Simulation of bilayers

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Mike Allen discussed the calculation of the pressure for a system in which a bilayer of amphiphilic molecules separates two regions of aqueous phase. This had come up in discussions with colleagues at Bristol and elsewhere. Since the number of amphiphiles is fixed, the situation is distinct from the one where a bulk oil layer (for example) separates two regions of aqueous phase. (In both cases we assume full periodic boundary conditions, so really there is just one region of aqueous phase). In the latter case, a change in cross-sectional area is associated with a surface free energy term (due to interfacial tension). In fact, it can be calculated from the profiles of the normal and transverse components of the pressure tensor, for a constant-volume simulation. For given numbers of oil and water molecules, a constant pressure simulation may be carried out with the cross-sectional area fixed and the box length (in the direction normal to the interface) varying. In the case of amphiphiles, there is also a free energy due to the surface, but it is not of the same form, and the surface tension is not well defined. The bilayer is (by definition) microscopically thin, and the pressure tensor profiles are not defined unambiguously on this length scale. The number of amphiphiles per unit cross sectional area must be specified. For fixed values of these parameters, constant pressure simulations allowing the longitudinal box dimension to vary, may be carried out. It is instructive to consider constant-pressure simulations with all three box dimensions varying. For the oil/water case, assuming an isotropic applied pressure, the surface free energy term would drive the box towards a long thin shape, so as to minimize the surface area; this could be prevented by applying an anisotropic pressure to oppose the surface energy term, but this would require prior knowledge of the surface tension. In the bilayer case, contant pressure box moves in the transverse direction would change the surface area per amphiphile and the system would stabilize at a certain value of surface area. This seems a reasonable method of equilibrating towards a typical, physically interesting, value for the ratio of surface area per amphiphile, prior to fixing the box area for production runs.