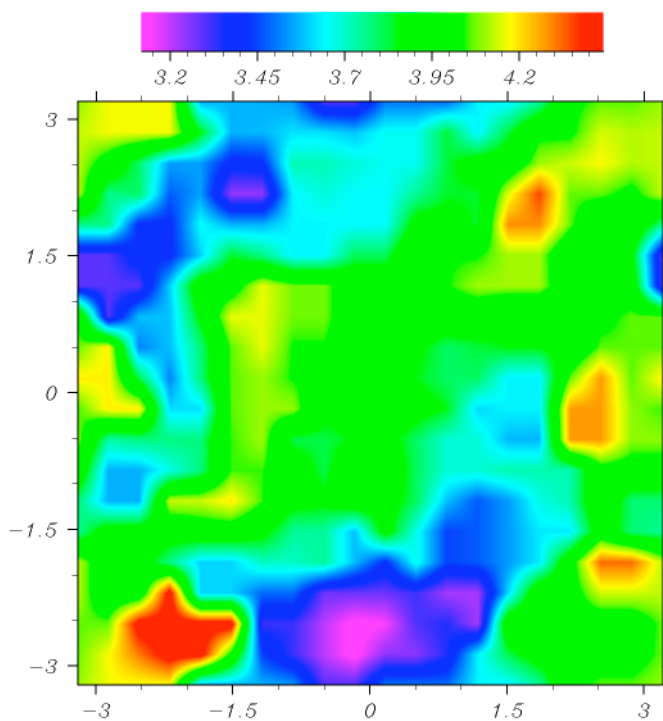


GridMAT-MD: A Grid-based Membrane Analysis Tool for use with Molecular Dynamics

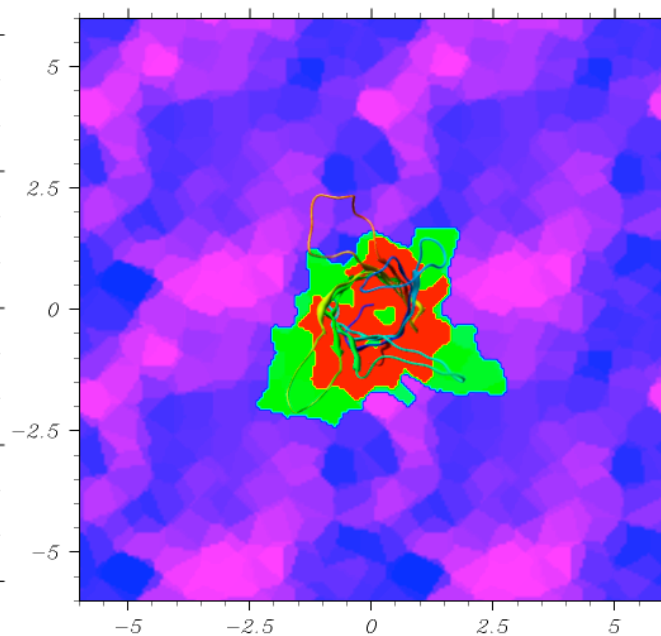
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Introduction. GridMAT-MD is a Perl program designed to assist in the analysis of lipid bilayers simulated by molecular dynamics. It measures two things - the apparent “thickness” of the bilayer, and the area per lipid head group of each individual lipid that comprises the bilayer. The output can then be visualized using a separate tool – we use the Xmatrix viewer (<http://www.matpack.de>). We believe this program to be superior to existing tools because (i) it is free to use and modify under the terms of the GNU public license, (ii) no installation is required, provided the Perl interpreter is installed, (iii) it calculates an explicit area for proteins, making no assumptions of “ideal proteins,” and (iv) it is very fast to run and easy to operate.

Examples. GridMAT-MD can analyze all kinds of bilayers: large and small, uniform or mixed. Below are two examples of analyses performed by the program. All molecular dynamics simulations were performed on System X at the Terascale Computing Facility at Virginia Tech, and GridMAT-MD itself was run on a local machine.



Simulation of a 128-lipid DPPC bilayer. The color gradient describes the average phosphate-to-phosphate thickness of the membrane. Thicker parts (red) are easily distinguished from thinner parts (blue). Periodic boundary conditions are also considered. Axes reflect system dimensions in the x - y plane.



Simulation of a protein in a 500-lipid DPPC bilayer. The cross-sectional area of the protein at the top interface (green) and at the bottom interface (red), is calculated explicitly and subtracted from the lateral area of the membrane for more accurate area per lipid headgroup calculations.

For more information and to download the program, please visit these sites and read our publication:

<http://bevanlab.biochem.vt.edu/GridMAT-MD/index.html>

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