Algorithmic Search for Flexibility using Resultants of Polynomial Systems

Robert H. Lewis
Fordham University
http://www.bway.net/~lewis/
rlewis@fordham.edu

Abstract

This talk describes the recent convergence of four topics: polynomial systems, flexibility of three dimensional objects, computational chemistry, and computer algebra.

We discuss a way to solve systems of polynomial equations with *resultants* by refining the Dixon method [KSY], [BEM] with new techniques.

Using ideas of Bricard [B] and Coutsias [C1], [C2], we find a system of six polynomial equations in six variables and eleven parameters that models a configuration of quadralaterals that is equivalent to some three dimensional structures. These structures are of interest in computational chemistry, as they represent molecules. We then describe and demonstrate an algorithm that examines the resultant and determines ways that the structure can be *flexible.* We review some ideas about flexibility, from Cauchy [Ca] to Bricard [B] to Connelly [Co].

Crucial in this work has been Lewis's computer algebra system "Fermat" [Lew] written especially for polynomial and matrix computations. Somewhat simliar problems were solved before in [LB] and [LS].

References:

[B] Bricard, Raoul, Memoire sur la theorie de loctaedre articule, J. Math. Pures Appl. **3** (1897), 113-150
(English translation: http://www.math.unm.edu/vageli/papers/bricard.pdf).

[BEM] L. Buse, M. Elkadi, and B. Mourrain, Generalized resultants over unirational algebraic varieties. J. Symbolic Comp. **29** (2000), p. 515-526.

[Ca] A. L. Cauchy, Sur les polygones et les polyhedres. Second Memoire. J. Acole Polytechn. **9** (1813), pp. 8.

[Co] R. Connelly, A counterexample to the rigidity conjecture for polyhedra. Publ. Math. I. H. E. S. **47** (1978), 333 - 338.

[C1] E. A. Coutsias, C. Seok, M. J. Wester and K.A. Dill, Resultants and Loop Closure, International Journal of Quantum Chemistry **106** (2005), no. (1), 176-189.

[C2] E. A. Coutsias, C. Seok, M.J. Jacobson, K.A. Dill, A Kinematic View of Loop Closure, Journal of Computational Chemistry **25** (2004), no. 4, 510 - 528.

[KSY] D. Kapur, T. Saxena, and L. Yang, Algebraic and geometric reasoning using Dixon resultants. In: *Proc. of the International Symposium on Symbolic and Algebraic Computation.* A.C.M. Press (1994).

[Lew] Robert H. Lewis, Computer algebra system *Fermat*.
www.bway.net/~lewis/

[LB] R. Lewis and S. Bridgett, Conic Tangency Equations Arising from Apollonius Problems in Biochemistry. Mathematics and Computers in Simulation **61** (2) (2003) p. 101-114.

[LS] R. Lewis and P. Stiller, Solving the Recognition Problem for Six Lines Using the Dixon Resultant. Mathematics and Computers in Simulation **49** (1999).