Research Project

Mathematical Modelling of Cell Membrane Dynamics

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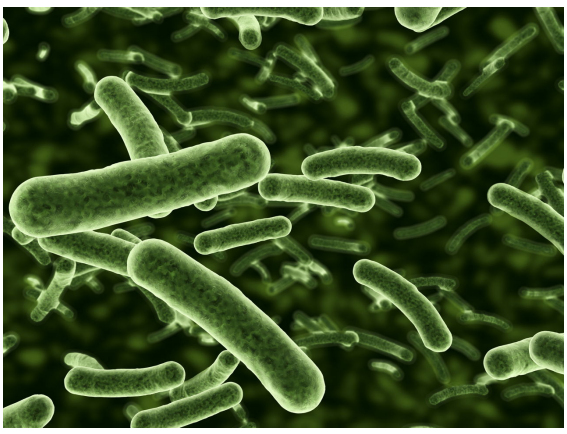

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1 Introduction

Cell membranes are the foundation of the origin of life, but also linked to the dynamics of virus al infections and genetic mutations since it controls what substances that can exit or enter the cell [1]. In fact, a good understanding of the cell membrane is important of engineering proteins to manipulate various intracellular processes in living systems [2].

One of the primary components of the cell membranes are lipids which serve many different functions. A key function is that it is consisting of a bilayer of lipids which controls the structural rigidity and the fluidity of the membrane. Thus, elastic bending forces, temperature and diffusion is essential on how a cell membrane will evolve [3, 4].

1.1 Elastic bending energy on evolving surfaces

Assuming that the system is a single-phase system, i.e., the lipids are uniformly distributed, can the elastic bending energy be modelled using the Canham-Helrich energy functional [5, 6, 3]. Let us denote b_b, b_k and H_0 as parameters based on physical models, then can the energy functional be denoted as,

$$\mathcal{E}_{CH}\left(\Gamma\left(t\right)\right) = \int_{\Gamma(t)} b_b \left(H - H_0\right)^2 + b_k K. \quad (1)$$

Here is $H = \kappa_1 + \kappa_2$ denoted as the mean curvature and $K = \kappa_1\kappa_2$ as the gaussian curvature with respectively and κ_1 and κ_2 as principal curvatures. $\Gamma\left(t\right)$ is here a evolving surface in $\mathbb{R}^3$, for more info see section 2. Using the Gauss-Bonnet theorem can it be shown that the problem above is equivalent to the so-called Willmore energy functional [7, 8],

$$\mathcal{E}_{W}\left(\Gamma\left(t\right)\right) = \int_{\Gamma(t)} \frac{1}{2} H^2. \quad (2)$$

This is a well known problem in the mathematical community [9, 10, 11, 12]. In fact, it is a mathematical tool used to study the geometry of surfaces because it can be used to study the diffeomorphism from a initial surface to a minimal energy configuration, which are surfaces with the least possible area for a given boundary. This is important in many areas of mathematics, including differential geometry, topology and mathematical physics [13, 14, 15].

It has been established many numerical methods for for shape optimization problems [16, 17], evolving surface partial differential equations (PDE) [18, 19, 20, 21, 22, 23, 24] and specific algorithms for the Willmore energy problem (2) [25, 26, 27, 28, 29].

1.2 Two-phase separation modelling on predefine evolving surfaces

It also turns out that the lipids often accumulate into so-called lipid rafts which serves as a rigid platform for proteins with special properties such as intracellular trafficking of lipids and lipid-anchored proteins [30]. Modelling of lipid rafts formation can be modelled as a two-phase separation problem based on minimization of the Ginzburg-Landau energy functional [31],

$$\mathcal{E}_{GL}\left(c\right) = \int_{\Gamma(t)} \Psi\left(c\right) + \frac{\gamma}{2}\left|\nabla c\right|^2, \quad (3)$$

which is describing the chemical energy for a concentration $c : \Gamma\left(t\right) \times [0, T] \mapsto [0, 1]$ and $\Psi\left(c\right)$ is a chemical potential function. Keep in mind that unlike the willmore energy functional (2), where the $\Gamma\left(t\right)$ is determined the elastic properties, should the energy functional (3) be interpreted as a chemical diffusion problem a predefined evolving domain $\Gamma\left(t\right)$. Usually is this problem solved by deriving equivalent variants of partial differential equations (PDE) such as Allen-Cahn equation (or Cahn-Hilliard equation if the total concentration is globally conserved) on evolving domains. See [31, 3, 32, 33, 34].

