New Advances in the Study of Generalized Willmore Surfaces

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Outline

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- - Part 1: Introduction; Generalized Willmore energies and surfaces in space forms
- - Part II: Willmore flow and Navier-Dirichlet BVP; Computational solutions

The Willmore energy (as originally defined) is expressed by the functional

$$W(S) = \int_S H^2 dS,$$

where H is the mean curvature of the surface. A Willmore surface in Euclidean 3-space $\mathbb{R}^3$ represents an immersion S that is locally critical for the Willmore functional.
The corresponding Euler-Lagrange equation is the (classical) Willmore equation:

$$\Delta H + 2H(H^2 - K) = 0$$

Famous Willmore conjecture

For every smooth immersed torus M in $\mathbb{R}^3$,

$$W(M) \geq 2\pi^2$$

This was proved by Fernando Codá Marques and André Arroja Neves using min-max theory of minimal surfaces in 2012.

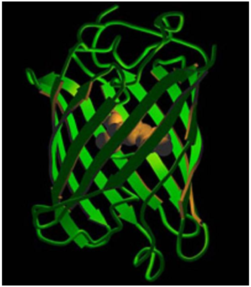
Some examples of Willmore-type surfaces and their real life models include:

- - all minimal surfaces/films/membranes in R^3
- - spheres
- - several Clifford-type tori
- - Mylar balloon models
- - Nanotubes
- - Red blood cells (discoids)
- - Certain elastic membranes; lipid bilayers (Helfrich surfaces as generalized Willmore)

Many well-established theoretical works in this field are due to:

Mladenov, I.; Pulov, V.; Hadzhilazova, M.; Djonjorov, V. at al.

Newer models of Willmore-type surfaces in molecular biology (2014-on):



http://www.aacc.org/resourcecenters/TestKnowledge/MOM/Pages/molecule2008.aspx GFP (green fluorescent protein) has a typical beta barrel structure. M. Chalfie, O. Shimomura, and R. Y. Tsien were awarded the 2008 Nobel Prize in Chemistry on 10 October 2008 for their discovery and development of the GFP.

Athukorallage, B. and Toda, M. interpreted beta-barrels as various rotational generalized Willmore surfaces with no self-intersections. The beta-barrel is a "smooth" surface shape that the centers of the beta "bead-like strands of atoms" would "lie on"... The following is the GFP beta barrel: it is a generalized Willmore that resembles a Delaunay profile with at least 2 inflection points. We proved that profiles of some beta-barrels can be catenoidal under certain conditions (depending on ratios between their diameter and height).

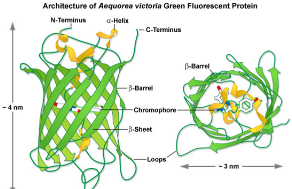


Figure 1

Generalized Willmore energy $\int(H^2 + c)dS$ motivated by Physics

The Generalized Willmore energy functional associated to a surface M immersed in $\mathbb{R}^3$ as:

$$E(M) = \int_M (kH^2 + \mu)\, dS, \tag{1}$$

- $k = 2k_c$: double of the usual bending rigidity.
- μ : superficial tension.
- dS: element of area with respect to the induced metric.

The corresponding Euler-Lagrange equation of (3) is

$$\Delta H + 2H(H^2 - K - \epsilon) = 0, \tag{2}$$

where $\epsilon = \frac{\mu}{k}$, and ΔH represents the Laplace-Beltrami operator of H, corresponding to the naturally induced metric.

Theorem 1 (Generalized Willmore energy in Mathematics)

