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The membrane inclusions curvature equations

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Abstract

We examine a system of equations arising in biophysics whose solutions are believed to represent the stable positions of N conical proteins embedded in a cell membrane. Symmetry considerations motivate two equivalent refomulations of the system which allow the complete classification of solutions for small $N < 13$. The occurrence of regular geometric patterns in these solutions suggests considering a simpler system, which leads to the detection of solutions for larger N up to 280. We use the most recent techniques of Gröbner bases computation for solving polynomial systems of equations.

1. Introduction

Both the shapes and positions of proteins which are embedded in a cell membrane can influence their biological function. It is the interaction between the proteins which dictates how they become arranged, but little is known about this interaction and its exact cause is uncertain. However, for conical proteins, a likely explanation is the bending of the membrane caused by the proteins. Specifically, an embedded conical protein induces a curvature in the two-dimensional membrane which influences the positions of neighboring proteins. There is an energy associated to this curvature and the proteins will tend to arrange themselves so as to minimize this energy. Recent work in [KJG98] shows that any minimum energy arrangement is a zero energy arrangement. Furthermore, if z_i is the

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position of the ith protein using complex coordinates, it was also shown that the energy at the ith protein is a constant multiple of $|f_i(z_1,\dots,z_N)|^2$ where

$$f_i(z_1,\dots,z_N)=\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{1}{(z_i-z_j)^2}.$$

Therefore the N proteins are at equilibrium if and only if $(z_1,\dots,z_N)$ is a solution to the Membrane Inclusions Curvature Equations, or MICE:

$$f_i(z_1,\dots,z_N)=0,\quad i=1,\dots,N. \tag{1}$$

For brevity, we refer to the Nth system of equations as M_N.

One possible application of knowing how these proteins arrange themselves is to deduce the form of proteins by examining the shapes they form. In this case, if they arrange themselves according to our solutions it is very likely that they are conical. Determining the shapes of proteins is still an unsolved problem in biology.

Gröbner bases are used to find the solutions of M_N for several N. In Section 2, we review the most efficient algorithms for computing Gröbner bases and their implementations. Direct application of these algorithms gives all the solutions of the problem for $N<7$ and is described in Section 3. Because the difficulty of computing Gröbner bases increases rapidly with respect to the complexity of the input equations, it is necessary to reformulate the system before most of the computations will successfully terminate. Two reformulations of M_N into equivalent systems are given in Section 4. The first reformulation employs an algorithm for converting the numerators of the M_N equations into symmetric polynomials, which are then expressed in terms of the elementary symmetric functions prior to computing. The second reformulation uses a differential equation describing the minimum polynomial for the coordinates of a solution and gives directly a system already formulated using the elementary symmetric functions. Both reformulations can be used jointly to decrease the computation time. Finally, we consider a much simplified system obtained from M_N by limiting our search to those solutions which have a certain geometric regularity to them; namely, we look for solutions whose coordinates form concentric rings of regular polygons. While this last approach does not detect all solutions for a given N, it does allow many to be found.

Our main result is a complete classification of the solutions for small values for N:

Theorem 1.1. *There are no solutions for $N\leqslant 12$ except for $N=5$ (finite number of solutions) and $N=8$ (M_8 form a 1-dimensional variety).*

The proof of this theorem is included in Sections 3 and 4. For larger values of N we have only a partial result:

Theorem 1.2. *There exist solutions to M_N for $N=5,8,16,21,33,37,40,56,65,85,119,$ $133,161,175,208,225,261,$ and 280. Moreover the number of solutions for M_{16} and M_{21} is infinite.*

We explain in Section 5 how we find this list of “regular solutions.”

2. Tools for solving polynomial equations

We now review some major algorithms for solving multivariate polynomial systems. The reader is also referred to [Dav93,Bec93,CLO92,CLO98] for a more detailed introduction.

Let $\mathbb{Q}[x_1, \ldots, x_n]$ be the polynomial ring with rational coefficients, F a finite list of polynomials and I the ideal generated by F.

The main tools we use are Gröbner bases [Buc65,Buc70,Buc79,Buc85]. We recall that, in general, when the number of equations equals the number of variables the shape of the Gröbner basis G for a lexicographical ordering is the following:

$$\begin{cases} h_n(x_n), \\ x_{n-1} = h_{n-1}(x_n), \\ \vdots \\ x_1 = h_1(x_n), \end{cases}$$

where all the h_i are univariate polynomials. Of course the shape of a lexicographical Gröbner basis is not always so simple but it will always be the case in this paper (except one very easy nonzero-dimensional system). From this Gröbner basis it is rather easy to compute numerically all the complex roots: we first solve numerically the first equation [DG99], and we find $z_1, \ldots, z_N$ a guaranteed approximation of all the complex roots of h_n. Then we substitute these values into the other coordinates.