1.3 Multiphysics problems on evolving surfaces

Ultimately will the cell membrane consists of interaction several kinds of physics (temperature, elasticity, chemical diffusion, internal fluid pressure etc.) [3]. Hence, being able to model several processes may give unforeseen results. An example is to try to the energy functionals (3) and (2), since the lipid-rafts formation is said to change the elasticity properties of the membrane, may be a good model for how cell membranes evolve to specific shapes or execute cell division. One way to couple the equations (1) and (3) is to let the parameters b_b, b_k and H_0 be some function of the concentration c , i.e.,

$$\begin{aligned}\mathcal{E}_{CHGL}\left(\Gamma\left(t\right), c\right) = &\int_{\Gamma(t)} b_b\left(c\right)\left(H - H_0\left(c\right)\right)^2 \\ &+ \int_{\Gamma(t)} b_k\left(c\right) K \\ &+ \int_{\Gamma(t)} \Psi\left(c\right) + \frac{\gamma}{2}\left|\nabla c\right|^2,\end{aligned}$$

For more information, see [35]. Recently have some authors also coupled diffusion processes and the so-called mean curvature energy, see [36, 37].

Some physical processes may require constant area and volume. This can simply be added by introducing respectively area and volume functionals, see [38, Definition 2.5].

Until now have all the models assumed that the membrane has no difference in internal and external pressure. As a matter of fact, osmotic pressure can be introduced by adding a energy functional using the van't Hoff formula. Let V_p be the volume of a closed evolving surface $\Gamma(t)$, we can then model the difference of internal and external pressure as,

$$\Delta P(V_p) = P_{in} - P_{out} = iRT\left(\frac{n}{V_p} - \bar{c}\right),$$

where $i, R, T, \bar{c}$ and n are the van't Hoff index, ideal gass constant, temperature , ambient molar concentration and molar amount of the enclosed solute. Then the energy functional have the form,

$$\mathcal{E}_p(\Gamma) = \int_\Gamma \Delta P(V_p),$$

For more information, see [39].

1.4 Outline of this report

The long-term goal would be to solve the multiphysics problems above. However, many of the problems above is fairly complicated to solve numerically and requires sophisticated techniques. Hence, in this report we focus on the latest research withing the numerical methods of finding the minima of the energy functional (2). However, we will first establish notation by including a section for definitions and important results from differential geometry and shape derivatives. We will then derive the underlying dynamics system of evolutionary system dynamics using the gradient flow technique inspired by shape optimization methods based on the work done in [40]. Lastly, we will establish the numerical methods of the system dynamics by applying recent methods using a evolutionary surface finite element method (FEM) [28, 29].

2 Background Theory

2.1 Differential Calculus

This subsection is inspired by the notation used in [28, 40]. Let some initial surface $\Gamma^0 \subset \mathbb{R}^3$ smooth compact and oriented surface with no boundary where we can assign a unique point $p \in \Gamma^0$. We define define the time evolutionary surface to be on the form,

$$\begin{aligned}\Gamma = \Gamma(t) &= \Gamma(X(\cdot, t)) \\ &= \{X(p,t) : \ p \in \Gamma^0\}\end{aligned}$$

transformed via the smooth mapping,

$$X : \Gamma^0 \times [0,T] \mapsto \mathbb{R}^3.$$

An important regularity result is that if Γ^0 is of class C^∞, then Γ is also of class C^∞ for $\forall t \in [0,T]$ [16, 40].

Formally in [16, p 48], it might be an idea to formulate normal unit-vector regularity as C^∞

We will define a unique evolutionary point $x \in \Gamma(t)$ based on the smooth mapping $X(p,t) = x$. A way to imagine this is to have a initial point in Γ^0 and the mapping X describes how this point will deform over time. The outer unit normal vector field of $\Gamma(t)$ is defined as the mapping $\nu : \Gamma \mapsto \mathbb{R}^3$.