Given an arbitrary constant k_1, the generalized Willmore functional $\widetilde{W}(M;k_1)$ for a surface immersed in $M^3(0) = \mathbb{R}^3$

$$\bar{W} = \int_M (H^2 + k_1)\, dS, \tag{3}$$

the Euler-Lagrange equation becomes

$$\Delta H + 2H(H^2 - K - k_1) = 0. \tag{4}$$

Willmore-type energies in spaceforms

Let $M^3(c)$ be a 3-dimensional space form of constant curvature c, namely,

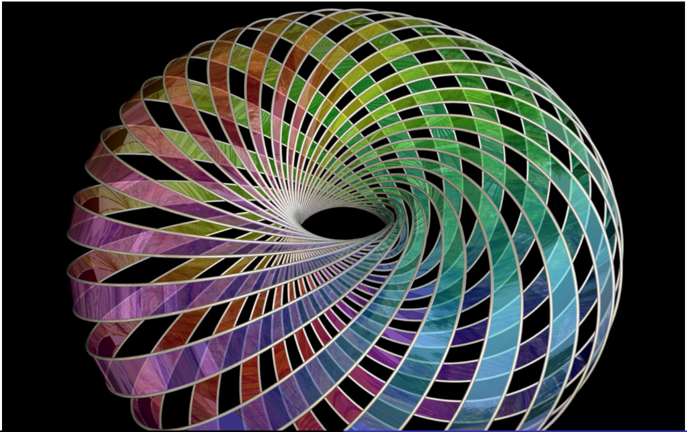
$$M^3(c) = \begin{cases} \mathbb{S}^3(c) = \left\{ x \in \mathbb{R}^4 | \langle x, x \rangle = \frac{1}{c} \right\}, & \text{if} \quad c > 0 \\ \mathbb{R}^3, & \text{if} \quad c = 0 \\ \mathbb{H}^3(c) = \left\{ x \in \mathbb{R}^4 | \langle x, x \rangle_{\mathbb{H}} = \frac{1}{c}, x^0 > 0 \right\}, & \text{if} \quad c < 0 \end{cases}$$

where $\langle \cdot, \cdot \rangle$ represents the standard inner product on $\mathbb{R}^4$, while

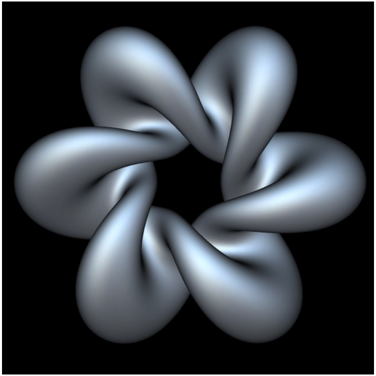
$$\langle x, y \rangle_{\mathbb{H}} = x^1 y^1 + x^2 y^2 + x^3 y^3 - x^0 y^0$$

represents the standard Lorenzian inner product on the Lorenz space $\mathbb{R}^4_1$.

Clifford Torus: - The Hsiang-Lawson conjecture states that any minimally embedded torus in S^3 with the round metric must be a Clifford torus. - Kilian, Schmidt and Schmitt proved (in 2014) that amongst the equivariant constant mean curvature tori in S^3, the Clifford torus is the only local minimum of the Willmore energy (other crit.pts.are maxima).



Other examples of Willmore surfaces in S^3: n-lobed tori in S^3 (credits due to D. Ferus and F. Pedit in 1990, graphics by N. Schmitt)



Theorem 2 Consider a given smooth immersion r of a surface M, with mean curvature H and Gauss curvature K, in the space form $M^3(k_0)$ of sectional curvature k_0. We consider two possible cases:
case 1): the surface M is closed and no boundary conditions have to be specified;
case 2): the surface M is not closed. In this case we assume that both $\mathbf{r}$ and $\frac{\partial \mathbf{r}}{\partial \mathbf{N}}$ are known smooth functions on the boundary ∂M.

Let $\mathbf{r}$ be a minimizer of the Willmore functional

$$W(M) = \int_M H^2 \, dS. \tag{5}$$

Then, the mean curvature H of $\mathbf{r}$ must satisfy the equation

$$\tilde{\Delta} H + 2H(H^2 - K + k_0) = 0 \,, \tag{6}$$

where $\tilde{\Delta}$ represents an extrinsic Laplace-Beltrami operator for the immersion in spaceform $M^3(k_0)$.

Remark: Other choices of boundary conditions can also be considered involving H and $\frac{\partial H}{\partial \mathbf{N}}$, but in this case extra boundary integrals should be included in functional (5).

Proof.