Even if all the algorithms for computing Gröbner bases do not depend on a specific order it is well known [Fau93] that it is more efficient to compute first a Gröbner basis for a Degree Reverse Lexicographical (DRL) ordering and then change the ordering with a specific algorithm. In this paper we have used a standard implementation of the Buchberger algorithm and the FGLM algorithm in Singular [Gre99] for easy cases. When the degree of the univariate polynomial is big (> 500), we have used:

- the F_4 [Fau99] algorithm for computing a DRL Gröbner basis;
- the F_2 [Fau94] algorithm to change the ordering. For the bigger computations we found that the dimension of $\mathbb{Q}[x_1, \ldots, x_n]/I$ is bigger than 10^6!

These two algorithms are implemented in an experimental software called FGb [Fau]. For generating the input equations we have used the Maple [Cha91] computer algebra system.

3. First experiments

First, we observe that the set of solutions to M_N is invariant under translation and multiplication by complex scalars. These considerations allow us to change coordinates so that $z_1 = 0$ and $z_2 = 1$.

Since the f_i in the system M_N are rational functions we need to transform the system into a polynomial system. In order to avoid “parasite" solutions, where $z_i = z_j$ for some

$i \neq j$, we introduce a new variable u and let P_i be the numerator of each f_i in M_N. That is to say

$$P_i(z_1, \dots, z_N) = \sum_{j \neq i} \prod_{\substack{k \neq i \\ k \neq j}} (z_i - z_k)^2 = 0, \quad i = 1, \dots, N,$$

$$M'_N = \begin{cases} u \prod_{i=1}^{N} \prod_{j=i+1}^{N} (z_i - z_j) = 1, \\ P_i(z_1, \dots, z_N) = 0, \quad i = 1, \dots, N, \\ z_1 = 0, \\ z_2 = 1. \end{cases} \tag{2}$$

Proposition 3.1. *There is no solution for $N \leqslant 4$ and $N = 6$. The only solution for M_5 is a regular pentagon.*

Proof. For $N \leqslant 5$ it takes less than 0.1 second to compute a lexicographic Gröbner basis with FGb on a PC Pentium II 300 Mhz. For $N < 5$ the Gröbner basis is $\{1\}$. For $N = 5$ we can factorize the univariate polynomial and find a decomposition into irreducible varieties: $V = V_1 \cup V_2 \cup V_3 \cup V_4 \cup V_5 \cup V_6$ and

$$I(V_1) = \left[z_3 - z_5^3 + z_5^2 - z_5, z_4 + z_5^2 - z_5, z_5^4 - z_5^3 + z_5^2 - z_5 + 1\right].$$

For any polynomial p in $x_1, \dots, x_N$ and any permutation σ, set $\sigma.p = p(x_{\sigma(1)}, \dots, x_{\sigma(N)})$ and $\sigma.I(V) = \{\sigma.p\colon \forall p \in I(V)\}$. It is easy to check that

$$(z_4, z_5).I(V_1) = I(V_6), \qquad (z_3, z_5).I(V_1) = I(V_3), \qquad (z_3, z_4).I(V_1) = I(V_2),$$
$$(z_3, z_4, z_5).I(V_1) = I(V_5), \qquad (z_3, z_5, z_4).I(V_1) = I(V_4).$$

Now we have

$$z_5^4 - z_5^3 + z_5^2 - z_5 + 1 = \frac{z_5^5 + 1}{z_5 + 1},$$

so that $z_5 = \mathrm{e}^{\alpha\imath\pi/5}$ and we see that the only solution is the regular pentagon.

The case $N = 6$ is a little more difficult: the degree of the polynomial

$$u \prod_{i=1}^{N} \prod_{j=i+1}^{N} (z_i - z_j) = 1$$

is $1 + N(N-1)/2 = 16$ and so big that it does not help the Gröbner basis computation. In that case we can replace this condition by $u z_3 z_4 z_5 z_6 = 1$ and it takes only 13.6 seconds to find $\{1\}$ with Fgb. $\square$

In conclusion, the straightforward approach solves the problem for small N but leads to several problems:

- intermediate computations contain the same solution several times (because solutions are invariant under permutations of the variables $z_3, \dots, z_N$),

so the degrees of the intermediate varieties are big;

- it is not easy to remove the parasite solutions $z_i = z_j$.

We have stopped the computation for $N = 7$ after 2000 seconds.