Using the notation presented in [40] and [28] can we define the basic surface differential operators. Consider a scalar function, $u : \Gamma \mapsto \mathbb{R}$, and a vector-valued function, $\hat{u} : \Gamma \mapsto \mathbb{R}^3$. We can then denote $\nabla_\Gamma u : \Gamma \mapsto \mathbb{R}^3$ as the tangential operator,

$$\nabla_\Gamma u = \nabla u - \langle \nu, \nabla u \rangle \nu.$$

May be an idea to define a extension $\widetilde{u}\ |_\Gamma$ and look into regularity. See definitions in [18].

Similarly, for the vector-valued function is the operator defined s.t.

$$\nabla_\Gamma \hat{u} = (\nabla_\Gamma u_1, \nabla_\Gamma u_2, \nabla_\Gamma u_3)^T.$$

The surface divergence for a vector-valued function is defined as

$$\nabla_\Gamma \cdot \hat{u} = \nabla \cdot \hat{u} - \nu^T D\hat{u} \cdot \nu$$

Here $D\hat{u}$ denotes the Jacobian of $\hat{u}$. Similarly, the Laplace-Beltrami operator $\Delta_\Gamma u : \Gamma \mapsto \mathbb{R}$ is proven to have the form [41, Lemma 1],

$$\begin{aligned}\Delta_\Gamma u &= \nabla_\Gamma \cdot \nabla_\Gamma u \\ &= \Delta u - \nu^T D^2 u \cdot \nu - H\partial_\nu u\end{aligned}.$$

Here is $D^2 u$ denotes as the Hessian of the scalar function u. In the case of a vector valued function is the operator defined as

$$\Delta_\Gamma \hat{u} = (\Delta_\Gamma u_1, \Delta_\Gamma u_2, \Delta_\Gamma u_3)^T$$

A method to compute the mean curvature and the so-called Frobenius norm of matrix A involves applying the extended Weingarten map, $A(x) = \nabla_\Gamma \nu(x)$, s.t. these identities holds ,

$$\begin{aligned}H &= tr(A) = k_1 + k_2, \\ |A|^2 &= k_1^2 + k_2^2,\end{aligned}.$$

see [28]. We may also want to use these definitions to introduce the following identities ,

$$\begin{aligned}\partial_\nu H &= -|A|^2, \\ \nabla_\Gamma H &= \Delta_\Gamma \nu + |A|^2 \nu.\end{aligned}$$

Again, see Lemma 3.3 and Lemma 3.2 in [40].

2.2 Evolutionary Surface Dynamics

In this section will we develop a framework evolutionary surface dynamics.

First of all, we can denote the velocity $v : \Gamma \mapsto \mathbb{R}^3$ to be

$$\frac{dx}{dt} = v(x) \quad \forall x \in \Gamma(t). \tag{4}$$

Given a model of the velocity v can we solve the ordinary differential equation (ODE) (4) and determine the evolution of a point on the surface $\Gamma(t)$. In this article will we assume that the velocity only has a normal component to the surface, i.e., it exists a scalar function $V : \Gamma \mapsto \mathbb{R}$ s.t. $v = V\nu$.

Recall that the point $x = X(p,t)$ is arising from the smooth mapping from the point p in Γ^0 to $\Gamma(t)$. Now, let some arbitrary energy functional have the form,

$$\mathcal{J}(\Gamma(t)) = \int_{\Gamma(t)} \varphi(x).$$

For instance, in the case presented in (2) we define $\varphi = H^2$.

Based on [40],the shape derivative of this energy functional at some time t in the direction of the velocity $v(x)$ from (4) is defined as

$$d\mathcal{J}(\Gamma(t); v) = \lim_{\varepsilon \to 0} \frac{\mathcal{J}(\Gamma(t+\varepsilon)) - \mathcal{J}(\Gamma(t))}{\varepsilon}.$$

For a more detailed description of the shape derivative, see [16, Definition 2.19].

