# Determining Flexibility of Molecules Using Resultants of Polynomial Systems

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We solve systems of multivariate polynomial equations in order to understand flexibility of three dimensional objects, including molecules.

Protein flexibility is a major research topic in computational chemistry. In general, a polypeptide backbone can be modeled as a polygonal line whose edges and angles are fixed while some of the dihedral angles can vary freely. It is well known that a segment of backbone with fixed ends will be (generically) flexible if it includes more than six free torsions. Resultant methods have been applied successfuly to this problem, see [3], [4].

In this work we focus on non-generically flexible structures (like a geodesic dome) that are rigid but become continuously movable under certain relations. The subject has a long history: Cauchy (1812), Bricard (1896), Connelly (1978).

In our previous work [8], we began a new approach to understanding flexibility, using not numeric but symbolic computation. We describe the geometry of the object with a set of multivariate polynomial equations, which we solve with resultants. Resultants were pioneered by Bezout, Sylvester, Dixon, and others. The resultant appears as a factor of the determinant of a matrix containing multivariate polynomials. Given the resultant, we described [8] an algorithm *Solve* that examines it and determines relations for the structure to be flexible. We discovered in this way the conditions of flexibility for an arrangement of quadrilaterals in Bricard [1], which models

molecules. Here we significantly extend the algorithm and the molecular structures.

### 0.1 First new result

We have now analyzed Bricard's original formulation of the quadrilaterals problem [1] in terms of three quadratic equations, with fifteen parameters and three variables. The resultant of this system has 5685 terms. The flexibility searching algorithm is more subtle now, and we have modified algorithm *Solve* to include these cases, with great success. We have discovered an apparently new flexible arrangement, which can be viewed at [10]. Although the physically meaningful flexible conformations of the cyclohexane are well known ("chair" versus "boat"), this appears to be the first fully algebraic approach for their derivation, as well as for deriving Bricard's flexible octahedra. Moreover, the identical set of equations arises in other contexts, and a variant gives the conformational equations of a protein or nucleic acid backbone [3] [4].

### 0.2 Second new result

Next we consider the cylo-octane molecule, pictured in figure 1.

Chemically relevant solutions fix the (bond) angles between the paler lines, introducing four constraint equations in the variables $\tau_i$. To save space, we show one equation here; the other three are similar.

$$-t\beta^4\,{\tau_4}^2\,{\tau_1}^2-4\,t\alpha_1\,t\beta^3\,{\tau_4}^2\,{\tau_1}^2+6\,t\beta^2\,{\tau_4}^2\,{\tau_1}^2+4\,t\alpha_1\,t\beta\,{\tau_4}^2\,{\tau_1}^2-{\tau_4}^2\,{\tau_1}^2-t\beta^4\,{\tau_1}^2+4\,t\alpha_1{}^2\,t\beta^2\,{\tau_1}^2+2\,t\beta^2\,{\tau_1}^2-{\tau_1}^2-8\,t\alpha_1{}^2\,t\beta^2\,\tau_4\,\tau_1-8\,t\beta^2\,\tau_4\,\tau_1-t\beta^4\,{\tau_4}^2+4\,t\alpha_1{}^2\,t\beta^2\,{\tau_4}^2+2\,t\beta^2\,{\tau_4}^2-{\tau_4}^2-t\beta^4+4\,t\alpha_1\,t\beta^3+6\,t\beta^2-4\,t\alpha_1\,t\beta-1=0$$

Here $\tau_i = \tan(z_i/2)$, $t\beta = \tan(\beta/2)$, and $t\alpha_i = \tan(\alpha_i/2)$.

We use the Dixon resultant to eliminate $\tau_2, \tau_3$, and $\tau_4$. An important **special case** is when the basic quadrilateral (heavy black lines) is planar.

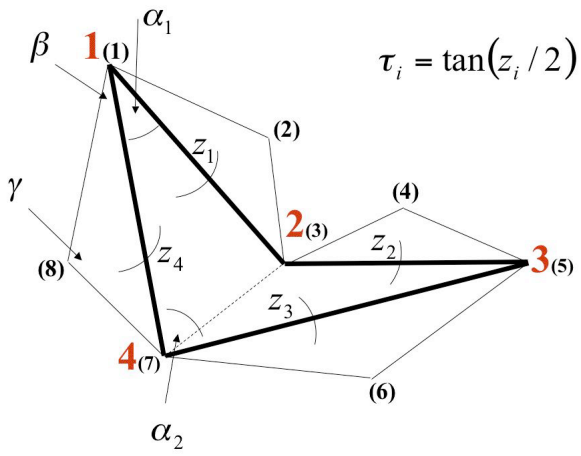


**Fig. 1.** Geometry of Octane Molecule.

The equations then simplify quite a bit, and we can describe all the solutions of this case. The Dixon matrix is $24 \times 24$. 57% of the entries are 0. On average there are 41 terms per entry. The Dixon-EDF method [9] takes 3 minutes 38 seconds to compute the resultant for $\tau_1$, which has 21715 terms. It is degree 32 in $\tau_1$ but has only even degree terms.

In the **general case** (three dimensional space) we have also made significant progress. The Dixon matrix is $64 \times 64$. 64% of the entries are 0. On average there are 107 terms per entry. The determinant of the Dixon matrix here, were it ever computed, would have many billions of terms. But our Dixon-EDF techniques [9] discover its hundreds of factors in about 67 hours of CPU time. The largest has 4872161 terms. Using some of these factors, we have verified some known chemical arrangements. We seem to have found new interesting flexible cases. Work is ongoing.

## References

1. Bricard, Raoul, Mémoire sur la théorie de l'octaèdre articulé, J. Math. Pures Appl. 3 (1897), p. 113 - 150
(English translation: http://www.math.unm.edu/∼vageli/papers/bricard.pdf).

2. Cauchy, A. L. Sur les polygones et les polyhedres. Second Memoire. Journal de l'École Polytechn. **9** (1813), pp. 8.
3. Coutsias, E. A., C. Seok, M. P. Jacobson and K. A. Dill A Kinematic View of Loop Closure, J. Comput. Chem., 25 (2004), no. (4), p. 510 - 528.
4. Coutsias, E. A., C. Seok, M. J. Wester and K. A. Dill, Resultants and loop closure, Int. J. Quantum Chem. 106 (2005), no. (1), p. 176 - 189.
5. Cromwell, P. R. *Polyhedra*. New York: Cambridge Univ. Press, 1997. p. 222 - 224.
6. Cox, D., J. Little, D. O'Shea. Using Algebraic Geometry. Graduate Texts in Mathematics, 185. Springer-Verlag. New York, 1998.
7. Dixon, A. L. The eliminant of three quantics in two independent variables. Proc. London Math. Soc., **6** (1908) p. 468 - 478.
8. Lewis, R. H. and E. A. Coutsias, Algorithmic Search for Flexibility Using Resultants of Polynomial Systems; in Automated Deduction in Geometry, 6th International Workshop, ADG 2006. Springer-Verlag. LNCS **4869** p. 68 - 79 (2007).
9. Lewis, R. H., Heuristics to accelerate the Dixon resultant. Mathematics and Computers in Simulation **77**, Issue 4, p. 400-407, April 2008.
10. Lewis, R. H., Flexible structures movie, http://home.bway.net/lewis/flex2.MOV. December 2008.
11. Thorpe, M., M. Lei, A. J. Rader, D. J. Jacobs, L. Kuhn. Protein flexibility and dynamics using constraint theory. J. Molecular Graphics and Modelling **19** (2001) p. 60 - 69.