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Dissipative dynamics of fluid vesicles

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ABSTRACT

Introduction. Vesicles consist of a closed lipid bilayer membrane being filled with and surrounded by a fluid. Membranes formed from multiple lipid components may exhibit coexisting phases or domains with distinct lipid compositions, which is expected to lead to a coupling of the vesicle morphology (e.g. the curvature) and the domain morphology (e.g. the line tension) inducing membrane deformations, budding or fission [1]. Among the various reasons to study vesicles let us mention that vesicles serve as a model system for the much more complicated biomembranes. For the latter, an interplay between geometric properties (like curvature) and biological properties (e.g. ion channel activity) is of great interest [2]. Also vesicles can be prepared experimentally and are explored and used as drug delivery systems.

In the following, the dynamics of vesicles with coexisting fluid domains will be consistently described in terms of generalized gradient flows, which guarantees a dissipative dynamics. This naturally introduces the dynamic laws in a variational form, i.e., in terms of weak formulations, which allow for a discretization using a finite element method. Here the membrane will we represented as a triangulated surface using parametric linear finite elements.

Model. The dynamics of the membrane is governed by the elastic properties of the membrane, which depend locally on the lipid phase, the phase separating processes in the membrane and the interaction with the surrounding fluid. Here we will stick to the local model, i.e., we neglect the interactions with the fluid. The membrane (lipid bilayer) itself may be viewed as a 2-dimensional incompressible fluid film. Let $\Gamma(t)$ denote the membrane (interface) at time t and $u(x,t)$, $x \in \Gamma(t)$, an order parameter describing the lipid phase. The total membrane free energy $\mathcal{F}[u,\Gamma] = \mathcal{F}_B[u,\Gamma] + \mathcal{F}_T[u,\Gamma] + \ldots$, consists of some phase-field approximation $\mathcal{F}_T$ of the line energy separating the domains in the membrane (e.g. a Cahn-Hillard type energy) and the following elastic bending energy $\mathcal{F}_B$ of the membrane, which is a generalization of the classical Helfrich model [3],

$$\mathcal{F}_B[\Gamma,u] = \frac{1}{2}\int_\Gamma b_n(u)\big(H - H_0(u)\big)^2\,\mathrm{d}\Gamma,$$

with mean curvature H, normal bending stiffness $b_n(u)$ and spontaneous curvature $H_0(u)$ depending on the order parameter u. Note that due to osmotic balance, the volume inside the fluid is constant and that the membrane is inextensible. Thus we have to deal with a local area and a global volume constraint.

Dissipative dynamics. To construct a dissipative dynamics, we proceed as follows: First, assuming u to be conserved, we expect u to obey some local balance law

$$\dot{u} + u\nabla_\Gamma \cdot \mathbf{v} + \nabla_\Gamma \cdot \mathbf{q} = 0, \tag{1}$$

with $\dot{u}$ denoting the material derivative and $\mathbf{q}$ some surface current $\mathbf{q}$. Second, the dynamics of u and Γ is required to be dissipative with respect to $\mathcal{F}[u, \Gamma]$, i.e., using (1), we postulate

$$0 \geq \frac{d}{dt}\mathcal{F} = D_u\mathcal{F}(\dot{u}) + D_\Gamma\mathcal{F}(\mathbf{v}) \tag{2}$$

$$= D_\Gamma\mathcal{F}(\mathbf{v}) - D_u\mathcal{F}(\nabla_\Gamma \cdot \mathbf{q}) - D_u\mathcal{F}(u\nabla_\Gamma \cdot \mathbf{v}) =: \frac{d}{dt}\mathcal{F}(\mathbf{q}, \mathbf{v}), \tag{3}$$

with $\mathbf{v}$ denoting the velocity of the membrane, D_u being the functional derivate corresponding to variations in u, and D_Γ the derivative corresponding to variations of the surface Γ, where, however, the order parameter u is evaluated at the fixed surface. Finally, we postulate

$$\frac{d}{dt}\mathcal{F}(\mathbf{q}, \mathbf{v}) = -g(\mathbf{q}, \mathbf{v}; \mathbf{q}, \mathbf{v}), \tag{4}$$

for some suitable metric $g = g(\mathbf{q}_1, \mathbf{v}_1; \mathbf{q}_2, \mathbf{v}_2)$, which clearly implies a dissipative dynamics. As an example one may choose (splitting $\mathbf{v} = v\mathbf{n} + \mathbf{t}$ into the normal and tangential components)

$$g(\mathbf{q}, \mathbf{v}; \mathbf{q}, \mathbf{v}) = \int_\Gamma \alpha_u |\mathbf{q}|^2 \, \mathrm{d}\Gamma + \int_\Gamma \alpha_v v^2 + \int_\Gamma \alpha_t |\mathbf{t}|^2,$$

for some strictly positive functions $\alpha_u, \alpha_v, \alpha_t$, which immediately yields equations for the unknowns $v, \mathbf{t}, \mathbf{q}$ in a variational form. Note that the expression for the flux $\mathbf{q}$ has to plugged into the balance law (1) to obtain an evolution equation for u. For the above metric, one does obtain some Willmore-Flow -type dynamics of the membrane coupled with a Cahn-Hillard-type dynamics for the order parameter u, which, however, are strongly coupled.

To account for the global volume and the local area constraint we introduce two Lagrange multipliers into the free energy functional $\mathcal{F}[u, \Gamma]$. A similar reasoning as above does lead to a dissipative dynamics and the constraints uniquely fix the Lagrange multilipliers, where for the local constraint multiplier an elliptic integro-differential equation has to be solved.

Numerics. We will give some first numerical examples. Here we use an operator splitting approach to first solve for the unconstrained dynamics – using methods introduced for the discretization of the Willmore flow in [4] – and then for the Lagrange multipliers to add the constraint correction. The discretization is based on linear parametric finite elements. Finally we will discuss the coupling of the membrane dynamics to the Stokes flow of the surrounding fluid.

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