Assume we have a scalar function $f : \Gamma(t) \mapsto \mathbb{R}$. Similarly, as for the shape derivative, we can now denote the material derivative at time t in the direction of the velocity $v(x)$ as

$$\begin{aligned}\frac{D}{Dt} f(x,t;v) &= \frac{d}{dt} f(X(p,t),t) \\ &= \lim_{\varepsilon \to 0} \frac{f(X(p,t+\varepsilon)) - f(X(p,t))}{\varepsilon},\end{aligned}$$

see [16, Definition 2.74].

We denote the $L^2(\Gamma)$ as the space of all functions that are square-integrable with respect to the surface measure, i.e.,

$$L^2(\Gamma) = \left\{ u : \Gamma \mapsto \mathbb{R} \mid \int_\Gamma |u|^2 < \infty \right\}$$

Let $u, v \in L^2(\Gamma)$, then can we define the norm and the inner-product

$$\begin{aligned}\|u\|^2_{L^2(\Gamma)} &= \int_\Gamma |u|^2 \\ (u,v)_{L^2(\Gamma)} &= \int_\Gamma uv\end{aligned}$$

In this paper will we also the shorthand notation $\|u\|_{L^2(\Gamma)} = \|u\|_\Gamma$ and $(u,v)_{L^2(\Gamma)} = (u,v)_\Gamma$. The Sobolev space $H^1(\Gamma)$ is defined as the space of all functions and its first weak derivative with a finite L^2-norm, i.e,

$$H^1(\Gamma) = \left\{ f : \Gamma \mapsto \mathbb{R} \mid \int_\Gamma |f|^2 + |\nabla_\Gamma f|^2 < \infty \right\},$$

with the following norm and inner product $u, v \in H^1(\Gamma)$,

$$\begin{aligned}\|u\|_{H^1(\Gamma)} &= \|u\|_\Gamma + \|\nabla_\Gamma u\|_\Gamma, \\ (u,v)_{H^1(\Gamma)} &= (u,v)_\Gamma + (\nabla_\Gamma u, \nabla_\Gamma v)_\Gamma.\end{aligned}$$

If we have a vector-valued function that $u : \Gamma \mapsto \mathbb{R}^3$ where each element is in $H^1(\Gamma)$ or $L^2(\Gamma)$, then do we denote is as a member of respectively $\left[H^1(\Gamma)\right]^3$ or $\left[L^2(\Gamma)\right]^3$.

The method we will use in this paper to minimize the energy functional (2) is to compute the so-called gradient flow. The fundamental idea of the gradient flow is to give rise of evolutionary dynamics to decrease the overall energy functional both in space and time, i.e., $\mathcal{J}(\Gamma(t_2)) < \mathcal{J}(\Gamma(t_1))$ for all $t_2 > t_1$. For more information about gradient flows, see [42, 43]. Now assume we have the velocity defined in (4) to be $v \in \left[L^2(\Gamma)\right]^3$, then we define the L^2 gradient flow s.t.

$$(v,\varphi)_\Gamma = -d\mathcal{J}(\Gamma;\varphi) \;\; \forall \varphi \in \left[L^2(\Gamma)\right]^3.$$

It turns out that if $v \neq 0$, then is this equivalent to

$$d\mathcal{J}(\Gamma; v) = -\|v\|^2_{L^2(\Gamma)} < 0.. \tag{5}$$

see [17]. Hence, we finally have a toolbox which can be used to model evolutionary dynamics for moving surfaces.

3 Evolutionary dynamics of the Willmore flow

The goal is to derive the evolutionary dynamics of the Willmore energy (2).

Recall that we define the velocity (4)to only have a normal component, i.e., $v(x) = V\nu$. The shape derivative for (2) in the direction of some velocity $v \in \left[H^1(\Gamma)\right]^3$ has the form

$$d\mathcal{E}_W(\Gamma; v) = \int_\Gamma \left(-\Delta_\Gamma H + \frac{1}{2}H^3 - H|A|^2 \right) V$$

A complete derivation of the shape derivative can be found in [40, Corally 4.7]. Consequently, by applying the gradient flow in (5) and using that $\|v\|_\Gamma = \|V\|^2_\Gamma$ can we easily see that,

$$\|V\|^2_\Gamma = \int_\Gamma V^2 = -d\mathcal{E}(\Gamma; v).$$

Hence, the gradient flow is equivalent to

$$V = \Delta_\Gamma H + Q, \tag{6}$$

where we denote the nonlinear term as $Q = -\frac{1}{2}H^3 + H|A|^2$.

