Functional Thin Films on Surfaces – supplemental material

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1 DERIVATION OF THE VARIATIONAL MODEL ON TRIANGULATED SURFACES

This appendix is a more detailed presentation of the material in section 3. We start from a set of basic geometrical identities, and based on those we present the Taylor expansions that are mentioned in various places in the paper. In particular, we shed more light on the derivation of the conservation law (§3.3), and the appearance of the rotated shape operator $\bar{S}$ therein, and provide explicit formulas for the viscous dissipation rate (§3.4).

Setup. As stated in §3.1, we consider a surface Γ, together with a height field $h : \Gamma \to \mathbb{R}$ and an approximate normal $n : \Gamma \to \mathbb{R}^3$. The fields and the surface itself are assumed to be Lipschitz continuous, which includes the important case where Γ is a triangular mesh and h, n are linearly interpolated within each face of Γ. We are indeed mainly interested in this particular case, where we also make the following consistency assumptions[1] on n:

1) approximation of the exact normal: $n = \nu + O(\delta x)$
2) symmetric surface gradient: $\nabla_\Gamma n - \nabla_\Gamma n^T = O(\delta x)$
3) directional derivatives are tangential: $\nabla_\Gamma n^T n = O(\delta x)$

where ν is the exact (piecewise constant) normal of the faces, δx is an appropriate measure of the size of the elements of the triangulation, and the surface gradient $\nabla_\Gamma = P\nabla_{\mathbb{R}^3}$ is defined via the projection $P = \mathrm{id} - \nu \otimes \nu$. Based on the consistency assumptions, we introduce the discrete shape operator

$$S = -\frac{1}{2}P\left(\nabla_\Gamma n + \nabla_\Gamma n^T\right)P = -\nabla_\Gamma n + O(\delta x) \quad (1)$$

The name will be justified when we look at the the expansion of the surface energy.

Geometrical Identities. Our main geometrical tool is a set of identities that describe the rate of change of various geometrical objects under the normal displacement

1. Note that these are all satisfied when $n = \nu + O(\delta x^2)$.

$\phi_{sh}(x) = x + sh(x)n(x)$, $x \in \Gamma$. In addition to the image $\phi_{sh}(U)$ of subsets $U \subset \Gamma$, we will also refer to their extrusion $\Phi_{sh}(U) = \{\phi_{rh}(x) \,|\, x \in U, r \in [0, s]\}$. Since we are studying *thin* films, the assumption is that the parameter s is always of order $\epsilon \ll 1$, thus justifying considering Taylor expansions in s. We have then, for a patch $U \subset \Gamma$

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_{\phi_{sh}(U)} \mathrm{d}a = \int_{\phi_{sh}(U)} \mathrm{Tr}(\nabla_\Gamma(hn))\mathrm{d}\,a$$
$$= -\int_{\phi_{sh}(U)} h\,\mathrm{Tr}(S)\,\mathrm{d}a + O(\delta x) \quad (2)$$

and for the associated volume $V_{sh}(U) = \Phi_{sh}(U)$

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_{V_{sh}(U)} \mathrm{d}x = \int_{\phi_{sh}(U)} hn \cdot \nu\,\mathrm{d}a$$
$$= \int_{\phi_{sh}(U)} h\,\mathrm{d}a + O(\delta x) \quad (3)$$

The approximations are based on the expansion $\nabla_\Gamma(hn) = n \otimes \nabla_\Gamma h + h\nabla_\Gamma n$. Using the map ϕ_{sh}, we can expand in a natural way the fields h and n into a neighbourhood of Γ, so that $\dot{h} = 0$ and $\dot{n} = 0$, if we use the notation $\dot{f} = \frac{\mathrm{d}}{\mathrm{d}s}f(\phi_{sh}(x))$. We also expand the exact normal ν by taking the normal[2] of the displaced surface $\Gamma_{sh} = \phi_{sh}(\Gamma)$ at the $y = \phi_{sh}(x)$. We can show then that

$$\dot{\nu} = -\nabla_\Gamma(hn)^T\nu = -\nabla_\Gamma h + O(\delta x) \quad (4)$$

