ABSTRACT
Liposomes are vesicles used in several domains: medicine, biology and biochemistry. The aim of this paper is to show how Dupin cyclides (Algebraic surfaces of degree 4) can be used to get a 3D representation of liposomes, which allows easy visualization and may facilitates the simulation of the various manipulation one can need to do with liposomes.

Dupin cyclides was introduced time in 1822 by the French mathematician Pierre-Charles Dupin. Although, they have a number of interesting geometric properties that make them suitable for geometric modeling and 3D representation, their use in the nowadays modeling tools is not yet considered. The conversion of Dupin cyclides into commonly used 3 D representation surfaces, such as rational biquadratic Bézier parametric surfaces, is therefore necessary and it also is discussed in this paper. We show examples of entire or part of liposome represented as Dupin cyclides together with their Bézier conversion.

KEY WORDS
Liposome, Dupin cyclides, torus of Willmore, Rational Biquadratic Bézier Patches, 3D representation.

1 Introduction

Since A. Bangham discovered liposomes about 30 years ago, these have been used in several domains as biology, biochemistry and medicine [14]. They can play the role of drug carriers and can be charged of a large variety of molecules: small drug molecules, proteins, nucleotides and plasmids. This method permits to introduce a gene of interest in a cell. Indeed, Dr. Xiaoyang Qi at the Cincinnati children’s research foundation has developed a unique composition for modulation of highly active growing cell. The complex is formed by a fusogenic protein or peptide derived from prosaposin associated with a liposome which may also contain a drug material in a pharmaceutically acceptable carrier to improve the delivery of that material across the biological membrane.

In 1990, U. Seifert [18] proved that, besides the spheres and surfaces which are characterized only by continuous deformations, there are blisters of toric kind: the torus of Willmore (the ratio of the major radius to the minor radius is $\sqrt{2}$) and the images of this torus by an inversion i.e. cyclides of Dupin. Topological genus of these two surfaces is 1, since it is necessary to add a handle to the sphere to obtain a surface equivalent to the one of these two surfaces [13]. In 1965, Willmore conjectured that directional surfaces of kind 1 having an axis of symmetry whose energy of curvature is weakest, are the torus of Willmore [21] and its images by inversion. This result was checked in experiments. The 3D representation of liposomes needs the use of two primitives: spheres and Dupin cyclides (a torus is a particular Dupin cyclide). Moreover, some particular Dupin cyclides are double spheres. So, Dupin cyclides seem to be sufficient to represent all the possible forms of liposomes.

Except the quadrics [4] and the tori of revolution [4], surfaces available in the modelers are parametric surfaces such as NURBS, B-Splines and Bézier [5, 15, 9], but Dupin cyclides are not proposed. Dupin cyclides are algebraic surfaces introduced for the first time in 1822 by the French mathematician Pierre-Charles Dupin [8]. They have a low algebraic degree: at most 4. Liposomes can be modelled by quartic Dupin cyclides. These Dupin cy-
clides have a parametric equation and two equivalent implicit equations [10, 7] and they have been studied by a several mathematicians [6, 7, 4]. Recently, a number of authors used them in Computer Aided Geometric Design, examples of such works are: Their use for the blending of quadrics [16, 17, 2, 3]; Their representation as Rational Biquadratic Bézier Patches (RBBPs) [16, 20, 1, 12]; Their NURBS conversion [22].

This paper is organized as follows: section 2 presents the needed mathematical background (RBBP, torus of revolution, Dupin cyclides). Section 3 presents the conversion of Dupin cyclides into RBBPs using an algorithm proposed by Pratt [16]. Section 4 presents two new conversion algorithms. Section 5 presents the conclusion.

2 Background

2.1 Rational Biquadratic Bézier Patches (RBBP)

The three Bernstein polynomial of degree 2 are:

\[ B_i(t) = \binom{2}{i} t^i (1-t)^{2-i} \]  \hspace{1cm} (1)

where \( i \in [0; 2] \). A point \( M(u, v) \in [0; 1]^2 \) on a RBBP is given by:

\[ \overline{OM}(u, v) = \frac{\sum_{i=0}^{2} \sum_{j=0}^{2} B_{ij}(u, v) \overline{OP}_{ij}}{\sum_{i=0}^{2} \sum_{j=0}^{2} B_{ij}(u, v)} \] \hspace{1cm} (2)

where \( (P_{ij})_{0 \leq i, j \leq 2} \) are control points, \( (w_{ij})_{0 \leq i, j \leq 2} \) are weights and \( B_{ij}(u, v) = w_{ij} B_i(u) B_j(v) \) [16].