Need to define a way to compute $\Delta_\Gamma H$ in the background theory.

From [28, Lemma 2.1] it derived that (6) must satisfy the following material derivatives,

$$\begin{aligned}\frac{D}{Dt}H &= -\left(\Delta_\Gamma + |A|^2\right)V,\\ \frac{D}{Dt}\nu &= \left(-\Delta_\Gamma + \left(HA - A^2\right)\right)z\\ &\quad + |\nabla_\Gamma H|^2\nu - 2\left(\nabla_\Gamma\cdot\left(A\nabla_\Gamma H\right)\right)\nu\\ &\quad - A^2\nabla_\Gamma H - \nabla_\Gamma Q.\end{aligned}$$

Here is the substitution variable introduced s.t. $z = \Delta_\Gamma\nu + |A|^2\nu$.

It exists methods which do not exploit the material derivatives [27, 44].However, it turns out that including these material derivatives brings additional computational costs, but provides so-called full-order approximation to the mean curvature, H, and the normal vector, ν, and ,thus, allows us to construct rigorous convergence proofs for evolving surface FEM, see [28, 20].

Should probably find sources with Reynolds theorem or something for why material derivatives is used.

Recent work has proposed that current method may not conserve the mesh quality while the surface is restricted to evolve along the normal velocity. Thus, a new variation of the standard methods has been considered by introducing an tangential velocity component via the equation $H = -v\cdot\nu$. Hence, also allowing the mesh to be less deformed, see more at [29]. However, in this report will we not consider it.

Finally, we end up with the following strong form of the second-order evolutionary system of PDE.

$$\frac{d}{dt}H = -\Delta_\Gamma V - |A|^2 V, \tag{7a}$$

$$V = \Delta_\Gamma H + Q, \tag{7b}$$

$$\begin{aligned}\frac{d}{dt}\nu &= \left(-\Delta_\Gamma + \left(HA - A^2\right)\right)z\\ &\quad + |\nabla_\Gamma H|^2\nu\\ &\quad - 2\left(\nabla_\Gamma\cdot\left(A\nabla_\Gamma H\right)\right)\nu\\ &\quad - A^2\nabla_\Gamma H - \nabla_\Gamma Q,\end{aligned} \tag{7c}$$

$$z = \Delta_\Gamma\nu + |A|^2\nu, \tag{7d}$$

$$\frac{d}{dt}x = v. \tag{7e}$$

where the terms are,

$$\begin{aligned}v &= V\nu,\\ Q &= -\frac{1}{2}H^3 + H|A|^2,\\ A &= \nabla_\Gamma\nu\end{aligned}$$

Recall that the material derivative operator $\frac{D}{Dt}$ is simply equivalent to the time derivative $\frac{d}{dt}$, thus, it is now possible to apply normal techniques for time discretization.

It turns out from basic numerical theory that rewriting an equivalent weak formulations (integral form) of the system dynamics (7) makes the problem suitable for numerical approximations since it involves complex shape dynamics. Hence, we will now introduce the weak formulation of the system dynamics.

Let us denote the following trial functions,

$$\begin{aligned}&(H\times V\times\nu\times z)\in\\ &\left(H^1(\Gamma), H^1(\Gamma), \left[H^1(\Gamma)\right]^3, \left[H^1(\Gamma)\right]^3\right),\end{aligned} \tag{8}$$

and similarly the test functions,

$$\begin{aligned}&(\chi^H\times\chi^V\times\chi^\nu\times\chi^z)\in\\ &\left(H^1(\Gamma), H^1(\Gamma), \left[H^1(\Gamma)\right]^3, \left[H^1(\Gamma)\right]^3\right),\end{aligned} \tag{9}$$

It has been proven that if you can find any trial functions (8) that does satisfy the following weak formulation (10) for all test functions (9), then the solution is equivalent to solving the dynamics presented in (7). See [28] for more information.