We take the first variation of the Willmore functional $\iint_M H^2 dS$ in $S^3(k_0)$, then we have

$$\delta \iint_M H^2 dS = \iint_M 2H\delta H \, dS + \iint_M H^2 \delta(dS)$$

Since $\delta(dS) = -2\phi H dS$,

$$\delta \iint_M H^2 \, dS = \iint_M 2H\delta H \, dS + \iint_M H^2(-2\phi H) \, dS$$

In order to find δH, we consider the normal variation of the immersion:

$$\bar{\mathbf{r}}(u^1, u^2, t) = \bar{\mathbf{r}}(u^1, u^2) + t\phi(u^1, u^2)\bar{\mathbf{N}},$$

- ϕ: smooth real valued function
- t: real number such that $-\epsilon < t < \epsilon$.

We define

$$\mathbf{r}_i = \frac{\partial \mathbf{r}}{\partial u^i}, \quad \mathbf{N}_i = \frac{\partial \mathbf{N}}{\partial u^i}, \quad \mathbf{r}_{ij} = \frac{\partial^2 \mathbf{r}}{\partial u^i \partial u^j}$$

$$g_{ij} = \langle \mathbf{r}_i, \mathbf{r}_j \rangle, \quad h_{ij} = -\langle \mathbf{N}_i, \mathbf{r}_j \rangle, \quad h_i^j = g^{jk} h_{ki}$$

Here, the coefficients h_i^j represent the “contracted” second fundamental form (or shape operator).

The first and second fundamental forms on M are respectively

$$I = g_{ij}du^i du^j = \langle d\mathbf{r}, d\mathbf{r}\rangle\,, \quad II = h_{ij}du^i du^j = -\langle d\mathbf{N}, d\mathbf{r}\rangle$$

Since

$$H = \frac{1}{2}\sum_{i,j}^{2} g^{ij}h_{ij}$$

$$\delta H = \delta\left(\frac{1}{2}g^{ij}h_{ij}\right) = \frac{1}{2}\delta(g^{ij})h_{ij} + \frac{1}{2}g^{ij}\delta(h_{ij}).$$

The Gauss and Weingarten equations in $S^3(k_0)$ are given by

$$\mathbf{r}_{ij} = \Gamma_{ij}^k \mathbf{r}_k + h_{ij}\mathbf{N} - g_{ij}k_0\mathbf{r}$$

and $\mathbf{N}_i = -\sum h_i^j \mathbf{r}_j$ respectively

- $r_{ij} = \frac{\partial^2 \mathbf{r}}{\partial u^i \partial u^j}$
- $h_i^j = g^{jk}h_{ki}$
- Γ_{ij}^k: classical Christoffel symbols.

we obtain

$$\begin{aligned}\delta H &= \frac{1}{2}2\phi g^{ik}h_k^j h_{ij} + \frac{1}{2}g^{ij}\left(\nabla_i\nabla_j\phi - \phi h_i^k h_{jk} + g_{ij}\phi k_0\right)\\ &= \frac{1}{2}\left(\Delta\phi + \phi h_k^i h_i^k + 2k_0\phi\right)\end{aligned}$$

Since $h_k^i h_i^k = \text{trace}(h^2) = 4H^2 - 2K + 2k_0$ we obtain

$$2\delta H = \Delta\phi + \phi(4H^2 - 2K + 4k_0)$$

Now let us consider the Green's second identity:

$$\int_M (H\Delta\phi - \phi\Delta H)\, dS = \oint_{\partial M} \left(H\frac{\partial\phi}{\partial\mathbf{N}} - \phi\frac{\partial H}{\partial\mathbf{N}}\right) d\Gamma,$$

- $\frac{\partial\phi}{\partial\mathbf{N}}$: the directional derivative in the direction of the outward normal.
- If surface M is closed: no boundary and the right-and side of the above equation is zero.
- If the surface M is not closed, we assumed that both $\mathbf{r}$ and $\frac{\partial\mathbf{r}}{\partial\mathbf{N}}$ are known smooth functions on the boundary ∂M. In this case both the test function ϕ and its normal derivative $\frac{\partial\phi}{\partial\mathbf{N}}$ vanish on the boundary, therefore also the right-hand side of equation vanishes.