2.2 Torus of Willmore

Let \( O \) be the center and \( r \) the radius of a circle \( C \) in a plane \( \mathcal{P} \). Let \( \Delta \) be a straight line such as \( O \) does not belong to \( \Delta \). The torus of revolution, figure 1, is produced by rotating the circle \( C \), called meridian [4], about the axis \( \Delta \). In the plane \( \mathcal{P} \), let \( \Omega \) be the intersection between \( \Delta \) and \( \Delta' \), its perpendicular straight line passing through \( O \).

So, in \( \mathcal{P} \), \( \Delta \) and \( \Delta' \) are the axis of the reference system. Let \( R = \Omega O \), the equation of \( C \) is \( y(\theta) = (R + r \cos \theta) \) and \( z(\theta) = r \sin \theta \) and the parametric equation of the torus is:

\[ \Gamma_T(\theta, \psi) = \left( (R + r \cos \theta) \cos \psi, (R + r \cos \theta) \sin \psi, r \sin \theta \right) \] \hspace{1cm} (3)

where \( \theta \in [0; 2\pi], \psi \in [0; 2\pi] \). If \( R = r\sqrt{2} \), the torus is called Willmore torus.

2.3 Inversion

Let \( \mathcal{E} \) be the affine space, \( \Omega \) a point belonging to \( \mathcal{E} \), \( k \) a number not equal to 0. An inversion is an application \( i : \mathcal{E} - \{ \Omega \} \longrightarrow \mathcal{E} - \{ \Omega \} \) [16] defined by: \( \forall M \in \mathcal{E} - \{ \Omega \}, M' = i(M) \iff \Omega M^3 = k \), i.e. \( \Omega \overline{M} = k\overline{\Omega M} \) \hspace{1cm} (4)

2.4 Quartic Dupin cyclides

So, in \( \mathcal{P} \), \( \Delta \) and \( \Delta' \) are the axis of the reference system. Let \( R = \Omega O \), the equation of \( C \) is \( y(\theta) = (R + r \cos \theta) \) and \( z(\theta) = r \sin \theta \) and the parametric equation of the torus is:

\[ \Gamma_T(\theta, \psi) = \left( (R + r \cos \theta) \cos \psi, (R + r \cos \theta) \sin \psi, r \sin \theta \right) \] \hspace{1cm} (3)

where \( \theta \in [0; 2\pi], \psi \in [0; 2\pi] \). If \( R = r\sqrt{2} \), the torus is called Willmore torus.

2.3 Inversion

Let \( \mathcal{E} \) be the affine space, \( \Omega \) a point belonging to \( \mathcal{E} \), \( k \) a number not equal to 0. An inversion is an application \( i : \mathcal{E} - \{ \Omega \} \longrightarrow \mathcal{E} - \{ \Omega \} \) [16] defined by: \( \forall M \in \mathcal{E} - \{ \Omega \}, M' = i(M) \iff \Omega M^3 = k \), i.e. \( \Omega \overline{M} = k\overline{\Omega M} \) \hspace{1cm} (4)

2.4 Quartic Dupin cyclides

Figure 2: Three kinds of Dupin cyclides. Left: ring, \( 0 < |c| \leq |\mu| \leq |a| \). Middle: horned, \( 0 < |\mu| \leq |c| < |a| \). Right: half spindle, \( 0 \leq |c| \leq |a| < |\mu| \).

It is possible to define Dupin cyclides in various equivalent ways: Liouville showed that a Dupin cyclide is the image of a cone of revolution or a torus of revolution or a cylinder of revolution under an inversion; A Dupin cyclide is the envelope of spheres centered on a given conic and orthogonal to a given fixed sphere, called sphere of
inversion: the latter is centered on the focal axis of the Dupin cyclide [6, 7]; A Dupin cyclide is the envelope surface of a set of spheres, the centers $M$ of which lies on a given conic with focus $F$, and the radius of which is such that the distance $FM + R$ is a given constant (this definition is due to Maxwell); A Dupin cyclide is the envelope surface of the spheres tangent to three given fixed spheres [8].