4. Using the symmetry

It is clear from (1) that if $(z_1, \dots, z_N) \in \mathbb{C}^N$ is a solution of M_N then $(z_{i_1}, \dots, z_{i_N})$ is also a solution of M_N for every possible permutation of $(i_1, \dots, i_N)$ of $(1, \dots, n)$. Hence it is enough to compute the polynomial

$$f(X) = (X - z_1) \cdots (X - z_N) = X^N - e_1 X^{N-1} + \cdots (-1)^N e_N,$$

where the $e_i = e_i(z_1, \dots, z_N)$ are the elementary symmetric functions in $z_1, \dots, z_N$. In this paper we will say that f is a solution to M_N.

In general solving efficiently a polynomial system with symmetries is an open issue especially when the group acting is a proper subgroup of the symmetric group. In our problem the solutions are invariant under the symmetric group but unfortunately f_i is not a symmetric polynomial in $(z_1, \dots, z_n)$ but only in $\{z_j\colon\ j \neq i\}$. If we exchange the role of z_j and z_k then f_i remain unchanged while f_j becomes f_k and reciprocally

$$z_j \leftrightarrow z_k \quad f_i = f_i \text{ for } i \neq j, k \quad f_j \leftrightarrow f_k.$$

4.1. nilCoxeter algebra

Let e_r be the rth elementary symmetric function in N variables. For $\lambda = (\lambda_1, \dots, \lambda_r)$ let

$$m_\lambda = \sum z_{i_1}^{\lambda_1} \cdots z_{i_r}^{\lambda_r} \tag{3}$$

denote the monomial symmetric functions, where the sum ranges over all monomials whose exponent vector is equal to a permutation of λ. Solving M_N is equivalent to finding a polynomial

$$\begin{cases} f = X^N - e_1 X^{N-1} + e_2 X^{N-2} - \cdots + (-1)^N e_N, \\ f \quad \text{is squarefree,} \end{cases} \tag{4}$$

whose roots are a solution to M_N. For any polynomial p in $z_1, \dots, z_N$, set

$$\partial_i(p) = \frac{p(z_1, z_2, \dots, z_N) - p(z_i, z_2, \dots, z_{i-1}, z_1, z_{i+1}, \dots, z_N)}{z_1 - z_i}. \tag{5}$$

Let I_1 be the ideal generated by $P_1, \dots, P_N$. We define by induction

$$I_k = I_{k-1} : \left(\prod_{i_1 < i_2} (z_{i_1} - z_{i_2}) \right) \tag{6}$$

and $I = I_\infty$. Note that $P_i = (1, i).P_1$ for $1 \leqslant i \leqslant N$ and P_1 is symmetric in $z_2, \dots, z_N$.

Theorem 4.1. *Define for* $1 \leqslant i_1 < \cdots < i_{k+1} \leqslant N$

$$P_{i_1,\dots,i_k,i_{k+1}} = \frac{P_{i_1,\dots,i_k} - P_{i_1,\dots,i_{k-1},i_{k+1}}}{z_{i_k} - z_{i_{k+1}}},$$

so that $P_{i_1,\dots,i_k} \in I_k$ *and* $P_{i_1,\dots,i_k}$ *is symmetric in* $z_{i_1}, \dots, z_{i_k}$ *and in the complementary set of variables. Hence*

$$H_k = \sum_{1 \leqslant i_1 < \cdots < i_k \leqslant N} P_{i_1,\dots,i_k}$$

is a true symmetric function.

The next theorem gives an efficient method for computing the H_k.

Theorem 4.2. *For* $1 \leqslant i_1 < \cdots < i_k \leqslant N$

$$P_{i_1,\dots,i_k} = (1, i_1).(2, i_2).\cdots.(k, i_k) Q_k,$$

where $Q_k = P_{1,2,\dots,k}$ *and we have*

$$Q_k = \partial_k Q_{k-1}.$$

The H_i were first computed in the monomial basis m_λ using code specifically written for this application in C++ in the small computer algebra system Gb; then the polynomials were expressed in the e_i basis using ACE [AS98], SF [J.98], and Symmetrica [Sym]. If we set $z_N = 0$ and $z_{N-1} = 1$ prior to computing the H_i, the reformulated system $\widetilde{S}_N$ consists of the polynomials $H_1, \dots, H_N, P_{N-1}, P_N$ in the variables $e_1, \dots, e_{N-2}$. It turns out that $\widetilde{S}_N$ is easier to solve: it takes 2 minutes to compute a Gröbner basis for $N = 10$ with FGb, while the calculation for M_7 was unsuccessfully stopped after 2000 seconds.

