Multiscale molecular simulation of membranes

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ABSTRACT

Fundamental advances in the understanding of the molecular mechanisms enable a guided strategy towards analysis, modeling, and design of nanoscale structures. An essential difficulty in molecular modeling is that relevant system sizes of interest are very large. Although molecular mechanics has developed accurate models of interactions between individual molecules, the difficulty is that it is simply infeasible to solve these models on existing – or even conceived – computers. Although accurate models of the individual interactions between the molecules are available, the engineered materials typically consist of well over a billion such molecules. However, multiscale methods are well-suited to such problems: near the region of activity, e.g., an indenter pushing through the substrate, we can use molecular resolution to understand the critical features of indenter/substrate interactions; away from the active region, we can coarse-grain to retain only the effective influence. On the other hand, existing molecular multiscale methods, such as Quasi-continuum, Bridging-scales, and Bridging-domain methods, are only suitable for crystalline materials. They rely on the Cauchy–Born rule to relate the lattice vectors to the deformation gradient tensor which is a continuum description. The main feature of crystals is the translational symmetry. However, several structures such as nanotubes, bended graphene sheets, biological structures, and animal cell membranes do not exhibit translational symmetry. In our study, a unique molecular multiscale method for noncrystalline, but highly symmetric structures, is developed. Our method is based on the Objective Structures framework. In other words our method not only exploits the translational symmetry, but also uses other symmetries such as rotational and screw symmetries. Our strategy is to approximate the energy of full atomistic system by the energy of coarse-grained particles. We incorporate the symmetries of the structure to find the neighborhood around the coarse-grained particles. We then use finite element analysis to minimize the energy.