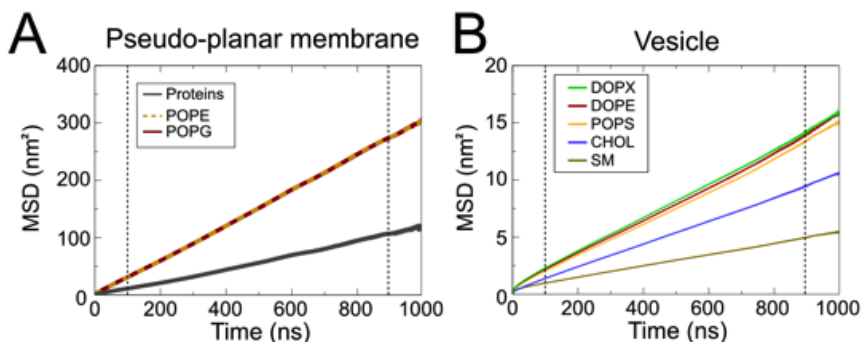
Sup. Fig. 1: Mean square deviation (MSD) plots for proteins and lipids. (A) MSD tracked for POPG, POPE and proteins in the planar membrane without filtering. (B) MSD tracked for lipid components of the vesicle without filtering. Dashed lines delineate 5 the time boundaries used to calculate diffusion coefficients presented in Table 1.
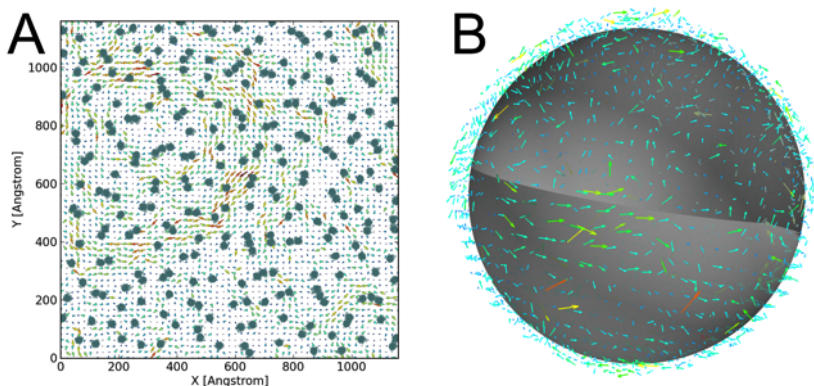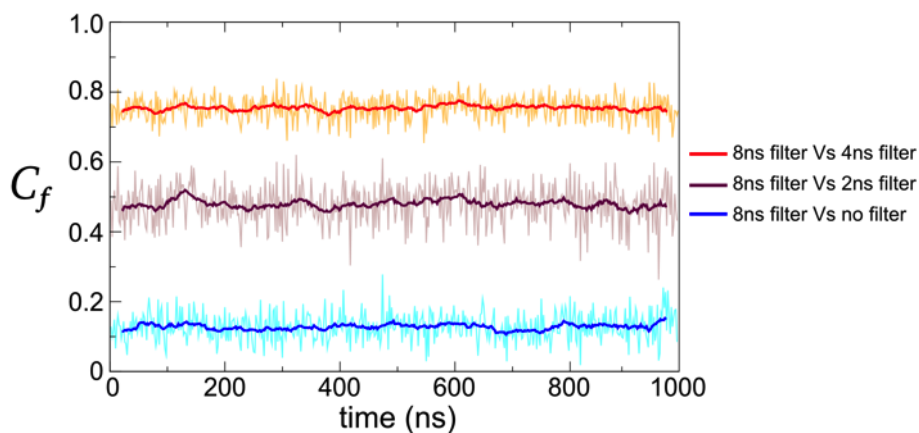