4.2. Harm Derksen's formulation

Our second reformulation was found by Harm Derksen [Der99], and appeals to the structure of the polynomial f in (5). First, a lemma.

Lemma 4.3. *For any* $(z_1, \dots, z_N) \in \mathbb{C}^N$,

$$\sum_{j=1}^{N} \frac{1}{z_j^2} = \frac{e_{N-1}^2 - 2e_N e_{N-2}}{e_N^2}.$$

Proof. Since $\sum_{j=1}^{N}(1/z_j) = e_{N-1}/e_N$ and $\sum_{i>j}(1/z_i z_j) = e_{N-2}/e_N$, we have

$$\sum_{j=1}^{N} \frac{1}{z_j^2} = \left(\sum_{j=1}^{N} \frac{1}{z_j}\right)^2 - 2\sum_{i>j} \frac{1}{z_i z_j} = \frac{e_{N-1}^2}{e_N^2} - 2\frac{e_{N-2}}{e_N}. \qquad \square$$

Theorem 4.4. $(z_1, \dots, z_N)$ *is a solution to* M_N *if and only if*

$$\begin{cases} f & \textit{is squarefree, and} \\ 3(f'')^2 - 4f'f''' & \textit{is divisible by } f, \end{cases}$$

where $f = \prod_{i=1}^{N}(x - z_i) = x^N - e_1 x^{N-1} + e_2 x^{N-2} - \cdots + (-1)^N e_N$.

Proof. Let S_r be the rth elementary symmetric polynomial in $x - z_1, \dots, x - z_N$. Note that replacing x by z_i in S_r gives the rth elementary symmetric polynomial in $z_i - z_1, \dots, z_i - z_{i-1}, z_i - z_{i+1}, \dots, z_i - z_N$, which we denote by E_r^i. Furthermore, the kth derivative of f is $f^{(k)} = k!S_{N-k}$ so that $f^{(k)}(z_i) = k!E_{N-k}^i$. Set $h := 3(f'')^2 - 4f'f'''$. Then

$$h(z_i) = 3\big(2E_{N-2}^i\big)^2 - 4E_{N-1}^i\big(3!E_{N-3}^i\big) = 12\big(\big(E_{N-2}^i\big)^2 - 2E_{N-1}^i E_{N-3}^i\big). \tag{7}$$

By Lemma 4.3

$$f_i = \sum_{j \neq i} \frac{1}{(z_i - z_j)^2} = \frac{(E_{N-2}^i)^2 - 2E_{N-1}^i E_{N-3}^i}{(E_{N-1}^i)^2}, \tag{8}$$

so that $h(z_i)$ is a constant multiple of the numerator of f_i. Therefore f divides h and the z_i are distinct $\Leftrightarrow$ $h(z_i) = 0$ for all i and the z_i are distinct $\Leftrightarrow$ $f_i(z_1, \dots, z_N) = 0$ for all i $\Leftrightarrow$ $(z_1, \dots, z_N)$ is a solution of M_N. $\square$

Let r be the remainder of dividing h by f, and let c_j, $1 \leqslant j \leqslant \deg(r)$, be the coefficient of x^j in r. Then each c_j is a polynomial in the e_i and Theorem 4.4 implies the system $c_j(e_1, \dots, e_N) = 0$, $1 \leqslant j \leqslant \deg(r)$, is equivalent to M_N.

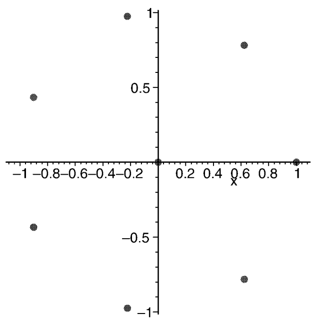
Computations with Singular [Gre99] using the formulation of Theorem 4.4 reveal a one-dimensional family of solution shapes for $N = 8$:

Proposition 4.5. *The coordinates of a solution to M_8 are given by the roots of the polynomial*

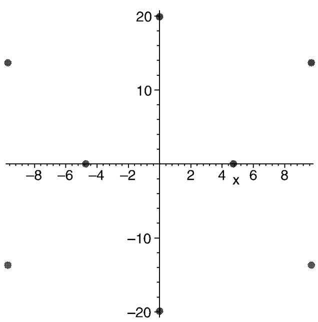
$$t^8 + \frac{28}{5}t^6 a + 14t^4 a^2 + 28t^2 a^3 - t - 7a^4,$$

where a is arbitrary. Setting $a = 0$, the roots form a regular heptagon with a point in the center. Varying a deforms this into irregular hexagons with two points in the interior.