Therefore, one has

$$\int_M H\Delta\phi \, dS = \int_M \phi\Delta H \, dS.$$

Combining the variations $\delta(dS)$,$2\delta H$ and using above Green's identity, the first variation of the Willmore functional is

$$\delta W = \int_M \phi(\Delta H + 2H(H^2 - K + 2k_0)) \, dS.$$

Therefore the Euler-Lagrange equation corresponding to the functional is

$$\Delta H + 2H(H^2 - K + 2k_0) = 0.$$

If instead of the *intrinsic Laplace-Beltrami operator* we use by definition the *extrinsic Laplace-Beltrami operator)*, $\tilde{\Delta}$ acting on any smooth function ψ of the given coordinates:

$$\tilde{\Delta}\psi = g^{ij}\nabla_i\nabla_j\psi + 2k_0\psi = g^{ij}(\psi_{ij} - \Gamma_{ij}^k\psi_k) + 2k_0\psi,$$

then the Willmore equation can be rewritten in the equivalent form

$$\tilde{\Delta}H + 2H(H^2 - K + k_0) = 0.$$

Theorem

Consider a surface M that is immersed in the ambient space $M^3(k_0)$. The generalized Willmore energy functional $\widetilde{W}(M;k_1)$ has the corresponding Euler-Lagrange equation

$$\tilde{\Delta}H + 2H(H^2 - K - k_1 + k_0) = 0\,, \tag{7}$$

where $\tilde{\Delta}$ is the extrinsic Laplace-Beltrami operator of the immersion in $M^3(k_0)$.

Proof.

Based on the previous two theorems, the proof is immediate. □

Generalized Willmore flow of graphs

We consider the following geometric evolution equation:

$$V = \Delta H + 2H(H^2 - K - \epsilon) \quad \text{on} \quad M(t)$$

where V is the normal velocity of the evolving surfaces $M(t)$.

Derivation of generalized Willmore flow equation of graphs

By the definition of Laplace Beltrami operator we can express it as a function of the type

$$\Delta = \frac{1}{A}\text{div}\left(\left(AI - \frac{\nabla u \otimes \nabla u}{A}\right)\nabla\right)$$

- $\nabla u \otimes \nabla u$: usual tensor product of ∇u with itself
- $A = \sqrt{1 + |\nabla u|^2} = \sqrt{1 + u_x^2 + u_y^2}$.

We may write

$$\Delta H = \nabla \cdot \left(\frac{1}{A} \left(I - \frac{\nabla u \otimes \nabla u}{A^2} \right) \nabla (AH) \right) - H \nabla \cdot \left(\frac{1}{A} \left(I - \frac{\nabla u \otimes \nabla u}{A^2} \right) \nabla A \right)$$

Since $2H = \nabla \cdot \left(\frac{\nabla u}{A} \right)$ for a graph we have

$$\frac{1}{A} \left(I - \frac{\nabla u \otimes \nabla u}{A^2} \right) \nabla A = \frac{1}{A} \left(\nabla A - \frac{\Delta u}{A} \nabla u \right) + 2H \frac{\nabla u}{A}$$

By a calculation we can obtain

$$\nabla \cdot \left(\frac{1}{A} \left(\nabla A - \frac{\Delta u}{A} \nabla u \right) \right) = -2K$$

Then we have

$$\Delta H = \nabla \cdot \left(\frac{1}{A} \left(I - \frac{\nabla u \otimes \nabla u}{A^2} \right) \nabla (AH) \right) + 2HK - \nabla \cdot \left(H^2 \frac{\nabla u}{A} \right) - 2H^3$$

Comparing the previous equation and the generalized Willmore flow equation:

$$\frac{u_t}{A} = V = \Delta H + 2H^3 - 2HK - 2H\epsilon$$

we obtain the following fourth oder PDE

$$u_t - A\Bigg(\nabla\cdot\left(\frac{1}{A}\left(I - \frac{\nabla u \otimes \nabla u}{A^2}\right)\left(\nabla(AH)\right) - \nabla\cdot\left(\frac{H^2\nabla u}{A}\right)\right. \\ \left. - \epsilon\nabla\cdot\left(\frac{\nabla u}{A}\right)\right)\Bigg) = 0$$

