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Molecular Dynamics Based Assessment of Electric Pulse Enhancements of Cell Membrane Poration by Pressure Waves

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Applications of electric pulses is known to create nanopores at the membranes of biological cells, which can then modulate the intracellular conductivity and permeabilization in a controlled manner. Applications of such membrane poration lies in the field of biomedical engineering, drug/gene delivery, cell fusion, and electrochemotherapy for cancer treatment. However, in addition to external voltage pulses, pressure transients (typically in the MHz range) have also been shown to create pores in plasma membranes by imparting mechanical stress due to these ultrasonic shock waves [1]. Sonoporation experiments show that the collapse of bubbles in water by ultrasound generates membrane pores, thereby allowing the intracellular delivery of drug or gene payload.
Here we focus on poration of lipid bilayers of cell plasma membrane by the interaction of transient shock waves through atomistic Molecular Dynamics (MD) simulations. The Gromacs simulator is used, with a simple point charge SPC model for water molecules incident on a nanometer-sized patch of a dipalmitoylphosphatidylcholine (DPPC) phospholipid membrane bilayer. The simulations were performed by having a sheet of water molecules with a pre-determined velocity (representing an incident shock-wave) impinge on a section of a DPPC bilayer. The simulations were carried out systems containing over 1 million atoms with dimensions of the corresponding MD cells taken to be 34x34x82 nm3.
In addition to simple shock, we have include the presence of an external electric field as an additional stimuli in concert with the pressure transient. With this superposition, the requirements on the electric field intensity were reduced. In principle such a dual mechanism would make it possible to spatially tune membrane poration effects. Besides, using electric fields alone can potentially slow the electrophoretic driving force for ions and dipolar molecules once pores have formed due to the reduced voltage drops associated with the high local conductivity. Hence, a dual strategy would likely have practical advantages. In this contribution, details of our simulation results along with the enhanced potential for cellular throughput at reduced fields will be discussed.

[1] S. P. Wrenn, S. M Dicker, E. F. Small, N. R. Dan, M. Mleczko, G. Schmitz, and P. A. Lewis, Bursting bubbles and bilayers, Theramostics, vol. 2, pp. 1140-1159, 2012.

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