$$\begin{aligned}\left(\frac{d}{dt}H, \chi^H\right)_\Gamma &= \left(\nabla_\Gamma V, \nabla_\Gamma\chi^H\right)_\Gamma\\ &\quad - \left(|A|^2 V, \chi^H\right)_\Gamma,\end{aligned} \tag{10a}$$

$$\begin{aligned}\left(V, \chi^V\right)_\Gamma &= -\left(\nabla_\Gamma H, \nabla_\Gamma\chi^V\right)\\ &\quad + \left(Q, \chi^V\right)_\Gamma,\end{aligned} \tag{10b}$$

$$\begin{aligned}\left(\frac{d}{dt}\nu, \chi^\nu\right)_\Gamma &= \left(\nabla_\Gamma z, \nabla_\Gamma\chi^\nu\right)_\Gamma\\ &\quad + \left((HA - A^2)z, \chi^\nu\right)_\Gamma\\ &\quad + \left(|\nabla_\Gamma H|^2\nu, \chi^\nu\right)_\Gamma\\ &\quad + \left(A^2\nabla_\Gamma H, \chi^\nu\right)_\Gamma\\ &\quad + 2\left(A\nabla_\Gamma H, \nabla_\Gamma\chi^\nu\nu\right)_\Gamma\\ &\quad + \left(Q, \nabla_\Gamma\cdot\chi^\nu\right)_\Gamma\\ &\quad - \left(QH\nu, \chi^\nu\right)_\Gamma,\end{aligned} \tag{10c}$$

$$\begin{aligned}\left(z, \chi^z\right)_\Gamma &= -\left(\nabla_\Gamma\nu, \nabla_\Gamma\chi^z\right)_\Gamma\\ &\quad + \left(|A|^2\nu, \chi^z\right)\end{aligned} \tag{10d}$$

$$\frac{d}{dt}x = v. \tag{10e}$$

Note that the time dependent variables ν, H and x is initialized at $t = 0$ based on Γ^0. It is also essential to take account that this is a highly nonlinear PDE, hence, proving uniqueness is a difficult task. However, it has been proved that the willmore flow has a unique solution if the initial surface Γ^0 is close to a sphere [45]. It has also been discussed that under some shapes, does the willmore functional, in fact, develop singularities [46]. Furthermore, no literature has shown the uniqueness of the willmore flow coupled with the material derivatives, i.e., dynamics presented in (7).

4 Numerical Methods

To be able to find a numerical approximation the weak formulation (10) will we to formulate a evolving surface element method (ESFEM) for the evolutionary equation PDE's coupled with the evolving surface velocity. We will mostly use the notation and methods described in [28, 29].

4.1 Triangular mesh for Γ^0

Let initial surface $\Gamma^0 \in \mathbb{R}^3$ have the triangular mesh $\mathcal{T}_h$ constisting of triangles T. We will assume that the mesh is inform, i.e., for any T_1, T_2 $T_1 \neq T_2$ and $T_1 \cap T_2 \neq \emptyset$, then must T_1 and T_2 share either a vertex or a facet. Let diameter of each triangle h_T be denoted as,

$$\begin{aligned} h_T &= \max_{x_1,x_2 \in \Gamma^0} dist(x_1, x_2), \\ h_{min} &= \min_{T \in \mathcal{T}_h} h_T, \\ h_{max} &= \max_{T \in \mathcal{T}_h} h_T, \end{aligned}$$

where h_{min} and h_{max} is the maximum and minimum diameter of an individual triangle T in $\mathcal{T}_h$. We define the chunkiness parameter $c_T = h_T / r_T$, where r_T is the largest ball inside inscribed in T. We will then assume that the mesh is shape regular and quasi-uniform, i.e., $c_T \leq c$ and $h_{max} \leq c h_{min}$ for a constant c independent of h_T and T. For more information, see [19].

Apparently some quasi-uniform and shape regular definitions in [19], need to check this.

4.2 Finite surface element

In this section is the goal to develop discrete analogs of the definitions we introduced in subsections 2.1 and 2.2.

Let $\mathcal{T}_h$ be the triangulation of Γ^0. Now denote the vector $\mathbf{x} = \mathbf{x}(t) \in \mathbb{R}^{3N}$ as a collection of all evolving nodes, $x_j(t) \in \mathbb{R}^3$, $j \in \mathcal{I}$, by a piecewise polynomial interpolation with degree k. Here is the index of all the nodes defined as $\mathcal{I} = \{1, \ldots, N\}$, where N is the total number of nodes.

