An advected-field method for deformable entities under flow

T. Biben and C. Misbah^a

Groupe de Recherche sur les phénomènes hors équilibre, Laboratoire de spectrometrie physique, Université Joseph Fourier, BP87 38402 Saint Martin d'Hères Cedex, France

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Abstract. We study dynamics of a deformable entity (such as a vesicles under hydrodynamical constraints). We show how the problem can be solved by means of Green's functions associated with the Stokes equations. A gauge-field invariant formulation makes the study of dynamics efficient. However, this procedure has its short-coming. For example, if the fluids are not Newtonian, then no Green's function is available in general. We introduce a new approach, the advected field one, which opens a new avenue of applications. For example, non-Newtonian entities can be handled without additional deal. In addition problems like budding, droplet break-up in suspensions, can naturally be treated without additional complication. We exemplify the method on vesicles filled by a fluid having a viscosity contrast with the external fluid, and submitted to a shear flow. We show that beyond a viscosity contrast (the internal fluid being more viscous), the vesicle undergoes a tumbling bifurcation, which has a saddle-node nature. This bifurcation is known for blood cells. Indeed red cells either align in a shear flow or tumble according to whether haematocrit concentration is high or low.

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1 Introduction

Studies of deformable entities under hydrodynamical constraints is a general problem of science. For example, this problematic is essential in the understanding of blood rheology, liquid suspensions of Newtonian and non Newtonian fluids, and so on. The deformation of these entities in a shear flow, their alignment, or their breakup into smaller entities affect the macroscopic behaviours of suspensions. For example, when blood is submitted to a shear flow red cells become elongated and oriented in the flow, conferring to the blood thixotropic properties; that is a collapse of the actual viscosity (which can attain a decade), also known as shear thinning effect [1]. In small vessels, at low concentration (haematocrit less than 2%), red blood cells tumble. In the field of emulsions, when a droplet is suspended in another fluid, the droplet may, under shear, break-up generating thus smaller droplets. It has been shown that the particle size can drastically affect the toughness of blend polymers. For example in one case it has been demonstrated that toughness decreased fourfold when the average particle size increased from 0.7 μ m to 0.8 μ m [2]. In the context of rheological properties, it seems natural to concentrate first on the behaviour of an isolated entity. On the other hand, there are several circumstances where cells in the body often act as individual entities. Examples of particular interest in the biological and medical science is cell locomotion, like leucocytes moving in response to

a tissue injury, or cell aggregation during embryo-genesis. Of course the cell dynamics, besides flow, must include a more realistic picture of cytoskeletton, cytoplasm, as well as adhesion centers, when the motion imply a substrate. For an introduction to vesicle migration, see [3,4].

The aim of this contribution is to introduce a new approach for studying deformable entities under external constraints, like, for example, under a shear flow. For definiteness most of the discussion will be oriented towards vesicle dynamics, but we must keep in mind that the method works perfectly well in a variety of situations. In order to put the study in the context we shall review the ordinary method, and the power of geometry when a boundary (like the vesicle surface) is treated in the sharp limit sense. This part should also be very useful when local models for dynamics are used. In Section 2 we introduce the system and basic ingredients, we also introduce a toy model which offers a nice ground for identifying several dynamical features. In Section 3 we introduce the realistic model where hydrodynamics are taken into account. Section 4 introduces the new approach, with an application to vesicles under shear flow. Summary and outlook will be presented in Section 5.

2 The model

We consider the following situation: a deformable entity, taken here to be a vesicle for definiteness, is filled with a

^a e-mail: chaouqi.misbah@ujf-grenoble.fr



Fig. 1. A schematic view of a vesicles. The membrane is made of a bi-layer, each is composed of a 2D fluid-like phase of phospholipid molecules.

fluid having viscosity η_{in} and is suspended in a fluid having a viscosity η_{out} . The vesicle is subject to a hydrodynamical external flow, which is taken to be (without restriction) a linear shear flow $v_x = \gamma y$, where γ is the shear rate.

Vesicles are closed membranes suspended in an aqueous solution (Fig. 1), and we shall concentrate on this system at least for two reasons. On the one hand it constitutes a model system (in comparison to red cells, where it is likely that the cytoskeletton plays an important role). They can be viewed as a minimal cytoplasmic membrane model. On the other hand it lends itself to a relatively well controlled experimental manipulation, and thus a comparison with models can be made.

