Abstract Submitted
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Lipid Bilayer Vesicle extrusion through nanopores: a coarse grained molecular dynamics study[1] MARTIN BERTRAND, BELA JOOS, University of Ottawa — We conducted Coarse-Grained Molecular Dynamics simulations of the pressure extrusion of vesicles in nanopores that confirm and help explain prior experimental observations (Patty, P. and Frisken, B., Biophys. J., 85, 2003). We demonstrate that, to a first approximation, the final size of extruded vesicles can be obtained by considering an invariable inner vesicle volume enclosed by a finitely extensible lipid bilayer. Using our data, we also describe in details the mechanics of vesicle rupture in a nanopore when pushed by various pressure gradients. This is made possible by tracking local variations of the stress in the lipid membrane via changes in surface area using a triangulation algorithm. The simulations are executed using state of the art GPU accelerated software. Our findings could potentially be useful in the design of liposome based drug delivery systems and in getting a better understanding of how the cell nucleus and the cell as a whole react in similar conditions.

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