Solutions $N = 8,\ a = 0$



Solutions $N = 8,\ a = 100$



This is a one-dimensional family of solution shapes.

Proposition 4.6. *There are no solutions to M_N for $N = 3, 4, 6, 7, 9, 10, 11$, and* 12.

Proof. For $N = 3, 4$, short (less than one minute by Maple on a Sun Ultra-5) Gröbner bases computations show that M'_N, hence M_N, has no solutions. For the remaining N, computations using one or both of the above reformulations show that there are no solutions of the equivalent systems. For $N > 7$ we use FGb for the computations. When $N > 9$ another difficulty arises in the computation: it is impossible to compute the discriminant of $g = x^{N-2} - e_1 x^{N-3} + e_2 x^{N-4} - \cdots + (-1)^N e_{N-2}$. At the beginning we add only the condition $g(0) = e_{N-2} \neq 0$ and $g(1) \neq 0$ and we compute a lexicographical Gröbner basis. Finally we remove the bad solutions. □

5. Regular solutions

The geometry of the solutions known thus far lead one to ask: What other regular polygons are solution shapes (with or without a point in the center)? What about two regular polygons, or n regular polygons? We use the notation $[n, m, p]$ to denote a solution shape consisting of n regular concentric m-gons and $p = 1$ or 0 as there is or is not a point in the center. Thus a solution $[n, m, p]$ will be a solution for M_{nm+p}. We begin this section by trying to find "by hand" some regular solutions and then give a more systematic way to find these solutions.

5.1. One regular m-gon: $[1, m, p]$

Since the solutions are invariant under translation and multiplication by complex numbers, it suffices to examine the mth roots of unity.

The main lemma we need is

Lemma 5.1. *Let ω be a primitive mth root of unity. Then*

$$\sum_{j=1}^{m} \frac{1}{(\omega^j)^2} = 0, \qquad \sum_{j=1}^{m-1} \frac{1}{(\omega^j - 1)^2} = -\frac{(m-1)(m-5)}{12},$$
$$\sum_{j=1}^{m} \frac{1}{(\frac{a}{b}\omega^j - 1)^2} = \frac{mb^m(b^m + a^m(m-1))}{(b^m - a^m)^2}. \tag{9}$$

Proof. From Lemma 4.3 we know

$$\sum_{j=1}^{N} \frac{1}{z_j^2} = \frac{e_{N-1}^2 - 2e_N e_{N-2}}{e_N^2},$$

where the e_i are the elementary symmetric polynomials in the z_j. The polynomials with roots ω^j $(1 \leqslant j \leqslant m)$, $\omega^j - 1$ $(1 \leqslant j \leqslant m-1)$, and $\frac{a}{b}\omega^j - 1$ $(1 \leqslant j \leqslant m)$ are

$$P(X) = X^m - 1,$$
$$P(X) = \frac{(X+1)^m - 1}{X} = X^{m-1} + mX^{m-2} + \cdots + \binom{m}{3}X^2 + \binom{m}{2}X + m,$$
$$P(X) = (X+1)^m - \left(\frac{a}{b}\right)^m, \tag{10}$$

respectively. Substituting in the corresponding values of e_N, e_{N-1}, and e_{N-2} gives the result. □

We first consider the case $p = 0$: $[1, m, 0]$, i.e., $N = m$. Let $z_i = \omega^i$ for all i, where ω is a primitive mth root of unity. Then the ith equation is

$$f_i = \sum_{j \neq i} \frac{1}{(z_i - z_j)^2} = \sum_{j \neq i} \frac{1}{(\omega^i - \omega^j)^2} = \frac{1}{(\omega^i)^2} \sum_{j \neq i} \frac{1}{(\omega^{j-i} - 1)^2} = \frac{1}{(\omega^i)^2} \sum_{j=1}^{m-1} \frac{1}{(\omega^j - 1)^2}.$$

By Lemma 5.1, for all i the ith equation is zero if and only if

$$\sum_{j=1}^{m-1} \frac{1}{(\omega^j - 1)^2} = -\frac{(m-1)(m-5)}{12} = 0,$$

i.e., if and only if $m = 5$ or $m = 1$. Thus the regular pentagon is the only solution shape for this case.