On the scale of the vesicle size $(10-100 \ \mu m)$, the width of the membrane is so small (few nm) that it can be viewed as a geometrical location, or surface of discontinuity. It will be shown later, however, that conferring a finite width to the membrane has proven to be extremely useful. For the sake of simplicity we shall confine ourselves to a two dimensional problem (the membrane is a contour). In order to show the benefit of the advected field approach, we shall first review the models used so far for the study of vesicle dynamics.

2.1 Geometry

This part is not only a review within the context of vesicles, but also regarded as a powerful method whenever one treats the boundaries as sharp (as a geometrical surface). From geometrical considerations it is a simple matter to derive an evolution equation for the contour in terms of the normal velocity v_n and the curvature. An elementary derivation is presented in [5]. The curvature κ is taken to be positive for a circle. The evolution equation for the curvature κ [5] involving derivatives with respect to the arclength s is

$$\frac{\partial \kappa}{\partial t} = -\left(\frac{\partial^2}{\partial s^2} + \kappa^2\right) v_n + v_t \frac{\partial \kappa}{\partial s} \tag{1}$$

where v_t is the tangential velocity. This equation is exact where only geometrical concepts are evoked. The tangential velocity appearing here is a gauge, it does not represent the velocity of matter, rather it is simply the velocity of a point at fixed curvilinear coordinate, and thus is fixed by the contour parameterization. Since a drift of the parametrization along the contour does not affects the shape, the tangential velocity is arbitrary. In the presence of hydrodynamics of course there is a tangential physical velocity which reacts on the normal one. Since in this part no hydrodynamics is included the tangential velocity is a gauge. A particular gauge, which will determine a particular definition of the tangential velocity, which has proven to be efficient in numerical treatments [5] is

$$\frac{\partial(s/L)}{\partial t} = 0, \qquad (2)$$

where L is the total arclength. This condition implies [5]

$$v_t(s) = -\int_0^s \mathrm{d}s' \kappa v_n + \frac{s}{L} \oint \mathrm{d}s' \kappa v_n \,. \tag{3}$$

Within this gauge, the evolution equation for the curvature becomes

$$\frac{\partial\kappa}{\partial t} = -\left(\frac{\partial^2}{\partial s^2} + \kappa^2\right) v_n + \frac{\partial\kappa}{\partial s} \left[\frac{s}{L} \oint \mathrm{d}s' \; \kappa v_n - \int_0^s \mathrm{d}s' \kappa v_n\right].$$
(4)

Gauge problems usually result in nonlocality. The physics is contained in the normal velocity, a question on which we direct our attention now.

A vesicle is a two dimensional fluid which does not resist to shear. The soft modes are *bending modes*, like in thin plates. If the membrane is viewed as a two dimensional geometrical surface, there are two invariants, which are the mean and the Gaussian curvatures. The energy associated with bending has the following form

$$E_b = \frac{\kappa_m}{2} \int \kappa^2 \mathrm{d}A + \frac{\kappa_g}{2} \int \kappa_1 \kappa_2 \mathrm{d}A + P \int \mathrm{d}V + \int \zeta \mathrm{d}A \tag{5}$$

where κ is the mean curvature $\kappa = \kappa_1 + \kappa_2$, κ_m and κ_g are the mean membrane rigidity and the Gaussian one; that the first term is quadratic in κ simply implies that for a geometrical surface the bending energy does not depend on the sign of κ . We have to keep in mind, however, that because of the membrane thickness this is not always correct; see the contribution of I. Bivas. The second term in the energy is a topological invariant owing to the Gauss-Bonnet theorem. Thus, if one is not interested in topological changes, this term can be disregarded, as we will adopt in what follows. For a two dimensional geometry, this term is of course absent as well. Finally P and ζ are two Lagrange multipliers enforcing a constant volume inside the vesicle (the fluid is incompressible), and a constant surface (the membrane is locally incompressible). ζ is a function of position along the membrane and of time. We only request a global condition for the fluid incompressibility (*i.e.* the pressure field is constant) rather than the usual local condition since the geometrical model we consider here does not incorporate hydrodynamics, and thus only provides informations on the global volume of the vesicle. When hydrodynamics is included the two conditions of incompressibility are formally the same. They

are both written as a vanishing of a divergence of velocity field (one in the bulk and the other along the contour). In the bulk the incompressibility is fulfilled thanks to the pressure field, while that along the surface is fixed thanks to a tension field. With the latter condition one has to follow the membrane which is advected by the velocity field.