We denote the discretized surface, $\Gamma_h[\mathbf{x}(t)]$, to be the numerical approximation of the surface $\Gamma(t)$. As an initial condition do we construct the initial nodes, $x_j(0) = p_j \forall j \in \mathcal{I}$, s.t. $\Gamma_h^0 = \Gamma_h[\mathbf{x}(0)]$ interpolates the initial surface, Γ^0 in the nodal points $p_j \in \Gamma^0$, $j \in \mathcal{I}$.

An essential piece of the puzzle is the finite element basis on $\Gamma_h[\mathbf{x}]$, which is denoted to have the form,

$$\phi_j[\mathbf{x}] : \Gamma_h[\mathbf{x}] \mapsto \mathbb{R}, \quad j \in \mathcal{I}.$$

How can the basis vectors move? And how is it related to the definition of X_h later in the subsection?

In fact, the basis satisfies the identity,

$$\phi_j[\mathbf{x}](x_i) = \delta_{ij} \quad \forall i, j \in \mathcal{I}.$$

Finally, we can now define the so-called evolving finite element space of $\Gamma_h[\mathbf{x}(t)]$ as,

$$\begin{aligned} S_h[\mathbf{x}] &= S_h(\Gamma_h[\mathbf{x}]) \\ &= span\left\{ \sum_{j \in \mathcal{I}} c_j \phi_j[\mathbf{x}] \mid c_j \in \mathbb{R} \right\}. \end{aligned}$$

The discretized surface mapping, $X_h : \Gamma_h^0 \mapsto \Gamma_h[\mathbf{x}(t)]$, is denoted as

$$X_h(p_h, t) = \sum_{j \in \mathcal{I}} x_j(t) \phi[x(0)](p_h), \; p_h \in \Gamma_h^0,$$

and the problem obviously does satisfy the identities; $X_h(p_h, 0) = p_h \forall p_h \in \Gamma_h$, the evolutionary property $X_h(p_j, t) = x_j(t) \forall j \in \mathcal{I}$, and

$$\begin{aligned} \Gamma_h &= \Gamma_h(t) = \Gamma_h[\mathbf{x}(t)] \\ &= \Gamma_h[X_h(\cdot, t)] \\ &= \left\{ X_h(p_h, t) : p_h \in \Gamma_h^0 \right\}. \end{aligned}$$

TODO: Need to check if the definition of $\Gamma_h[\mathbf{x}] = \Gamma_h[X_h(\cdot, t)]$ makes sense. Also made $\Gamma_h = \Gamma_h[\mathbf{x}(t)]$ som et kunstig innslag.

For shorthand notation do we define the discretized point as $x_h = X_h(p_h, t) \in \Gamma_h$. Thus discretized velocity $v_h(x_h, t) : \Gamma_h \mapsto \mathbb{R}^3$ is defined as

$$v_h(x_h, t) = \sum_{j \in \mathcal{I}} v_j(t) \phi_j[\mathbf{x}(t)](x_h)$$

Hence, by introducing $\mathbf{v} = \mathbf{v}(t)$ as a collection of the velocity nodes, $v_j \in \mathbb{R}^3$, can we define the evolutionary dynamics of the nodal points $\mathbf{x}$ s.t. this holds,

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{v}(t).$$

Ultimately, the discrete material derivative of a function $f_h : \Gamma_h \mapsto \mathbb{R}$ is simply defined in the direction in the velocity v_h as

$$\begin{aligned} \frac{D}{Dt} f_h(x_h, t; v_h) &= \frac{d}{dt} f_h(x_h, t; v_h) \\ &= \sum_{j \in \mathcal{I}} \frac{df_j(t)}{dt} \phi_j[\mathbf{x}](x_h) \end{aligned}$$

where f_j is the nodal variables.

Is $\frac{df_j(t)}{dt}$ this consistent with with the similar definition of the velocity? I guess so since $\dot{x}_j = v_j$. Anyhow, I am also wondering if the basis functions should have time derivative as well.