If $p = 1$ we are looking at polygons of the shape $[1, m, 1]$ with $N = m + 1$ and then we have $z_i = \omega^i$ for $i = 1, \dots, m$ and $z_{m+1} = 0$. Then the $(m+1)$st equation

$$f_{m+1} = \sum_{j=1}^{m} \frac{1}{(\omega^j - 0)^2} = 0$$

by Lemma 5.1. For $i = 1, \dots, m$, the ith equation is

$$\begin{aligned} f_i &= \sum_{j \neq i} \frac{1}{(z_i - z_j)^2} = \sum_{j \neq i} \frac{1}{(\omega^i - \omega^j)^2} + \frac{1}{(\omega^i)^2} = \frac{1}{(\omega^i)^2}\left(\sum_{j \neq i} \frac{1}{(\omega^{j-i} - 1)^2} + 1\right) \\ &= \frac{1}{(\omega^i)^2}\left(\sum_{j=1}^{m-1} \frac{1}{(\omega^j - 1)^2} + 1\right). \end{aligned} \tag{11}$$

So for all $i = 1, \dots, m$ the ith equation is zero if and only if

$$\sum_{j=1}^{m-1} \frac{1}{(\omega^j - 1)^2} = -\frac{(m-1)(m-5)}{12} = -1,$$

i.e., $m = 7$ or $m = -1$. Therefore the regular heptagon with a point in the center is the only solution shape in this case.

5.2. Two regular m-gons $[2, m, x]$

Again we may fix one m-gon, P_1, to be the mth roots of unity. We introduce a new complex variable, x, to describe the second m-gon, $P_2 = xP_1$, where multiplication of a polygon P with x means x times each vertex of the polygon.

Proposition 5.2. *There are no solution shapes of the form* $[2, m, 0]$ *or* $[2, m, 1]$.

Proof. We include in square brackets facts for the case $[2, m, 1]$. Let

$$z_i = \begin{cases} \omega^i & \text{if } i = 1, \dots, m, \\ x\omega^i & \text{if } i = m+1, \dots, 2m, \\ [0 & \text{if } i = 2m+1]. \end{cases} \tag{12}$$

Dividing by $(1/\omega^i)^2$ in the ith equation when $i = 1, \ldots, m$, or $(1/(x\omega^i))^2$ when $i = m+1, \ldots, 2m$, we get two equations in one unknown:

$$-\frac{(m-1)(m-5)}{12}[+1] + \frac{m(1+x^m(m-1))}{(1-x^m)^2} = 0, \tag{13}$$

$$-\frac{(m-1)(m-5)}{12}[+1] + \frac{mx^m(x^m+m-1)}{(x^m-1)^2} = 0, \tag{14}$$

where we have used the third part of Lemma 5.1. Subtracting one equation from the other gives

$$1 - x^{2m} = 0, \tag{15}$$

so the solution set would have to consist of $2m$th roots of unities. But we have already seen that in the single polygon case the only solutions are $m = 5$ and $m = 7$, neither of which is divisible by two. Therefore no shapes of the form $[2, m, 0]$ or $[2, m, 1]$ can be a solution. $\square$

5.3. The generalization

Using the differential equation of Theorem 4.4 we can find some more conditions not only for the case of regular polygons but for any set of roots to a polynomial $N(X)$. For the case of regular polygons this raises the chances of successful computations since we can add the new equations to our old systems.

Definition 5.3. Let N, M, P be univariate polynomials of degree n, m, p. We use the notation $[N, M, P]$ to denote the set of solutions of M_{nm+p} with the shape $P(X)N(M(X))$. In the particular case $P(X) = X^p$, $M(X) = X^m$ we use the simplified notation $[N, m, p]$.

Theorem 5.4. *Let $N(x) = \sum_{i=0}^{n} a_i X^i$ be a square free polynomial of degree n such that $a_0 \neq 0$. Then $[N, m, p]$ (with $m > 1$) is a solution of M_{nm+p} if and only if $p \leqslant 1$ and $N(X)$ divides*

$$\sum_{\substack{i=1\\j=1}}^{n} ija_ia_j(mi-1)(3mj+5-4mi)X^{i+j} \quad \text{if } p = 0$$

and $N(X)$ divides

$$\sum_{\substack{i=0\\j=1}}^{n} a_ia_j jm(jm+1)(im+1)(3im-4jm+4)X^{i+j} \quad \text{if } p = 1.$$

Proof. Let $f(X) = X^p N(X^m)$. We know from Theorem 4.4 that f is a solution of M_{nm+p} if and only if f is square free and $U(X) = 3(f'')^2 - 4f'f'''$ is divisible by $f(X)$. The first condition is true as soon as $p \leqslant 1$ since 0 is not a root of $N(X)$.