The reaction force of the vesicle is obtained from the functional derivative of E_b , and one obtains in 2D:

$$\mathbf{f} \equiv -\frac{\delta E_b}{\delta \mathbf{r}} = \left[\left\{ \kappa_m \left(\frac{\partial^2 \kappa}{\partial s^2} + \frac{\kappa^3}{2} \right) - \kappa \zeta - P \right\} \mathbf{n} + \frac{\partial \zeta}{\partial s} \mathbf{t} \right]$$
(6)

n and **t** are respectively the normal and tangential unit vectors at current point **r** of the membrane. One has to relate now the force to the velocity field. This relation is nonlocal due to hydrodynamics. Intuitively, a force of a portion of the membrane acting on the fluid in which it is suspended disturbs the flow around it, affecting thereby other portions of the membrane. Since hydrodynamics possess no intrinsic lengthscale (like in electrostatics), the effect is of long range. Before presenting full dynamics is is instructive, however, to consider a local model.

2.2 A local model

A local model where dynamics depends on local velocity is the first example of dynamics to be considered here. We introduce the following dissipation functional

$$F_d = \frac{\eta}{2} \int |\mathbf{v}|^2 \mathrm{d}s \;. \tag{7}$$

The coefficient η is here an effective viscosity and has the dimension of a viscosity per unit length (due to the 2D geometry of the model). Neglecting inertial terms, the Euler-Lagrange equations for a dissipative dynamics provides

$$\eta v_n = \kappa_m \left(\frac{\partial^2 \kappa}{\partial s^2} + \frac{\kappa^3}{2} \right) - \kappa \zeta - P , \quad \eta v_t = \frac{\partial \zeta}{\partial s} . \tag{8}$$

The tangential velocity is defined up to an additive gauge, as we have seen. For example if $\frac{\partial \zeta}{\partial s} = 0$, then there is no physical tangential velocity, and the only remaining contribution is a gauge. In order to determine an equation for ζ , the membrane local incompressibility is imposed, entailing

$$\mathbf{t} \cdot \frac{\partial \mathbf{v}}{\partial s} = \frac{\partial v_t}{\partial s} + v_n \kappa = 0 \tag{9}$$

a relation fixing ζ as a function v_n and κ . Dynamics can thus be determined completely as a function of κ only. We have [6] solved numerically the problem of vesicles moving by *haptotaxis*, a terminology referring to a motion induced by an adhesion gradient along the substrate. Figure 2 shows a typical shape. The adhesion potential is chosen as

$$w(\mathbf{r}) = w_0(1+u_0x) \left(\frac{y_0^4}{y^4} - \frac{2y_0^2}{y^2}\right),\tag{10}$$



Fig. 2. A typical profile of a vesicle moving to the right in an adhesion gradient.

 y_0 fixes the characteristic distance between the substrate and the membrane, and $\hat{w}(x) = -w_0(1 + u_0 x)$ the minimum of the potential interaction, occurring for $y = y_0$. It depends linearly on x with an adhesion gradient u_0 . We must supplement the force by the adhesion contribution. Writing the adhesion energy as $\int w(x) dx$ we obtain for the additional force

$$\mathbf{f}_w = -(cw + \nabla w \cdot \mathbf{n})\mathbf{n} \ . \tag{11}$$

The Lagrange multiplier P is fixed by imposing that the enclosed area (volume in 3D) is fixed, due to the incompressibility of the fluid. This means that $\int v_n ds = 0$, from which we obtain

$$P = -\zeta \langle \kappa \rangle + \langle v_n^0 \rangle \tag{12}$$

where we have defined $v_n = v_n^0 - P - \kappa \zeta$, and $\langle ... \rangle$ stands for $(1/L) \int ... ds$, L being the vesicle perimeter.