By considering $W = AH$ the previous fourth order PDE can be expressed as a system of second order PDE as follows:

$$\begin{aligned} u_t &= A\nabla \cdot \left(\frac{B}{A} \nabla W - \frac{W^2}{A^3} \nabla u - \epsilon \left(\frac{\nabla u}{A} \right) \right) \text{in} \quad \Omega \times (0, T) \\ W &= \frac{A}{2} \nabla \cdot \left(\frac{\nabla u}{A} \right) \end{aligned}$$

where $A = \sqrt{1 + |\nabla u|^2}$, $B = I - \frac{\nabla u \otimes \nabla u}{A^2}$ and $V = \frac{u_t}{A}$.

Weak formulation of the Steady state problem

$$\begin{aligned} \int_\Omega \left(\frac{2W}{A}\varphi_u + \frac{\nabla u}{A} \cdot \nabla \varphi_u \right) d\Omega &= 0, \forall \varphi_u \in H_0^1(\Omega) \\ \int_\Omega \left(-\frac{B}{A} \nabla W \cdot \nabla \varphi_v + \left(\frac{W^2}{A^3} + \frac{\epsilon}{A} \right) \nabla u \cdot \nabla \varphi_v \right) d\Omega &= 0, \forall \varphi_v \in H_0^1(\Omega) \end{aligned}$$

with $u(\Gamma) = 0$ and $W(\Gamma) = 0$, where Γ is the boundary of Ω.

For solving the nonlinear problem

$$\mathbf{F}(\mathbf{v}) = 0$$

we use automatic differentiation (AD) to exactly evaluate the Jacobian matrix in the Newton iteration step

$$\mathbf{J}(\mathbf{v}_n)\mathbf{w}_{n+1} = -\mathbf{F}(\mathbf{v}_n),$$
$$\mathbf{v}_{n+1} = \mathbf{v}_n + \mathbf{w}_{n+1},$$

where

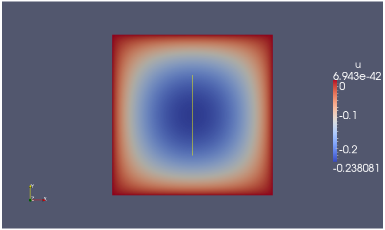
$$\mathbf{J}(\mathbf{v}_n) = \frac{\partial \mathbf{F}}{\partial \mathbf{v}}(\mathbf{v}_n).$$

AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically.

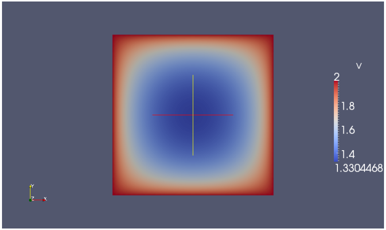
Code modification for AD

C++

```
#include ''adept.h''
adept:: Stack & s = FemusInit::_adeptStack;
vector <  adept::adouble > solu;
vector <  adept::adouble > aResu;
s.new_recording();
adept::adouble soluGauss =0;
vector < adept::adouble > soluGauss_x(dim,0.);
s.dependent(&aResu[0],nDofs);
s.independent(&solu[0],nDofs);
s.jacobian(&Jac[0]);
s.clear_independents();
s.clear_dependents();
```



: Generalized Willmore variation profile with $u(\Gamma) = 0$.