Considering the case $p = 0$, we find:

$$\begin{aligned} U(X) = 3&\left(\sum_{i=1}^{n} im(mi-1)a_i X^{mi-2}\right)^2 \\ &- 4\left(\sum_{i=1}^{n} ima_i X^{mi-1}\right)\left(\sum_{i=i_3}^{n} im(mi-1)(mi-2)a_i X^{im-3}\right), \end{aligned}$$

where $i_3 = 2$ if $m = 2$ and $i_3 = 1$ else. Since X and $f(X)$ are relative prime, f divides U iff f divides $X^4 U = V$ with

$$\begin{aligned} V(X) = 3&\left(\sum_{i=1}^{n} im(mi-1)a_i X^{mi}\right)^2 \\ &- 4\left(\sum_{i=1}^{n} ima_i X^{mi}\right)\left(\sum_{i=i_3}^{n} im(mi-1)(mi-2)a_i X^{im}\right), \end{aligned}$$

hence $V = W(X^m)$ is divisible by $N(X^m)$ iff $W(X)$ is divisible by $N(X)$. We can rewrite the sum:

$$W(X) = m^2 \sum_{\substack{i=1 \\ j=1}}^{n} ija_i a_j (mi-1)(3mj+5-4mi)X^{i+j}.$$

We consider now the case $p = 1$ and find:

$$\begin{aligned} U(X) = 3&\left(\sum_{i=1}^{n} a_i(im+1)(im)X^{im-1}\right)^2 \\ &- 4\left(\sum_{i=0}^{n} a_i(im+1)X^{im}\right)\left(\sum_{i=1}^{n} a_i(im+1)(im)(im-1)X^{im-2}\right) \end{aligned}$$

must be divisible by X and $N(X^m)$, so that $m > 2$ and $V_1(X) = X^2 U(X)$ should be divisible by $N(X^m)$.

$$V_1(X) = 3\left(\sum_{i=1}^{n} a_i(im+1)(im)X^{im}\right)^2$$

$$-4\left(\sum_{i=0}^{n} a_i(im+1)X^{im}\right)\left(\sum_{i=1}^{n} a_i(im+1)(im)(im-1)X^{im}\right).$$

This equivalent to divisibility of

$$\begin{aligned}W_1(X) = 3&\left(\sum_{i=1}^{n} a_i(im+1)(im)X^i\right)^2\\ &-4\left(\sum_{i=0}^{n} a_i(im+1)X^i\right)\left(\sum_{i=1}^{n} a_i(im+1)(im)(im-1)X^i\right)\\ &= \sum_{\substack{i=0\\ j=1}}^{n} a_i a_j jm(jm+1)(im+1)(3im-4jm+4)X^{i+j}. \qquad \square\end{aligned}$$

Remark 5.5. We can always suppose that $N(X) = X^n + X^{n-1} + \sum_{i=0}^{n-2} a_i X^i$.

Remark 5.6. In the following we give an explicit value to n and p and we consider m as a variable.

Corollary 5.7. *There are no solutions of the form* $[N, 2, 1]$.

Proof. From the proof of Theorem 5.4, $f(X) = XN(X)$ does not divide $U(X)$ because X does not divide $U(X)$. $\square$

Corollary 5.8. *For* $\deg(N) = 1$, $[N, m, 0]$ *is a solution iff* $(m-1)(m-5) = 0$ *and* $N(X) = 1 + X$.

Proof. We apply Theorem 5.4 to $N = 1 + X$ and we find $W(X) = -X^2(m-1)(m-5)$. $\square$

Corollary 5.9. *For* $\deg(N) = 1$, $[N, m, 1]$ *is a solution iff* $m = 7$ *and* $N(X) = 1 + X$.

Proof. We apply Theorem 5.4 to $N = 1 + X$ and we find

$$W_1(X) = X\left(-4 + 4m^2\right) + X^2\left(m^3 - 2m^2 - 7m - 4\right)$$

and the remainder of W_1 divided by N should be zero:

$$-m(-7+m)(m+1)x. \qquad \square$$

Corollary 5.10. $\deg(N) = 2$, $[N, m, 0]$ *there is no solution.*

Proof. We apply Theorem 5.4 to $N = a_0 + X + X^2$ and we find

$$W(X) = -\bigl(4(2m-1)(2m-5)X^2 + 4(m-1)(4m-5)X + (m-1)(m-5)\bigr)X^2$$

and the remainder of W divided by N should be zero:

$$-\bigl(-5 - m^2 + 18m - 60a_0m + 16a_0m^2 + 20a_0\bigr)X \\ - \bigl(-m^2 + 18m - 5 + 16a_0m^2 - 48a_0m + 20a_0\bigr)a_0 = 0.$$

We can compute a lexicographical Gröbner of the coefficients:

$$\bigl[20a_0 - m^2 + 18m - 5, m\bigl(m^2 - 18m + 5\bigr)\bigr]$$

and the number of solutions is 0.