Sup. Fig. 2: Vector field rendering using the Python module. (A) 2D results on the 10 planar membrane. (B) 3D results on the vesicle system. The transparent sphere was added to clarify the visualization.
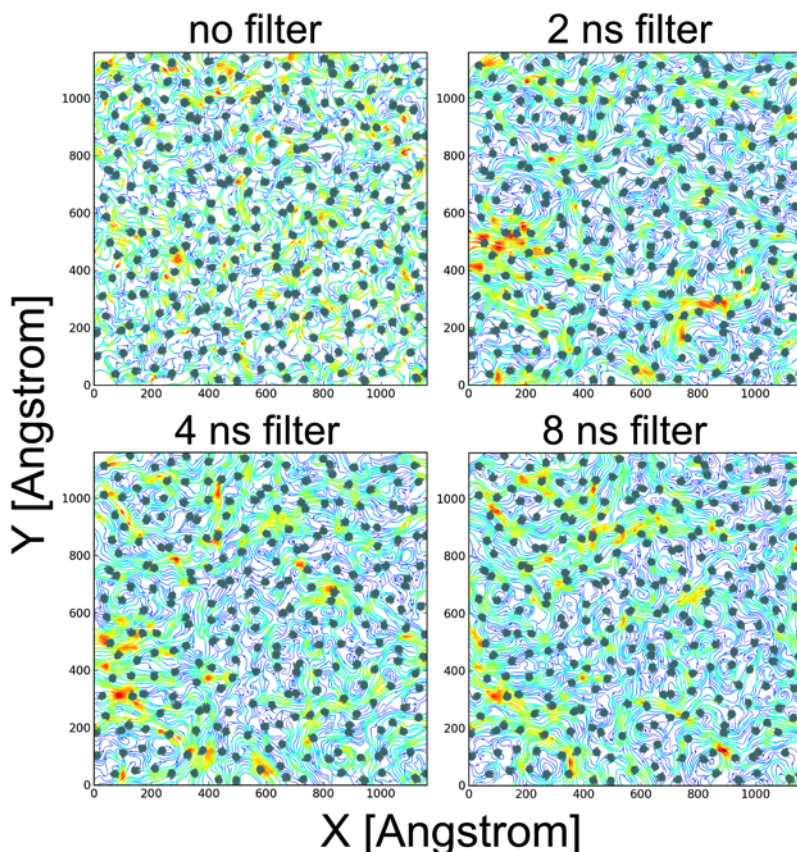
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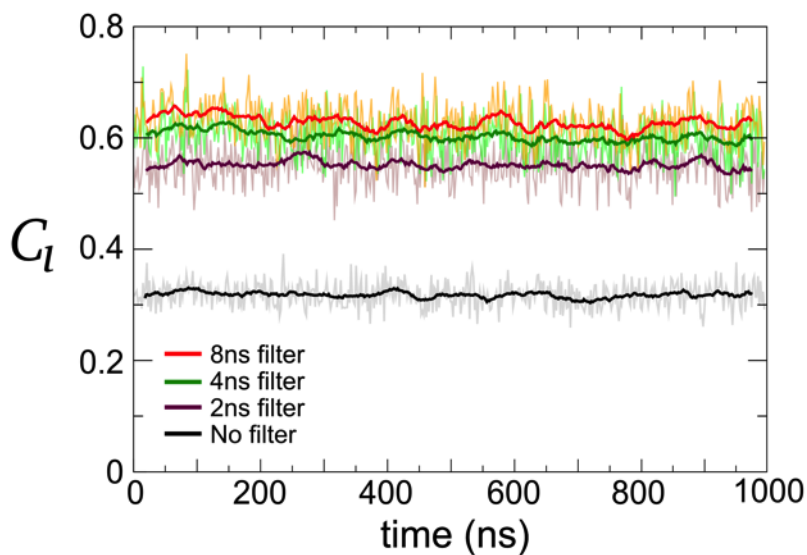
Sup. Fig. 3: Effect of filter time window size on the leaflet lipid motion correlation values for the planar membrane.

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Sup. Fig. 4: Correlation graph comparing the 8 ns window filter with other filters and raw data.

Sup. Fig. 5: Comparison of the different filter time window sizes for the planar membrane system. Streamline plots are shown for the different filter window sizes.

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Sup. Movie 1: Lipid path lines rendering for the planar system based on VMD visualization. A longer and high-resolution version is available at https://vimeo.com/user22894882.

10 **Sup. Movie 2:** Lipid path lines rendering for the vesicle system based on VMD visualization. A longer and high-resolution version is available at https://vimeo.com/user22894882.

Sup. Movie 3: Streamline rendering for the planar system based on Python-Matplotlib 15 visulization. A longer and high-resolution version is available at https://vimeo.com/user22894882.

Sup. Movie 4: Streamline rendering for the vesicle system based on VMD visualization. A longer and high-resolution version is available at https://vimeo.com/user22894882.
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Sup. Movie 5: Streamline rendering with z coloring of the membrane for the planar system based on Python-Matplotlib visulization. A longer and high-resolution version is available at https://vimeo.com/user22894882.