3 Nonlocal model

As stated before the motion of vesicles is nonlocal owing to the long range hydrodynamical equations. Thus for the sake of comparison with realistic situations we must include nonlocal interactions. The Reynolds number is small so that the hydrodynamics equations become linear (the Stokes limit). By means of Green's functions the velocity field at any point in the fluid can be related to the forces by (where the viscosities inside and outside the vesicle are equal)

$$\mathbf{v}(\mathbf{r}, t) = \int_{memb} \overline{\overline{T}} \cdot \mathbf{f}' \, \mathrm{d}s' + \int_{subs} \overline{\overline{T}} \cdot \left(-\eta \frac{\partial \mathbf{v}'}{\partial y'} + p' \hat{\mathbf{y}}\right) \, \mathrm{d}x' \,.$$
(13)

 $\overline{\overline{T}}$ is the Oseen tensor [7,8] and $\hat{\mathbf{y}}$ is a unit vector. For brevity we set $\mathbf{v}' \equiv \mathbf{v}(\mathbf{r}', t)$ and $\overline{\overline{T}} \equiv \overline{\overline{T}}(\mathbf{r}, \mathbf{r}')$. The first term in equation (13) represents the membrane contribution, with \mathbf{f} the membrane forces (the sum of 6 and 11). The second term accounts for the presence of the wall. Here p' denotes the pressure field, and because that pressure is compatible with the fluid incompressibility condition (used in order to obtain the Oseen tensor), there is no need for introducing the analogue of the Lagrange multiplier P met in the last section. The determination of ζ follows for the membrane incompressibility as before. The wall reaction term can be determined by requiring $\mathbf{v} = 0$ on the substrate, and inverting numerically the integral equation (13). The membrane velocity is equal to the fluid velocity, providing us with the tangential and normal velocity to be used in dynamics as in the last section. This method allows to handle several problems such as migration in an adhesion gradient, lift force of viscous nature [3,4], and so on. This method is powerful, but is limited to a restricted range of situations. This is why we have developed a new approach which opens many new lines of inquiries.

4 New approach: the advected field

Although the integral formulation presented above, combined with geometry, is powerful, the general applicability is limited to problems where the underlying field equations (like the hydrodynamics equations) are linear, otherwise the Green's function techniques can not be used. Thus, in principle one has to discretize the full field equations and solve them with boundary conditions, and especially on the vesicle contour, which changes dynamically. This requires at each time a front tracking procedure, which is, in general, difficult to implement. In addition, if several deformable entities are present one has to track each boundary, and to specify rules (by hand, and thus often in an ad-hoc manner) on their possible coalescence, bud emission, and so on. We introduce a new powerful method, the advected field approach. This method bypass front tracking, notwithstanding their straightforward numerical implementation.

The basic ingredient of the method consists in introducing an auxiliary field, $\phi(\mathbf{r}, t)$ which is continuous across the boundary, albeit it varies quite rapidly. That field takes a value, say $\phi = -1$, inside the vesicle and $\phi = 1$ outside. The profile has a tanh-like shape across the boundary. The rapid variation of ϕ encodes the boundary position. This field must be coupled to the hydrodynamical field, and possibly to other fields, and written in such a way that the usual equations (in the sharp limit sense) are recovered when letting the extent of the rapid variation go to zero (a step function). The field will be advected (*i.e.* transported by the flow), and this induces the shape evolution. This is why we name this method as the advectedfield. The field ϕ is governed by the following equation

$$\frac{\partial \phi}{\partial t} = -\mathbf{v} \cdot \nabla \phi + \epsilon_{\phi} \left(-\frac{\delta E_{intrinsic}}{\delta \phi} - \kappa \epsilon^2 \left| \nabla \phi \right| \right) \quad (14)$$

where we recognize an advection (transport) term, the $-\mathbf{v} \cdot \nabla$ contribution, which couples the auxiliary field to the flow, and a relaxation term which produces a tanhlike profile across the boundary according to the intrinsic energy functional

$$E_{intrinsic}[\phi] = \int \int dx dy \, \left\{ \frac{1}{4} (1 - \phi^2)^2 + \frac{\epsilon^2}{2} \left(\nabla \phi \right)^2 \right\}_{(15)}$$