Two equivalent implicit equations of a Dupin cyclide were obtained using two principal circles of the Dupin cyclide [16, 11].

A Dupin cyclide has a parametric equation:

$$\Gamma_d(\theta, \psi) = \left( \begin{array}{c} \mu (c - a \cos \theta \cos \psi) + b^2 \cos \theta \\ a - c \cos \theta \cos \psi \\ b \sin \theta \times (a - \mu \cos \psi) \\ a - c \cos \theta \cos \psi \\ b \sin \psi \times (c \cos \theta - \mu) \\ a - c \cos \theta \cos \psi \end{array} \right)$$

(5)

where $\theta \in [0; 2\pi]$, $\psi \in [0; 2\pi]$.

### 3 Conversion of Dupin cyclides into RBBP

In this section, the parameters $a$, $c$ and $\mu$ of the Dupin cyclide and the bounds $\theta_0$, $\theta_1$, $\psi_0$ and $\psi_1$ of the part of the Dupin cyclide to convert are given.

Curves plotted on a RBBP with one variable $u$ or $v$ constant are conics. The lines of curvature of Dupin cyclides are particular conics: circles. So, it is possible to convert a part (region) of a Dupin cyclide into a RBBP. This part is defined by four lines of curvature: $\gamma_{\theta_0}: \psi \mapsto \Gamma_d(\theta_0, \psi)$, $\gamma_{\theta_1}: \psi \mapsto \Gamma_d(\theta_1, \psi)$, $\gamma_{\psi_0}: \theta \mapsto \Gamma_d(\theta, \psi_0)$, $\gamma_{\psi_1}: \theta \mapsto \Gamma_d(\theta, \psi_1)$. To this end, we have to compute nine control points $(P_{ij})_{0 \leq i, j \leq 2}$ and the nine weights $(w_{ij})_{0 \leq i, j \leq 2}$.

Several conversion algorithms have been presented: K. Ueda uses matrix and resolve systems of linear equations [20]. G. Albrecht converts a piece of a cone of revolution into RBBP. The image of this RBBP is an RBBP representing a piece of symmetric horned Dupin cyclide ($\mu = 0$ and $c \neq 0$). The kind of the Dupin cyclide can be modified by taking a $\varepsilon$-offset of Dupin cyclide [1]. Some examples of results can be found on site: [http://www.univ-valenciennes.fr/macacompacs/dupin.htm](http://www.univ-valenciennes.fr/macacompacs/dupin.htm). We have developed an algorithm that uses barycentric properties of Dupin cyclides and the Bézier representations of circular arcs [12]. In this paper, we consider in more details the conversion algorithm presented by M. Pratt in [16]. We show and discuss some results of this algorithm with possible improvements.

In this algorithm, the coordinates of control points and weights are calculated directly from the parametric equation of the Dupin cyclide, equation (5), and from the

---

**Figure 3**: Left: Three medical images of Liposomes. Right: Liposomes modelled with Willmore torus and Dupin cyclide.
Moreover, if \( \theta_0, \theta_1, \psi_0 \) and \( \psi_1 \). In fact, M. Pratt writes circular functions as rational fractions (\( \cos \theta = \frac{1 - \tan^2 \left( \frac{\theta}{2} \right)}{1 + \tan^2 \left( \frac{\theta}{2} \right)} \) and \( \sin \theta = \frac{2 \tan \left( \frac{\theta}{2} \right)}{1 + \tan^2 \left( \frac{\theta}{2} \right)} \)) in using trigonometric relations:

\[
\begin{align*}
\cos(\theta) &= \frac{1 - \tan^2 \left( \frac{\theta}{2} \right)}{1 + \tan^2 \left( \frac{\theta}{2} \right)}, \\
\sin(\theta) &= \frac{2 \tan \left( \frac{\theta}{2} \right)}{1 + \tan^2 \left( \frac{\theta}{2} \right)}.
\end{align*}
\] (6)

