XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

SuAVE: a computational tool for the assessment of curved surfaces

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Abstract: Data analysis is an inevitable and necessary step for engineering predictive models for a studied system. The success of the model depends directly on how precise, and preferably, efficient are the analyses in measuring properties of interest. The program SuAVE (Surface Assessment Via grid Evaluation) is a Fortran-based program developed to analyze geometrical properties of surfaces taking into account the structural morphology of the systems. To do so, this ensemble of numerical routines relies on a surface fitting process established over the basis of differential and computational geometry and numerical calculus[1] (Figure 1).

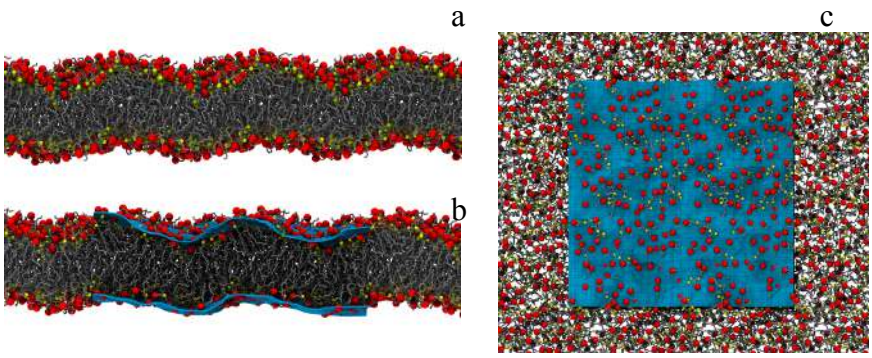

Figure 1. Representation of the generation and fitting of grid along the surface of a bilayer of Lipid A. Lateral (a, b) and top (c) views of the membrane surface. Grid surface is represented in blue, phosphorous and oxygen from phosphate groups are represented in red and yellow respectively, and acyl chains in gray.

The program has been developed to handle any organic, inorganic, or biological system containing a surface or an interface, presenting or not curvature and displaying a wide range of morphologies. It can take as input trajectory files from molecular dynamics (MD) and Monte Carlos simulations as well as any other numerical methodology once an input file in PDB format is provided. The program can efficiently calculate the area and volume per molecule composing an interface, membrane thickness, surface topology maps, density profiles, curvature order parameters and Gaussian curvatures. The accuracy of the numerical methodology implemented in SuAVE to assess the above-mentioned geometrical properties of curved surfaces has been validated via the analysis of four different Lipid A chemotypes[2] and compared with conventional

methodologies which does not take into account the membrane curvature. The different Lipid A chemotype bilayers displays distinct morphologies, namely gel, lamellar and ripple-shaped phases as shown by MD simulations. MD simulations were carried out for 100 ns after equilibration of the bilayers using GROMOS 53A6 force field[3] at the NpT ensemble. The average deviation of the SuAVE fitted points in relation to the system surface was 0,11 nm with a grid refinement of 50X50 points applied to each analysis. The comparison of the area per lipid head-group can exemplify the two most important conclusions in the systematic evaluation of SuAVE efficiency. For bilayers with a lamellar planar shape, the values calculated with SuAVE are in excellent agreement with the same analysis performed with conventional methodologies. However, when comparing the results for bilayers in the ripple phase, conventional analysis underestimates the area per lipid molecule in about 19% because they neglect membrane curvature. Likewise, density profiles for the ripple phase bilayers are rather distinct when the membrane curvature is taken into account or not in the calculations while they are identical for lamellar phase bilayers. The density profiles calculated with SuAVE for the former systems show that even if not planar they conserve a lamellar structure. On the other hands, density profiles obtained via the use of conventional analysis imply the presence of water within the membrane which clearly leads to the equivocal interpretation of the data. Further, the SuAVE code calculates the curvature order parameter which provides a quantitative estimate of how curved is a given surface on average. By using the surface curvature angles with respect to the normal axis to the system, it is possible to demonstrate that for gel and lamellar systems about of 90% of the surface exhibits a surface curvature angle below 30º while for ripple shaped membranes it can increase up to a value of 60º. Through all these examples SuAVE has demonstrated capabilities for evaluating structural properties for different systems taking into account their constitutional geometry, not observed in conventional numerical analysis, displaying a potential for contributing in the evaluation of a wider range of organic, inorganic or biological systems.

Key-words: Membrane Curvature, Voronoi Tesselation, Helfrich Equation, Lamellar Phase, Ripple Phase, Structural Transitions
Support: This work has been supported by CNPq, BioMol, CAPES.
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