which is the classical double-well potential for a fluid-fluid equilibrium, for example. The width of the boundary is $\epsilon\sqrt{2}$. ϵ_{ϕ} is a constant related to the relaxation time of the profile to its tanh-like shape. The term which is proportional to $|\nabla\phi|$ in (14) is here to suppress the wall energy associated with ϕ [9]. A vesicle exchanges no matter with the underlying bulk phase, so that its area is constant; a vesicle has no intrinsic surface tension. The next step is to specify dynamics of the velocity field in the whole domain, *i.e.* which is valid in the interior as well as in the exterior. For that purpose one must determine the membrane forces. The Helfrich free energy in the advected-field sense takes the form

$$E_b = \frac{\kappa_m}{2} \int \int \mathrm{d}x \,\mathrm{d}y \,\kappa^2 \frac{|\nabla \phi|}{2} + \int \int \mathrm{d}x \,\mathrm{d}y \,\zeta \frac{|\nabla \phi|}{2} \cdot \quad (16)$$

The curvature field κ can easily be expressed in terms of ϕ if we define the normal vector field \mathbf{n} and the tangential one \mathbf{t} as: $\mathbf{n} = \nabla \phi / |\nabla \phi|$, $\mathbf{t} = \mathbf{n} \wedge \mathbf{z}$. This definition corresponds to the choice: $d\mathbf{t}/ds = -\kappa \mathbf{n}$ in curvilinear coordinates. One can easily check that $\kappa = +\nabla \cdot \mathbf{n} \cdot \zeta(\mathbf{r}, t)$ is, in the sharp-boundary spirit (as seen before), a Lagrange multiplier which enforces local incompressibility of the vesicle area in the course of time. The functional derivative of E_b provides us with the membrane force

$$\mathbf{f} = \left[\kappa_m \left\{\frac{\kappa^3}{2} + \mathbf{t} \cdot \nabla(\mathbf{t} \cdot \nabla\kappa)\right\} \mathbf{n} - \zeta\kappa \mathbf{n} + \mathbf{t} \cdot \nabla\zeta \mathbf{t}\right] \frac{|\nabla\phi|}{2} \cdot (17)$$

This expression coincides with (6) when $\epsilon \to 0$. Once the force is known, the velocity field equation in the whole domain can be written. This takes the form

$$\epsilon_v \frac{\partial \mathbf{v}}{\partial t} = \eta \Delta \mathbf{v} - \nabla P + \mathbf{f} \tag{18}$$

where ϵ_v is a density scale which is related to the relaxation time. ϵ_v is chosen in such a way that inertia are small enough (the Stokes limit). The pressure field must be adjusted to ensure incompressibility:

$$\nabla \cdot \mathbf{v} = 0.$$

In the presence of a viscosity contrast between the interior and exterior of the vesicle $\eta \Delta \mathbf{v}$ in the Stokes equation is substituted by $\partial_i(\eta(\partial_i v_j + \partial_j v_i))$. Summation over repeated indices is implied. A convenient prescription for the viscosity is $\eta = \eta_{out}(1+\phi)/2 + \eta_{in}(1-\phi)/2$. Finally, in order to ensure local incompressibility of the membrane, the field ζ is governed by the following dynamical equation

$$\frac{\partial \zeta}{\partial t} = -\mathbf{v} \cdot \nabla \zeta + T \, \mathbf{t} \cdot (\mathbf{t} \cdot \nabla) \mathbf{v} \tag{19}$$

where T is a tension-like constant and $\mathbf{t}.(\mathbf{t}.\nabla)\mathbf{v}$ represents $\mathbf{t} \cdot \partial \mathbf{v}/\partial s$ in the sharp boundary limit, which is nothing but the local lateral extension rate of the membrane (see Eq. (9)). ζ is then a tension field proportional to the local lateral elongation of the membrane, and as the auxiliary



Fig. 3. A typical situations where the vesicle undergoes a tanktreading motion characterized by an angle $\psi(t)$, and the arrows represent the velocity field. On sees that the membrane is advected by the flow, causing a tank-treading, which in turn induces a flow inside the vesicle.

field ϕ it is transported by the flow $(-\mathbf{v} \cdot \nabla$ term). Choosing a large enough T enforces incompressibility. Note that the field ζ , like the advected field ϕ is defined over the entire domain. Its action is however only limited close to the membrane thanks to the gradient of ϕ appearing in the force (17). We can show that the equations of motion reduces to the usual sharp boundary set, when $\epsilon \to 0$. This is a singular perturbation problem which will be treated elsewhere [10].

