Numerical Vesicle Dynamics and Rheology: a Phase Field Approach

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Abstract

Vesicles are droplets with arbitrary viscosity surrounded by a fluid phospholipidic membrane. They constitute a simple model to describe the mechanical properties of cells. Despite their simplicity compared to the biological systems, vesicles show an extremely rich behaviour even in simple situations as when embedded in an external linear shear flow. Vesicle dynamics has been studied for few years, and now the investigation is starting to address the rheological properties of a suspension of vesicles.

A suspension of vesicles is a complex fluid, in the sense that its constitutive equation is non newtonian and actually still unknown.

From a numerical point of view, the first technique used for simulations of vesicles is the *Boundary Integral Method*, which involves the direct tracking of the membrane and is based on the linearity of the hydrodynamical equation (Stokes law). Now this creates some difficuleties as the advection of the grid to follow the movement of the surface, and cannot be used when the velocity equation is not linear (as for arbitrary Reynolds number or for a nonlinear constitutive equation of the embedding fluid).

These are the main reasons for introducing *diffuse interface models* in this field. The phase field model is one of them. It is based on the introduction of an auxiliary field, the phase field, which assumes a constant value inside the vesicle, another constant value outside and has a rapid but continuous variation between the two regions. The position of the membrane is then encoded in the variation of the phase field. The velocity evolution equation is then coupled to the phase field evolution.

The advantages of this technique are the possibility to use a fixed mesh, the fact that the membrane is not tracked directly and that topology changes do not need any special care: they are just automatic.

The main challenges of this technique is the lack of agreed governing equations, fact due to the arbitrarity in the definition of the phase field, and the need to compute the limit of sharp interface, in whick the phase field becomes discontinuous across the interface, to get quantitatively precise results. Only in this limit the phase field model reproduces the known evolution equations for a thin interface.

To address the issue concerning the derivation of the evolution equations, a new model has been derived, based on the thermodynamical consistency for the equations even at finite interface thickness.

We have used the phase field model to study the rheology properties of a suspension of vesicles in a linear shear flow. The first topic has been the study of the constraints generated by a single vesicle. This study is not of primary importance for biological applications, where often cells in suspension are not isolated. But it is of a big conceptual importance, because understanding the individual behaviour is the key to link macroscopic behaviours to microscopic dynamics. Moreover, for a single vesicle analytical computations are possible (and already

done in the form of perturbation analysis) and a direct comparison with the Einstein model of a suspension of non-interacting rigid spheres is possible.

The numerical computations have been carried out in two dimensions. Nevertheless they show all the main caracteristics of its three-dimensional analogous. An extremely rich rheology has been found exploring its dependence on the viscosity contrast of the vesicle. this parameter is one of the most significative for the dynamics of the vesicle. Infact it allows to pass from a stationary solution (*tank-treading* regime, where the vesicle is elongated in the flow) to a periodic one (*tumbling*, where the vesicle rotates in the shear plane). Both instant and mean values of rheological properties show behaviours that can be explained through the presence of a membrane and the elasticity of the whole vesicle, giving a satisfactory explanation of macroscopic rheology as a function of microscopic dynamics.