Finally, we consider a curve $\gamma \in \Gamma$ with (unit) tangent vector τ. The normal displacement transforms the curve $\gamma \mapsto \phi_{sh}(\gamma)$ and therefore also the tangent vector, with

$$\dot{\tau} = \nabla_\Gamma(hn)\tau - (\tau^T\nabla_\Gamma(hn)\tau)\tau$$
$$= \frac{\partial h}{\partial \tau}n + h(\frac{\partial n}{\partial \tau} \cdot \rho)\rho + O(\delta x) \quad (5)$$

where $\rho = \nu \times \tau$ is the (inward pointing) conormal of γ. Then for line integrals we have

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_{\phi_{sh}(\gamma)} \mathrm{d}l = \int_{\phi_{sh}(\gamma)} \tau^T\nabla_\Gamma(hn)\tau\,\mathrm{d}l$$
$$= \int_{\phi_{sh}(\gamma)} h(\frac{\partial n}{\partial \tau} \cdot \tau)\,\mathrm{d}l + O(\delta x) \quad (6)$$

2. The underlying assumption is that the values that s takes are small enough, so that the images Γ_{sh} do not intersect.

and for the area integrals over the extrusion $\Phi_{sh}(\gamma)$

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_{\Phi_{sh}(\gamma)}\mathrm{d}a = \int_{\phi_{sh}(\gamma)}|hn\times\tau|\,\mathrm{d}l \tag{7}$$

where $n\times\tau$ is the (almost unit) normal of the surface $\Phi_{sh}(\gamma)$.

Mass density. The relation between the mass density u and the height follows directly by integrating (3) with $U=\Gamma$ w.r.t. s:

$$\int_{V_{\epsilon h}}\mathrm{d}x = \int_0^\epsilon\int_{\Gamma_{sh}}h\,\mathrm{d}a\,\mathrm{d}s + \mathrm{O}(\delta x)$$

$$= \int_0^\epsilon\left\{\int_\Gamma h\,\mathrm{d}a + s\int_\Gamma h^2\,\mathrm{Tr}(\nabla_\Gamma n)\,\mathrm{d}a + \mathrm{O}(s^2)\right\}\mathrm{d}s + \mathrm{O}(\delta x)$$

$$= \epsilon\int_\Gamma\left(h-\frac{\epsilon}{2}h^2\,\mathrm{Tr}(S)\right)\mathrm{d}a + \mathrm{O}(\delta x+\epsilon^3)$$

where we recall that $\Gamma_{0h}\equiv\Gamma$. From the defining property $\int_{V_{\epsilon h}}\mathrm{d}x = \epsilon\int_\Gamma u\,\mathrm{d}a$ we deduce then that $u = h-\frac{\epsilon}{2}h^2\,\mathrm{Tr}(S)+\mathrm{O}(\delta x+\epsilon^3)$. Conversely, we will make extensive use of the substitution $h = u+\frac{\epsilon}{2}u^2\,\mathrm{Tr}(S)+\mathrm{O}(\delta x+\epsilon^3)$.

Gravitational Energy. The Taylor expansion for the gravitational energy $\mathcal{E}_g = \int_{V_{\epsilon h}}z\,\mathrm{d}x$ is very similar to the previous paragraph, with the major difference that, whereas $\dot{h}=0$ by construction, $\dot{z}=\nabla z\cdot(hn) = h\cos\theta + \mathrm{O}(\delta x)$. It follows that

$$\int_{V_{\epsilon h}}z\,\mathrm{d}x = \int_0^\epsilon\int_{\Gamma_{sh}}zh\,\mathrm{d}a\,\mathrm{d}s =$$

$$\int_0^\epsilon\left\{\int_\Gamma zh\,\mathrm{d}a + s\int_\Gamma(h\dot{z}-zh^2\,\mathrm{Tr}(S))\mathrm{d}a+\mathrm{O}(s^2)\right\}\mathrm{d}s+\mathrm{O}(\delta x)$$

$$= \epsilon\int_\Gamma\left(zh+\frac{\epsilon}{2}h^2\cos\theta-\frac{\epsilon}{2}h^2 z\,\mathrm{Tr}(S)\right)\mathrm{d}a + \mathrm{O}(\delta x+\epsilon^3)$$

$$= \epsilon\int_\Gamma\left(zu+\frac{\epsilon}{2}u^2\cos\theta\right)\mathrm{d}a + \mathrm{O}(\delta x+\epsilon^3)$$

Note that the change of variables $h = u+\frac{\epsilon}{2}u^2\,\mathrm{Tr}(S)$ in the last line introduces a term $\frac{\epsilon}{2}u^2 z\,\mathrm{Tr}(S)$ that cancels out with the existing term.