where \( \theta \in \mathbb{R} - \pi \mathbb{Z} \). To determine the nine control points \( (P_i)_{0 \leq i \leq 2} \) and the nine weights \( (w_{ij})_{0 \leq i, j \leq 2} \), he defines the numbers:

\[
\begin{align*}
g_0 &= \tan \frac{\theta_0}{2}, \\
h_0 &= \tan \frac{\psi_0}{2}, \\
g_1 &= \frac{g_0 + g_2}{2}, \\
h_1 &= \frac{h_0 + h_2}{2}, \\
g_2 &= \tan \frac{\theta_1}{2}, \\
h_2 &= \tan \frac{\psi_1}{2}, \\
G_0 &= \tan^2 \frac{\theta_0}{2}, \\
G_1 &= g_0 \times g_1, \\
G_2 &= \tan^2 \frac{\theta_1}{2}, \\
H_0 &= \tan^2 \frac{\psi_0}{2}, \\
H_1 &= h_0 \times h_1, \\
H_2 &= \tan^2 \frac{\psi_1}{2}.
\end{align*}
\] (7)

Immediately, we note that \( \pi \) is a forbidden value. For \( (i, j) \in [0, 2]^2 \), let be \( \hat{P}_{ij} = \left\{ \begin{array}{ll}
\psi_0^2 & (1 - G_i) (1 + H_j) - c (1 - G_i) (1 - H_j) \\
2b & c (1 - G_i) (1 + H_j) - \mu h_j \\
2 & a \end{array} \right. \)

and the weight \( w_{ij} \) is given by:

\[
w_{ij} = a \left( 1 + G_i \right) \left( 1 + H_j \right) - c \left( 1 - G_i \right) \left( 1 - H_j \right).
\] (8)

The trigonometric values of angles \( \theta_0, \theta_1, \psi_0 \) and \( \psi_1 \) are used to determine the elements of the equation (7), which are thereafter introduced into the formula (8) to obtain the coordinates of control points, and into formula (9) to obtain weights. In case one \( \theta_0 = \frac{2 \pi}{3} \) and \( \theta_1 = \frac{4 \pi}{3} \), the discontinuity of the function \( x \to \tan \left( \frac{x}{2} \right) \) in \( \pi \) modulo \( 2\pi \) makes that weights and control points will be calculated as if \( \theta_0 = -\frac{2 \pi}{3} \) and \( \theta_1 = \frac{2 \pi}{3} \), which makes it impossible to obtain the correct conversion [12].

One way to deal with the above mentioned drawback is to take the absolute value in the weights computation formula as follows (for \( (i, j) \in [0; 2]^2 \)):

\[
w_{ij} = |a \left( 1 + G_i \right) \left( 1 + H_j \right) - c \left( 1 - G_i \right) \left( 1 - H_j \right)|.
\] (9)

Moreover, if \( \theta_0 = 0 \) and \( \theta_1 = 4 \frac{\pi}{3} \), control points are computed as if \( \theta_0 = -\frac{2 \pi}{3} \) and \( \theta_1 = 0 \), which does not allow to obtain the right conversion. So, the conditions are:

\[
|\theta_0 - \theta_1| < \pi \quad \text{and} \quad |\psi_0 - \psi_1| < \pi
\] (10)

The non-observance of the constraint \( |\theta_0 - \theta_1| < \pi \) is showed by figure 4. On the left picture, one can see the patch of Dupin cyclide. On the right picture, one can see the Dupin cyclide patch and its wrong corresponding RBBP. In fact, the RBBP is the complementary of the Dupin cyclide patch (for the values \( \theta \)). However, it is now possible to take values \( \theta_0, \theta_1, \psi_0 \) and \( \psi_1 \) such as \( \pi \in [\theta_0; \theta_1] \) and/or \( \pi \in [\psi_0; \psi_1] \). Indeed, a piece of liposome, figure 3, is converted into RBBP, figure 5.

The bounds of the piece are: \( \theta_0 = 0, \theta_1 = \frac{\pi}{3}, \psi_0 = \frac{\pi}{2} \) and \( \psi_1 = \frac{4 \pi}{3} \). Left picture shows the Dupin cyclide and the piece to convert. Pratt’s algorithm produces a wrong RBBP, middle picture, whereas the new algorithm gives a correct conversion, right picture. So, it is now possible to convert some new liposomes pieces.

