Methodological problems in pressure profile calculations for lipid bilayers

From molecular dynamics simulations of a dipalmitoyl-phosphatidyl-choline (DPPC) lipid bilayer in the liquid crystalline phase, pressure profiles through the bilayer are calculated by different methods. These profiles allow us to address two central and unresolved problems in pressure profile calculations: The first problem is that the pressure profile is not uniquely defined since the expression for the local pressure involves an arbitrary choice of an integration contour. We have investigated two different choices leading to the Irving-Kirkwood (IK) and Harasima (H) expressions for the local pressure tensor. For these choices we find that the pressure profile is almost independent of the contour used, which indicates that the local pressure is well defined for a DPPC bilayer in the liquid crystalline phase. This may not be the case for other systems and we therefore suggest that both the IK and H profiles are calculated in order to test the uniqueness of the profile. The second problem is how to include electrostatic interactions in pressure profile calculations when the simulations are conducted without truncating the electrostatic potential, i.e., using the Ewald summation technique. Based on the H expression for the local pressure, we present a method for calculating the contribution to the lateral components of the local pressure tensor from electrostatic interactions evaluated by the Ewald summation technique. Pressure profiles calculated with an electrostatic potential truncation (cutoff) from simulations conducted with Ewald summation are shown to depend on the cutoff in a subtle manner which is attributed to the existence of long-ranged charge ordering in the system. However, the pressure profiles calculated with relatively long cutoffs are qualitatively similar to the Ewald profile for the DPPC bilayer studied here.