Surface Energy. For the surface energy, the Taylor expansion is very similar in spirit to the well-known Steiner formulas. The main difficulty is that the leading order term is simply the area of Γ which is fixed, and therefore we need to calculate the second variation of the surface area. Although it is an established result for smooth surfaces, we will sketch its calculation to illuminate the way $\nabla_\Gamma n$ shows up in the case of a triangular surface. The main idea is that a parametrization of Γ can be pushed forward onto the images Γ_{sh}. If we write the metric of Γ as $g = X^T X$, where X is the matrix whose columns are the coordinate vectors X_i of the parametrization, then the X_i are pushed forward by the normal displacement map ϕ_{sh} so that $\dot{X}_i = \nabla_\Gamma(hn)X_i \Rightarrow \dot{X} = \nabla_\Gamma(hn)X$. For the induced metric g of the Γ_{sh}, we have then $\dot{g} = X^T(\nabla_\Gamma(hn)+\nabla_\Gamma(hn)^T)X$ and this is exactly where the matrix $\nabla_\Gamma(hn)$ comes into all the geometrical measure calculations. In particular, with the help of the identities $\frac{\mathrm{d}}{\mathrm{d}s}\,\mathrm{Tr}(g) = \mathrm{Tr}(\dot{g})$ and $\frac{\mathrm{d}}{\mathrm{d}s}\det(g) = \det(g)\,\mathrm{Tr}(g^{-1}\dot{g})$ and the fact that the tangential projection can be written

as $P = Xg^{-1}X^T$, we can show that the area element $\sqrt{\det(g)}\,\mathrm{d}x_1\,\mathrm{d}x_2$ grows with

$$\frac{\mathrm{d}}{\mathrm{d}s}\sqrt{\det(g)} = \mathrm{Tr}(\nabla(hn))\sqrt{\det(g)}$$

$$= -h\,\mathrm{Tr}(S)\sqrt{\det(g)} + \mathrm{O}(\delta x)$$

and, together with the fact that $\dot{h}=0$ and $\dot{n}=0$ by construction,

$$\frac{\mathrm{d}^2}{\mathrm{d}s^2}\sqrt{\det(g)} =$$

$$\left\{\mathrm{Tr}(\nabla(hn))^2 - \mathrm{Tr}(\nabla(hn)^2) + |\nabla_\Gamma(hn)^T\nu|^2\right\}\sqrt{\det(g)}$$

$$= \left\{h^2(\mathrm{Tr}(S)^2-\mathrm{Tr}(S^2)) + |\nabla_\Gamma h|^2\right\}\sqrt{\det(g)} + \mathrm{O}(\delta x)$$

Considering these for a uniform film $h=1$, and recalling the relation between the variation of the surface area and the curvatures given by the Steiner formulas, we naturally identify $H = \mathrm{Tr}(S)$ as the discrete mean curvature, and $K = \frac{1}{2}(\mathrm{Tr}(S)^2-\mathrm{Tr}(S^2))$ as the discrete Gaussian curvature. Recall that S is a 3×3 matrix with a zero eigenvalue, since $S\nu=0$. If we denote κ_1,κ_2 the other two eigenvalues (and $\kappa_3=0$), then we can easily show that $H = \kappa_1+\kappa_2+\kappa_3 = \kappa_1+\kappa_2$. Furthermore, $K = \kappa_1\kappa_2+\kappa_2\kappa_3+\kappa_3\kappa_1 = \kappa_1\kappa_2$, whereas $\det(S)=0$, justifying the unexpected expression for K. Using the derivatives above, we can prove the first variation (2) and derive a similar identity for the second variation. An expansion similar to the ones we used above, with the change of variable form h to u in the end, yields then the relevant terms in expression (9).