5.4. Summary of the regular solutions

An extended version of this paper including a complete list of solutions, pictures and all the polynomials can be found at http://calfor.lip6.fr/~jcf/MICE/mice.ps.gz. We summarize all the results:

Theorem 5.11. *For fixed values of n and p we give all the possible values of m and for each m all the solutions $[n, m, p]$. The results are summarized in Table 1.*

Table 1

Shape	Values of m	Values of N
$[1, m, 0]$	$m = 5$	$N = 5$
$[1, m, 1]$	$m = 7$	$N = 8$
$[2, m, 0]$	$\emptyset$	
$[2, m, 1]$	$\emptyset$	
$[3, m, 0]$	$m = 7$, $m = 11$	$N = 21$, $N = 33$
$[3, m, 1]$	$m = 5$, $m = 13$	$N = 16$, $N = 40$
$[4, m, 0]$	$m = 2$, $m = 4$	$N = 8$, $N = 16$
$[4, m, 1]$	$m = 5$	$N = 21$
$[5, m, 0]$	$m = 13$, $m = 17$	$N = 65$, $N = 85$
$[5, m, 1]$	$m = 11$, $m = 19$	$N = 56$, $N = 96$
$[6, m, 0]$	$\emptyset$	
$[6, m, 1]$	$\emptyset$	
$[7, m, 0]$	$m = 19$, $m = 23$	$N = 133$, $N = 161$
$[7, m, 1]$	$m = 17$, $m = 25$	$N = 119$, $N = 175$
$[8, m, 0]$	$m = 5$, $m = 7$	$N = 40$, $N = 56$
$[8, m, 1]$	$m = 4$, $m = 8$	$N = 33$, $N = 65$
$[9, m, 0]$	$m = 25$, $m = 29$	$N = 225$, $N = 261$
$[9, m, 1]$	$m = 23$, $m = 31$	$N = 208$, $N = 280$

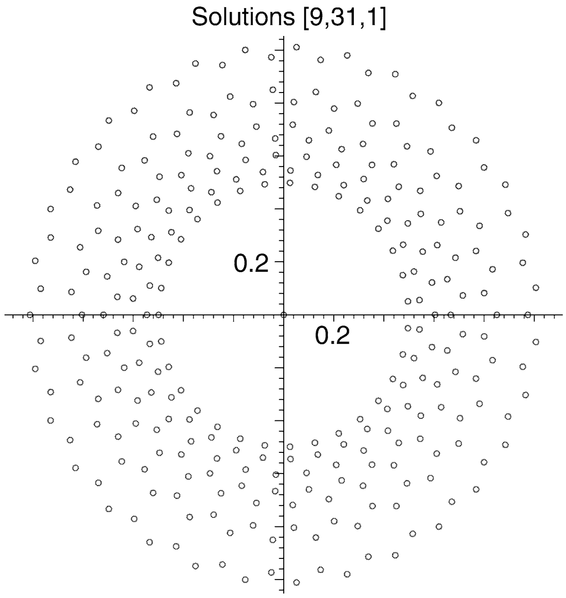


Fig. 1. One regular solution for $N = 280$.

Corollary 5.12. *Using this information we could find the following solution families*:

$$f(x) = -32\lambda x^5 + \lambda + x^{16} + x^{11} + \frac{11}{8}x^6 - \frac{11}{128}x,$$
$$f(x) = -\lambda x + 25\lambda x^8 + x^{21} + x^{14} - \frac{13}{10}x^7 + \frac{13}{400},$$

for $N = 16$ *and* $N = 21$.

Conjecture 5.13. *For n odd, there will be solutions for* $[n, m, 0]$ *with* $m = 3n - 2$ *and* $m = 3n + 2$ *and for* $[n, m, 1]$ *with* $m = 3n - 4$, $m = 3n + 4$. □

6. Conclusion

We have a new application of computer algebra in biological physics. We were able to solve the system completely up to $N = 12$ using the symmetry and the most recent techniques for the Gröbner bases computation. Starting with solution shapes of regular polygons we found solution families for $N = 8, 16, 21$ as well as single solutions for N up to 280 for which we have reason to assume that they are part of solution families as well.

From the biophysical point of view, solutions for N about 1000 are needed since there are thousands of proteins in a cell membrane [Kim99]. But even small numbers of proteins can give some interesting insights. We have extended the results in the original paper [KJG98] from $N = 5$ to 12.

This work is a particular instance of the more general problem of finding a global minimum of an energy function and in particular we want to point out similar work related to the classification of the stable solutions of the n body problem.

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