Flexibility of Molecules via Computer Algebra

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This is joint work with
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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. A polypeptide backbone can be modeled as a polygonal line whose edges and angles are fixed while dihedral angles can vary. Resultant methods have been applied successfuly to this problem to determine flexibility [3], [4].

In this work we focus on non-generically flexible structures (like a geodesic dome) that are usually rigid but can become flexible (continuously movable) under certain relations. We compute the resultant of a polynomial system, then analyze it to determine the conditions for flexibility.

0.1 Background

The subject has a long history: Cauchy (1812), Bricard (1896), Connelly (1978) [2], [1].

In our previous work [5], [9], [10], 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. Given the resultant, we described [5] 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.

0.2 Previous Result

We 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 *Solve* was successful in 2008 [9], [10]. We discovered an apparently new flexible arrangement, which can be viewed at [6]. This was the first fully algebraic approach, and applies as well 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].

0.3 New Result One

Next we considered 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 τ_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 used the Dixon resultant to eliminate τ_2, τ_3, and τ_4. An important **special case** is when the basic quadrilateral (heavy black lines) is planar. The equations then simplify quite a bit, and we can described all the solutions of this case.

In the **general case** (three dimensional space) we have also made significant progress. Our Dixon-EDF techniques [7] discover hundreds of factors

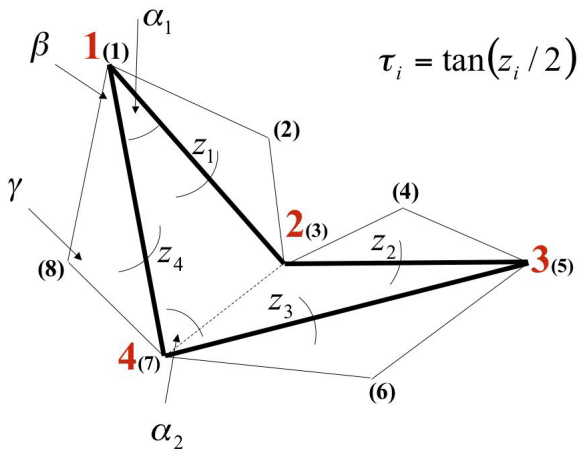

Fig. 1. Geometry of Octane Molecule.

of the resultant in about 30 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.

0.4 New Result Two

We have returned to the Bricard quadrilaterals. As mentioned above, they are equivalent to Bricard's flexbible octahedra [1]. In that paper he described three essentially different ways the octahedra can be flexible.

Our previous work found many relations among the sides yielding flexibility. However, apparently all of them were examples of two of Bricard's three cases. We have now modified the *Solve* algorithm to find examples of the third case. This is a significant modification, as *Solve* can now work hierarchically. In other words, the set of equations can be broken down into stages, as in function composition. This is very promising for analyzing more complex structures.

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