Conservation Law. We consider the volume of fluid $V_{\epsilon h}(U)$ in the part of the thin film above a patch $U\subset\Gamma$. As the height function h changes in time, we require that *the rate of change of the volume $V_{\epsilon h}(U)$ matches the flux of the velocity field* $\mathfrak{v}$ through the sides[3] $F_{\epsilon h}(U) = \Phi_{\epsilon h}(\partial U)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_{\epsilon h}(U)}\mathrm{d}x = \int_{F_{\epsilon h}(U)}\mathfrak{v}\cdot\mu\,\mathrm{d}a \tag{8}$$

where $\mu = \frac{n\times\tau}{|n\times\tau|}$ is the (inward pointing) normal of the surface $F_{\epsilon h}(U)$. For the left hand side, we have already essentially shown that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_{\epsilon h}(U)}\mathrm{d}x = \epsilon\int_\Gamma\partial_t u\,\mathrm{d}a + \mathrm{O}(\delta x+\epsilon^3)$$

The right hand side can be written as

$$\int_{F_{\epsilon h}(U)}\mathfrak{v}\cdot\mu\,\mathrm{d}a = \int_0^\epsilon\int_{\phi_{sh}(\partial U)}h\,\mathfrak{v}\cdot(n\times\tau)\,\mathrm{d}l\,\mathrm{d}s$$

$$= \int_0^\epsilon\left\{\int_{\partial U}h\,\mathfrak{v}\cdot(n\times\tau)\,\mathrm{d}l + s\int_{\partial U}h^2\mathfrak{v}\cdot(n\times\frac{\partial n}{\partial\tau})\,\mathrm{d}l\right\}\mathrm{d}s$$

$$= \int_{\partial U}h\int_0^\epsilon\left\{\mathfrak{v}_{\Gamma,s}\cdot(n\times\tau) + sh\,\mathfrak{v}_{\Gamma,s}\cdot(n\times\frac{\partial n}{\partial\tau})\right\}\mathrm{d}s\,\mathrm{d}l$$

$$+ \mathrm{O}(\delta x+\epsilon^3)$$

where $\mathfrak{v}_{\Gamma,s}$ is the tangential part (since the triple product with n eliminates the normal component) of the velocity on

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3. Since the boundary $\Phi_{\epsilon h}(\partial U)$ is itself time-dependent, we should consider the relative velocity $V(y) = \mathfrak{v}(y) - \dot{y}$ instead. But $\dot{y} = s\,h_t n$ and $n\cdot\mu=0$, and therefore $V\cdot\mu = \mathfrak{v}\cdot\mu$.

the layer Γ_{sh}. The term $\frac{\partial n}{\partial \tau}$ comes in fact from the sum of $\dot{\tau}$ (from the variation of $\mathfrak{v} \cdot \mu$) and $h(\frac{\partial n}{\partial \tau} \cdot \tau)\tau$ (from the variation of $\mathrm{d}l$ via (6)). By (5), then $\dot{\tau} + h(\frac{\partial n}{\partial \tau} \cdot \tau)\tau = \frac{\partial h}{\partial \tau}n + h\frac{\partial n}{\partial \tau}$ and the cross product with n eliminates the first term. Next, we need to apply the divergence theorem to get an integral over U. For this, we note that $n \times \tau = \nu \times \tau + \mathrm{O}(\delta x)$ and $\nu \times \tau = \rho$ is exactly the conormal of ∂U that we need. The problem is the second term, which we need to rewrite. For any vector $a \in \mathbb{R}^3$, we introduce the skew-symmetric matrix $[a]_\times = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}$, which is defined so that $[a]_\times b = a \times b$ for any vector b. In other words, it is the matrix representation of the cross product with a fixed vector. Applying this for the normal ν, it is easy to show that the projection $P = -[\nu]_\times^2$. Then $\mathfrak{v}_{\Gamma,s} \cdot (n \times \frac{\partial n}{\partial \tau}) = \mathfrak{v}_{\Gamma,s} \cdot (n \times \nabla_\Gamma n\, P\tau) = -\mathfrak{v}_{\Gamma,s} \cdot ([n]_\times \nabla_\Gamma n[\nu]_\times^2 \tau) = -([n]_\times \nabla_\Gamma n[\nu]_\times)^T \mathfrak{v}_{\Gamma,s} \cdot [\nu]_\times \tau = -\bar{S}\mathfrak{v}_{\Gamma,s} \cdot (\nu \times \tau) + \mathrm{O}(\delta x)$ with $\bar{S} = -[\nu]_\times S[\nu]_\times$. This is exactly what we need to apply the divergence theorem:

