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CAN NANO-BUBBLES PERMEABILISE CELL MEMBRANES?

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Abstract. The mechanical properties of cells have been studied for decades, with the intent to understand the underlying physical and chemical processes required to fulfil their basic functions. The presence of defects in cell membranes, such as pores and domain borders, plays an important role in many cellular processes, such as drug delivery and ion transport. Computer simulations have demonstrated themselves to be a powerful tool in the study of membranes and their defects. In this investigation we use computational models to simulate the behaviour of transient pores in lipid membranes, while in the vicinity of nano-bubbles. We employ a classical, coarse-grained force field, MARTINI, to simulate a 1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC) lipid bilayer in water. Simulations of the lipid-water system are performed using the molecular dynamics (MD) code, LAMMPS. We use the Plumed tool to introduce a bias in the simulations in order to induce the formation of transmembrane pores. Other computational tools are used to analyse the structural and energetic aspects of the simulated systems. In our simulations, we observe a drastic reduction in the local lipid density upon the formation of pores. By comparing systems both in the absence and in the presence of a nano-bubble, we are able to estimate the difference in energy cost for opening transmembrane pores of different sizes. We find that the presence of a nano-bubble in the proximity of the membrane leads to a reduction in the energy required to open the pore. In addition, the pore formed has a greater radius, and therefore volume, than that formed in the absence of the nano-bubble. We conclude that nano-bubbles promote the formation of hydrophobic membrane pores which is expected to enhance membrane permeability.