Abstract Submitted
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Computing osmotic permeabilities of aquaporins AQP4, AQP5, and GlpF from near-equilibrium simulations[1] THIERRY WAMBO, ROBERTO RODRIGUEZ, LIAO CHEN, The University of Texas at San Antonio — Measuring or computing the single-channel permeability of aquaporins/aquaglyceroporins (AQPs) has long been a challenge. We report large scale simulations of osmotic current under sub M gradient through three AQPs (water channels AQP4 and AQP5 and glycerol-water channel GlpF. These simulations were implemented with hybrid periodic boundary conditions devised to avoid the artifactitious mixing across the membrane in a regular PME simulation. The computed single-channel permeabilities at 5 C and 25 C are in agreement with recently refined experiments on GlpF. The Arrhenius activation energies extracted from our simulations for all the three AQPs agree with the *in vitro* measurements. We observe that AQP4, that is particularly rich in the central nervous system, is more efficient in water conduction and more temperature-sensitive than other water-only channels (excluding glycerol channels that also conduct water when not inhibited by glycerol).

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