$$\int_{\partial U} h \int_0^\epsilon \left\{ \mathfrak{v}_{\Gamma,s} \cdot (n \times \tau) + sh\, \mathfrak{v}_{\Gamma,s} \cdot (n \times \frac{\partial n}{\partial \tau}) \right\} \mathrm{d}s\, \mathrm{d}l =$$

$$\int_{\partial U} \left\{ h \int_0^\epsilon (\mathfrak{v}_{\Gamma,s} - sh\bar{S}\mathfrak{v}_{\Gamma,s})\, \mathrm{d}s \right\} \cdot \rho\, \mathrm{d}l =$$

$$-\int_U \operatorname{div}_\Gamma \left\{ h \int_0^\epsilon (\mathfrak{v}_{\Gamma,s} - sh\bar{S}\mathfrak{v}_{\Gamma,s})\, \mathrm{d}s \right\} \mathrm{d}a$$

$$= -\int_U \operatorname{div}_\Gamma \left\{ h \int_0^\epsilon Q_s \mathfrak{v}_{\Gamma,s}\, \mathrm{d}s \right\} \mathrm{d}a$$

with the tensor $Q_s = \mathrm{id} - sh\bar{S}$. Making, as usual, the change of variables from h to u yields the form of the tensor Q_s that we use in §3.3.

Dissipation. As noted in §3.4, we know that the viscous dissipation rate $\int_{V_{\epsilon h}} |\nabla \mathfrak{v} + \nabla \mathfrak{v}^T|^2\, \mathrm{d}x$ is dominated by the vertical shear stress, i.e. the normal derivative of the tangential velocity. The problem is that the tangential velocities $\mathfrak{v}_{\Gamma,s}$ live on different tangent spaces $T\Gamma_{sh}$ for various s, and so the derivative $\frac{\partial}{\partial s}\mathfrak{v}_{\Gamma,s}$ can not be used as is for the calculation of the dissipation. The correct idea turns out to be to

1) pull back the velocities to the common tangent space $T\Gamma$
2) take the derivative w.r.t. s there
3) push forward the derivative up to $T\Gamma_{sh}$ and take its norm there

This leads to the following expression for the shear-dominated viscous dissipation rate:

$$\int_{V_{\epsilon h}} h^{-2} \left| d\phi_{sh} \frac{\partial}{\partial s} d\phi_{sh}^{-1} \mathfrak{v}_{\Gamma,s} \right|^2 \mathrm{d}x$$

where $d\phi_{sh}(x)$ is the push forward of the normal displacement, and $d\phi_{sh}^{-1}$ its pull back. Again using Taylor expansion we obtain as an approximation the quadratic form

$$\mathcal{D}_h(\mathfrak{v}, \mathfrak{v}) = \int_\Gamma \int_0^\epsilon \lambda_s \left| \Lambda_s \frac{\partial}{\partial s}(\Lambda_s^{-1} \mathfrak{v}_{\Gamma,s}) \right|^2 \mathrm{d}s\, \mathrm{d}a\,.$$