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4.3 Evolving surface finite element method

Let us denote the following trial functions,

$$(H_h \times V_h \times \nu_h \times z_h) \in \left(S_h[\mathbf{x}], S_h[\mathbf{x}], S_h[\mathbf{x}]^3, S_h[\mathbf{x}]^3\right), \tag{11}$$

and similarly the test functions,

$$(\chi_h^H \times \chi_h^V \times \chi_h^\nu \times \chi_h^z) \in \left(S_h[\mathbf{x}], S_h[\mathbf{x}], S_h[\mathbf{x}]^3, S_h[\mathbf{x}]^3\right), \tag{12}$$

Define the helping functions

$$\begin{aligned} v_h &= V_h \nu_h, \\ Q_h &= -\frac{1}{2} H_h^3 + H_h |A_h|^2, \\ A_h &= \frac{1}{2}\left(\nabla_{\Gamma_h} \nu_h + (\nabla_{\Gamma_h} \nu_h)^T\right) \end{aligned}$$

For the error analysis is it the discrete velocity denoted as, $v_h = \widetilde{I}_h(V_h \nu_h)$, where the interpolation operator is defined s.t. $\widetilde{I}_h : C(\Gamma_h[\mathbf{x}] \mapsto S_h[\mathbf{x}])$, however, in this article will this not be discussed, hence, we will note use the interpolation estimate. For more information see [28, Remark 3.1].

Why is the A_h symmetric, and maybe v_h has to be interpolated. [28, p.13]

It has been proven that if you can find any trial functions (11) that does satisfy the following weak formulation (10) for all test functions (9), then the solution is equivalent to solving the dynamics presented in (7). See [28] for more information.

$$\begin{aligned} \left(\frac{d}{dt} H_h, \chi_h^H\right)_{\Gamma_h} &= \left(\nabla_{\Gamma_h} V_h, \nabla_{\Gamma_h} \chi_h^H\right)_{\Gamma_h} \\ &\quad - \left(|A_h|^2 V_h, \chi_h^H\right)_{\Gamma_h}, && \text{(13a)} \\ \left(V_h, \chi_h^V\right)_\Gamma &= -\left(\nabla_{\Gamma_h} H_h, \nabla_{\Gamma_h} \chi_h^V\right) \\ &\quad + \left(Q_h, \chi_h^V\right)_{\Gamma_h}, && \text{(13b)} \\ \left(\frac{d}{dt} \nu_h, \chi_h^\nu\right)_{\Gamma_h} &= \left(\nabla_{\Gamma_h} z_h, \nabla_{\Gamma_h} \chi_h^\nu\right)_{\Gamma_h} \\ &\quad + \left((H_h A_h - A_h^2) z_h, \chi_h^\nu\right)_{\Gamma_h} \\ &\quad + \left(|\nabla_{\Gamma_h} H_h|^2 \nu_h, \chi_h^{\nu_h}\right)_{\Gamma_h} \\ &\quad + \left(A_h^2 \nabla_{\Gamma_h} H_h, \chi_h^{\nu_h}\right)_{\Gamma_h} \\ &\quad + 2\left(A_h \nabla_{\Gamma_h} H_h, \nabla_{\Gamma_h} \chi_h^{\nu_h} \nu_h\right)_{\Gamma_h} \\ &\quad + \left(Q_h, \nabla_{\Gamma_h} \cdot \chi_h^{\nu_h}\right)_{\Gamma_h} \\ &\quad - \left(Q_h H_h \nu_h, \chi_h^{\nu_h}\right)_{\Gamma_h}, && \text{(13c)} \\ \left(z_h, \chi_h^z\right)_{\Gamma_h} &= -\left(\nabla_{\Gamma_h} \nu_h, \nabla_{\Gamma_h} \chi_h^{z_h}\right)_{\Gamma_h} \\ &\quad + \left(|A_h|^2 \nu_h, \chi_h^z\right) && \text{(13d)} \\ \frac{d}{dt} x_h &= v_h. && \text{(13e)} \end{aligned}$$

Remark that we have not yet discretized in the time-dimension, but, we will try Note that the time dependent variables ν_h, H_h and x_h is initialized at $t = 0$ based on Γ^0.

4.4 The matrix formulation

Fundamentally, solving (13) straight forward can be cumbersome.

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