# Coarse Grained Molecular Dynamics Simulations of the Fusion of Vesicles Incorporating Water Channels

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| **Session Title:** | Platform O: Molecular Dynamics of Protein-Lipid Interactions |
| **Presentation Number:** | 127-Plat |
| **Abstract Title:** | Coarse Grained Molecular Dynamics Simulations of the Fusion of Vesicles Incorporating Water Channels |
| **Presentation Start/End Time:** | Sunday, Feb 19, 2006, 4:30 PM - |
| **Location:** | Room 250 A |
| **Topic:** | 8E Molecular Dynamics |
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As the dynamics of the cell membrane and the working mechanisms of proteins cannot be readily asserted at a molecular level, many different hypotheses exist that try to predict and explain these processes, for instance vesicle fusion. Therefore, we use coarse grained molecular dynamics simulations to elucidate the fusion mechanism of vesicles. The implementation of this method with hydrophilic and hydrophobic particles is known for its valid representation of bilayers. With a minimalistic approach, using only 3 atom types, 12 atoms per two-tailed phospholipids and incorporating only a bond potential and Lennard-Jones potential, phospholipid bilayers and vesicles can be simulated exhibiting authentic dynamics. We have simulated the spontaneous full fusion of both tiny (6 nm diameter) and larger (13 nm diameter) vesicles.

We showed that, without applying constraints to the vesicles, the initial contact between two fusing vesicles, the stalk, is initiated by a bridging lipid tail that extends from the membrane spontaneously. Subsequently it is observed that the evolution of the stalk can proceed via two pathways, anisotropic and radial expansion, which is in accordance with literature.

Contrary to the spherical vesicles of in vitro experiments, the fused vesicles remain tubular since the internal volume of these vesicles is too small compared to their membrane area. While the lipid bilayer has some permeability for water, it is not high enough to allow for the large flux required to equilibrate the vesicle content in the time accessible to our simulations. To increase the membrane permeability, we incorporate proteinaceous water channels, by applying the coarse grained technique to aquaporin. Even though incorporating water channels in the vesicles does significantly increase water permeability, the vesicles do not become spherical. Presumably the lipids have to be redistributed as well.

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| **Commercial Relationship:** | **A.F. Smeijers**, None; **A.J. Markvoort**, None; **K. Pieterse**, None; **P. Spijker**, None; **P.A.J. Hilbers**, None. |