The factors $\lambda_s = h^{-1}(1 - hsH)$ and $\Lambda_s = \mathrm{id} - shS$, which is a linearization of the push forward $d\phi_{sh}$, again capture the effect of the geometry. At this point, as in §3.4, we write the tangential velocity in the fluid as $\mathfrak{v}_{\Gamma,s} = \Pi_s v$, where Π_s is a (tensor) velocity profile and v is an average

velocity (independent of s) such that the conservation law is equivalent to $\partial_t u = -\operatorname{div}_\Gamma(uv)$. The dissipation then can be written as

$$\mathcal{D}_u(\Pi_s v, \Pi_s v) = \int_\Gamma \int_0^\epsilon \lambda_s |R_s v|^2\, \mathrm{d}s\, \mathrm{d}a = \int_\Gamma v \cdot C[\Pi_s] v\, \mathrm{d}a$$

with $R_s = \Lambda_s \frac{\partial}{\partial s}(\Lambda_s^{-1}\Pi_s)$ and $C[\Pi_s] = \int_0^\epsilon \lambda_s R_s^T R_s\, \mathrm{d}s$. We wish to optimize the transportation cost tensor $C[\Pi_s]$ for given boundary conditions $\Pi_0 = 0$ (no-slip at substrate) and $R_\epsilon = 0$ (zero shear stress at free surface) under the integral constraint $\int_0^\epsilon Q_s \Pi_s\, \mathrm{d}s = \mathrm{id}$. The optimum profile matches in the flat case to leading order the well-known Hagen-Pouseuille profile. For flat domains this is discussed in detail in [1]. The curved case for smooth substrate surfaces is discussed via perturbation arguments in [2]. Our approach is with respect to the optimization closest to [3]. We use the constraint to introduce the partial flux profile $\Sigma_s = \int_0^s Q_r \Pi_r\, \mathrm{d}s \Rightarrow \Pi_s = Q_s^{-1} \frac{\partial}{\partial s}\Sigma_s$. The constraint itself takes then the simple form $\Sigma_\epsilon = \mathrm{id}$, and we can think of the transportation cost as a function $C[\Sigma_s]$ of the partial flux profile with $R_s = \Lambda_s \frac{\partial}{\partial s}(\Lambda_s^{-1} Q_s^{-1} \frac{\partial}{\partial s}\Sigma_s)$. Taking the variation of $C[\Sigma_s]$ w.r.t. Σ_s, together with the boundary conditions in the form

- $\Sigma_0 = 0$ (by construction),
- $\Sigma_\epsilon = \mathrm{id}$ (by the constraint),
- $\frac{\partial}{\partial s}\Sigma_s|_{s=0} = 0$ (no slip at the substrate),
- $\frac{\partial}{\partial s}(\Lambda_s^{-1} Q_s^{-1} \frac{\partial}{\partial s}\Sigma_s)|_{s=\epsilon} = 0$ (no shear stress at the free surface),

we arrive at the criticality condition

$$\frac{\partial}{\partial s}\left\{ \Lambda_s^{-1} Q_s^{-1} \frac{\partial}{\partial s}\left(\lambda_s \Lambda_s^2 \frac{\partial}{\partial s}\left(\Lambda_s^{-1} Q_s^{-1} \frac{\partial}{\partial s}\Sigma_s \right) \right) \right\} = 0$$

Note that both Q_s and Λ_s are symmetric, hence the conspicuous absence of their transpose. Successive integrations, with the limits determined by the boundary conditions, give

$$\Sigma_s = \int_0^s Q_c \Lambda_c \int_0^c \lambda_b^{-1} \Lambda_b^{-2} \int_b^\epsilon Q_a \Lambda_a C\, \mathrm{d}a\, \mathrm{d}b\, \mathrm{d}c$$

with C a (tensor) integration constant. By the constraint $\int_0^\epsilon Q_s \Pi_s\, \mathrm{d}s = \mathrm{id} \Rightarrow \Sigma_\epsilon = \mathrm{id}$, we determine it uniquely as $C = \left(\int_0^\epsilon Q_c \Lambda_c \int_0^\epsilon \lambda_b^{-1} \Lambda_b^{-2} \int_b^\epsilon Q_a \Lambda_a\, \mathrm{d}a\, \mathrm{d}b\, \mathrm{d}c \right)^{-1}$. Successive integrations and truncations of the tensors with respect to the integration variables a, b, c (which are all of order ϵ), gives us Σ_s and from that we can determine the profile $s \mapsto \Pi_s$. The mobility then is $M(u) = C[\Pi]^{-1}$, which after a change of variables from h to u, yields the form of the mobility in (11).

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