Several tests have been performed in order to ascertain the numerical validity of the advected field approach. (i) We have checked that starting from an arbitrary initial shape the vesicle relaxes towards its equilibrium shape in the absence of any external constraint (external flow for example). (ii) We have checked that under a linear shear-flow the vesicle aligns at an angle ψ with respect to the flow direction. That angle decreases monotonously when the swelling factor decreases; the swelling factor is defined as $\tau = 4\pi S/\mathcal{P}^2$, S is the internal area, \mathcal{P} the perimeter (2D); for a circle $\tau = 1$, and $\tau < 1$ otherwise. The overall behaviour is in agreement with the finding of Kraus et al. [11] based on an integral formulation. This work was limited to the situation with no viscosity contrast, $r \equiv \eta_{in}/\eta_{out} = 1$. Even including just a viscosity contrast requires some deal within the boundary integral formulation, due to the so-called double layer contribution [7]. In contrast, within the advected field approach the implementation of a viscosity contrast is automatically performed; it suffices to choose the numbers η_{in} and η_{out} at will. In addition, if the constitutive fluid equation is nonlinear (not of Stokes type), obviously a boundary integral formulation can not be used at all. This circumstance is the rule rather than the exception in the industrial rheological liquids, in the physiological transports, and so on.



Fig. 4. A schematic view of the behaviour of the angle ψ as a function of the viscosity contrast r for a given swelling factor τ . At $r = r_c$ the stable branch (solid line) merges with the unstable one (dashed line), whereby a new time-dependent solution characterized by $\psi(t)$ takes place. This is a saddle node bifurcation.

This method is used first in order to study the behaviour of a vesicle in a shear flow with a viscosity contrast. The overall finding of this study can be summarized as follows. For $r < r_c$ (where r_c is a function of the swelling factor $\tau)$ the vesicle assumes an orientation with an angle ψ , like for the case with r = 1. The membrane (which is fluid-like) executes a tank-treading like motion as depicted in Figure 3. Note that in a tank only the treads rotate, the tank itself does not, while here the fluid inside is moving as well. The angle decreases upon increasing r. The interesting feature is that if $r = r_c$ the solution corresponding to a steady orientation of the vesicle ceases to exist whereby a new solution appears. The vesicles undergoes a *tumbling* motion, while its membrane continues to tank-tread. The tumbling threshold r_c is a function of τ . The tumbling is not an ordinary instability where below threshold the system withstands infinitesimal perturbations, while beyond it is unstable. Here in contrast the stable branch disappears after merging with an unstable one (see Fig. 4). This is called a saddle-node bifurcation. It must be noted that this transition does not exist for rigid particles since tank-treading is then impossible. A rigid particle placed in a shear flow always tumble, and thus the tank-treading regime is characteristic of deformable objects.

In blood red cells align under shear flow. If the same blood is diluted enough for the cell-cell interaction to be negligible, the red cell assumes a tumbling motion [12]. The viscosity of the interior of the human red cell is about 6-7 that of water, while the plasma has a viscosity of about 1.2–1.3 times the water viscosity. The tumbling threshold found here depends on the swelling factor. If one considers the swelling factor of a human of red cells $\tau \sim 0.7$, we find that the threshold for tumbling is of about $r \sim 6$. In other words it seems that the value of the viscosity ratio between interior and exterior of red cells is to put them close to a critical value for tumbling. We are not yet aware of whether this is accidental or rather it does have a physiological basis.

5 Summary

We have presented a new approach for the study of deformable entities under hydrodynamical constraints. The method has been presented for vesicles in 2D. An extension to 3D is straightforward and is currently under study. This method is powerful and has a much wider scope than the traditional boundary integral formulation based on the Green's functions. Of course the method can be used for the study of various situations such as droplet dynamics suspended in another fluid. The method has no special restriction on whether the fluids are Newtonian or not. Thus extension to non Newtonian fluids can be made along the same strategy.

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