For each variable \( \theta \) and \( \psi \), conditions of formula (11) imply that at least three values are necessary. So, to represent a complete Dupin cyclide, at least nine RBBPs are necessary. Figure 6 shows two examples of conversion.

Of course, the problem with \( \pi \) remains. So, it is not possible to use this algorithm to convert some Dupin cyclides carrying out a blending between a plane and a cylinder of revolution. For this reason, we have to present the
4 Re-parametrisation and affine transformation

Until now, the parameters $a$, $c$ and $\mu$ of Dupin cyclides have always been positive. In this section, parameters $\mu$ and $c$ can be negative. Theorem 1 gives the affine transformation to apply when we modify the sign of $c$ and/or $\mu$. The conversion algorithm proposed here is based on the Pratt’s algorithm discussed in the previous section. Using the new method, the conversion can be done in three steps: re-parametrization of the Dupin cyclide; use for Pratt’s algorithm; choice of the appropriate affine transformation.

**Theorem 1:**

Let $S$ be a Dupin cyclide with positive parameters $a$, $c$ and $\mu$. Let $S_c$ (resp. $S_\mu$) be the Dupin cyclide obtained by replacing $c$ with $-c$ (resp. $\mu$ with $-\mu$). In the same way, $S_{c,\mu}$ is the Dupin cyclide with parameters $a$, $-c$ and $-\mu$.

Let $\theta_+ (\Gamma_d)$ (resp. $\psi_+ (\Gamma_d)$) be the surface obtained by the re-parametrization $\theta \mapsto \theta + \pi$ (resp. $\psi \mapsto \psi + \pi$).

Let $\theta_- (\Gamma_d)$ (resp. $\psi_- (\Gamma_d)$) be the surface obtained by the re-parametrization $\theta \mapsto \pi - \theta$ (resp. $\psi \mapsto \pi - \psi$).

Let $r_z$ (resp. $r_y$) be the rotation by $\pi$ around the axis $(O, \overrightarrow{0z})$ (resp. $(O, \overrightarrow{0y})$). Let $s_y$ (resp. $s_z$) be the reflexion compared with the plane $(O, \overrightarrow{0y}, \overrightarrow{00})$ (resp. $(O, \overrightarrow{0z}, \overrightarrow{00})$). Then:

1. $S = r_z (\theta_+ (S_c))$ and $S = s_z (\theta_- (S_c))$.
2. $S = s_y (\psi_+ (\theta_- (S_{c,\mu})))$ and $S = r_y (\psi_- (\theta_+ (S_{c,\mu})))$.
3. $S = \psi_+ (S_{c,\mu})$ and $S = s_z (\psi_- (S_{c,\mu}))$.

Two conversions of a part of liposome (figure 3), into RBBP, which were impossible until now, are shown on figures 7 through 9. First, figure 7, the Pratt’s algorithm is applied using item 1. The bounds of the liposome piece are: $\theta_0 = \frac{2\pi}{7}$, $\theta_1 = \pi$, $\psi_0 = \frac{-2\pi}{7}$ and $\psi_1 = -\frac{\pi}{7}$.

Second, figure 8, the Pratt’s algorithm is applied using item 3. The bounds of the part of liposome are $\theta_0 = -\frac{\pi}{7}$, $\theta_1 = 0$, $\psi_0 = -\pi$ and $\psi_1 = -\frac{\pi}{7}$.

Moreover, it is possible to convert a complete liposome using a combination of algorithms, figure 9. The bounds of the part of liposome are $\theta_0 = \frac{2\pi}{7}$, $\theta_1 = \frac{7\pi}{10}$, $\psi_0 = \frac{3\pi}{10}$ and $\psi_1 = \frac{5\pi}{10}$. $S_1$ is obtained by using Pratt’s algorithm. $S_2$ (resp. $S_3$, $S_4$) is obtained by using the second improvement, item 2 (resp. item 3, item 1).
5 Conclusion

To make 3D representations of liposomes with classical modelers, we have studied the use of Dupin cyclides, some examples of these representations are shown. The conversion of Dupin cyclides into RBBPs simplifies the use of the proposed representations in common geometric modeling tools, we have discussed two conversion algorithms and given two illustrating conversion results.

References