: Mean curvature with $v(\Gamma) = 2$
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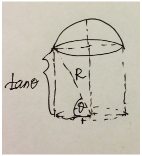
Analytical solution for spherical cap

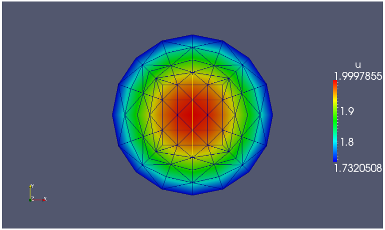
$$\begin{aligned} u(x,y) &= \sqrt{\sec^2\theta - (x^2+y^2)} \\ W(x,y) &= -\frac{1}{\sqrt{\sec^2\theta - (x^2+y^2)}} \end{aligned}$$

$u(\Gamma) = \tan\theta$ and $W(\Gamma) = -\frac{1}{\tan\theta}$
$\Gamma := \{(x,y) \in \mathbb{R}^2 : x^2+y^2 = 1\}.$

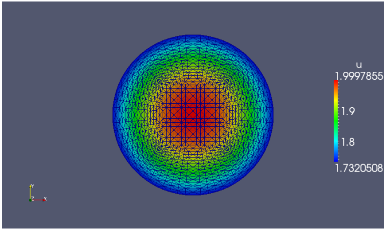


L^2 ERROR and CONVERGENCE ORDER			
level	Linear	Quadratic	Bi-quadratic
1	0.06102453786745	0.00083062986070	0.00042310259291
	1.870	3.317	3.805
2	0.01669876331327	0.00008337542370	0.00003026532805
	1.967	3.393	3.550
3	0.00427147988844	0.00000793617301	0.00000258367131
	1.992	3.418	3.246
4	0.00107407384676	0.00000074232788	0.00000027236276
	1.998	3.405	3.078
5	0.00026891145988	0.00000007006968	0.00000003225800

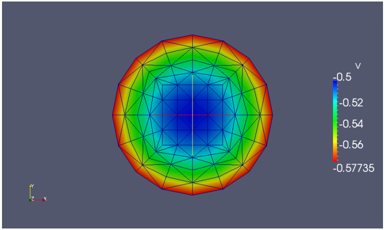
SEMINORM ERROR and CONVERGENCE ORDER			
level	Linear	Quadratic	Bi-quadratic
1	0.16877286773614	0.01228182955731	0.00338110240898
	0.880	2.207	2.275
2	0.09168463446034	0.00266020047043	0.00069867923079
	0.969	2.341	2.095
3	0.04683041645609	0.00052517415525	0.00016355640024
	0.992	2.384	2.027
4	0.02354274838120	0.00010061420639	0.00004012133746
	0.998	2.373	2.007
5	0.01178764066304	0.00001942679282	0.00000998152245



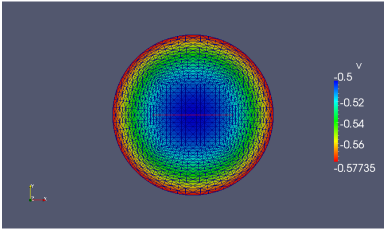
: Variation of the profile for the sphere with $u = \tan\theta$ on the boundary and $\theta = \pi/3$(Mesh level 1).



: Variation of the profile for the sphere with $u = \tan\theta$ on the boundary and $\theta = \pi/3$(Mesh level 3).



: Mean curvature $v = -1/\tan\theta$ on the boundary and $\theta = \pi/3$ (Mesh level 1)



: Mean curvature $v = -1/\tan\theta$ on the boundary and $\theta = \pi/3$ (Mesh level 3).

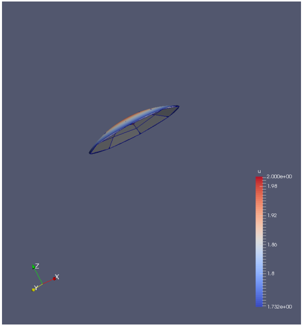
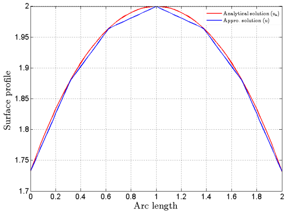
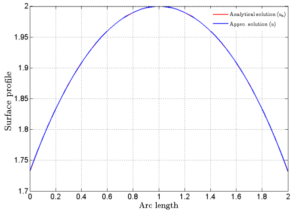


Figure: 3D plot of Analytical solutions vs Numerical solutions



: 1D plot of Analytical solution vs Numerical solution(Mesh level 0)



: 1D plot of Analytical solution vs Numerical solution(Mesh level 4)

Thank you!