

Conformational Search Using Real Algebraic Geometry

J. Maurice Rojas &

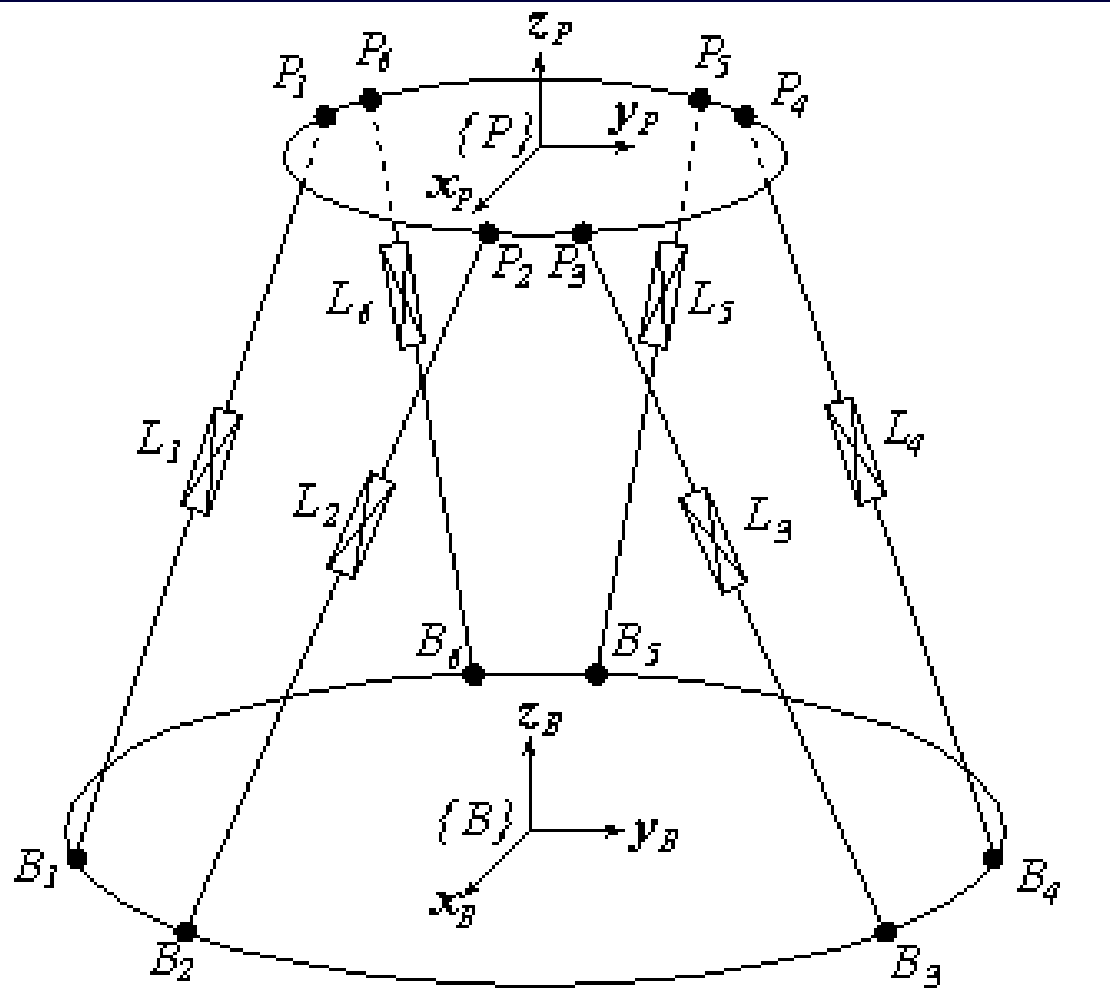
Ming Zhang

Texas A&M, Mathematics

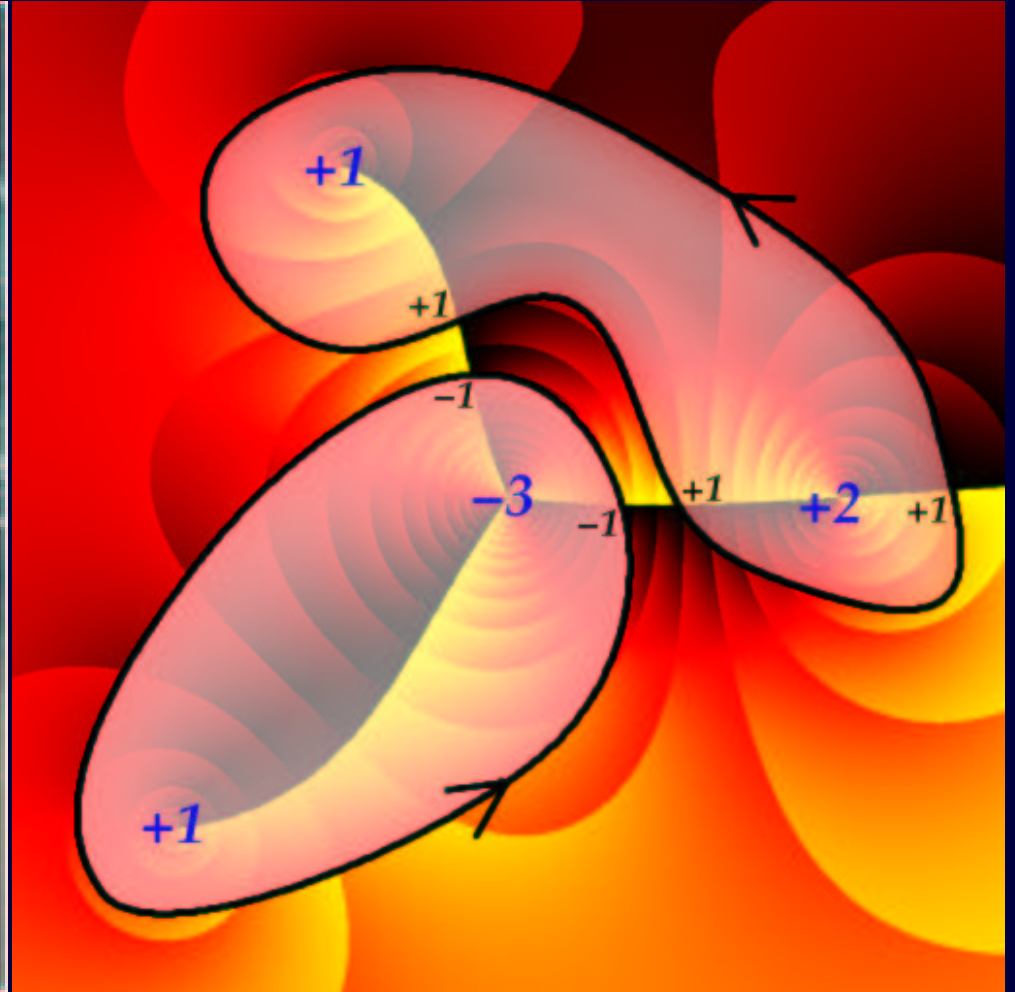
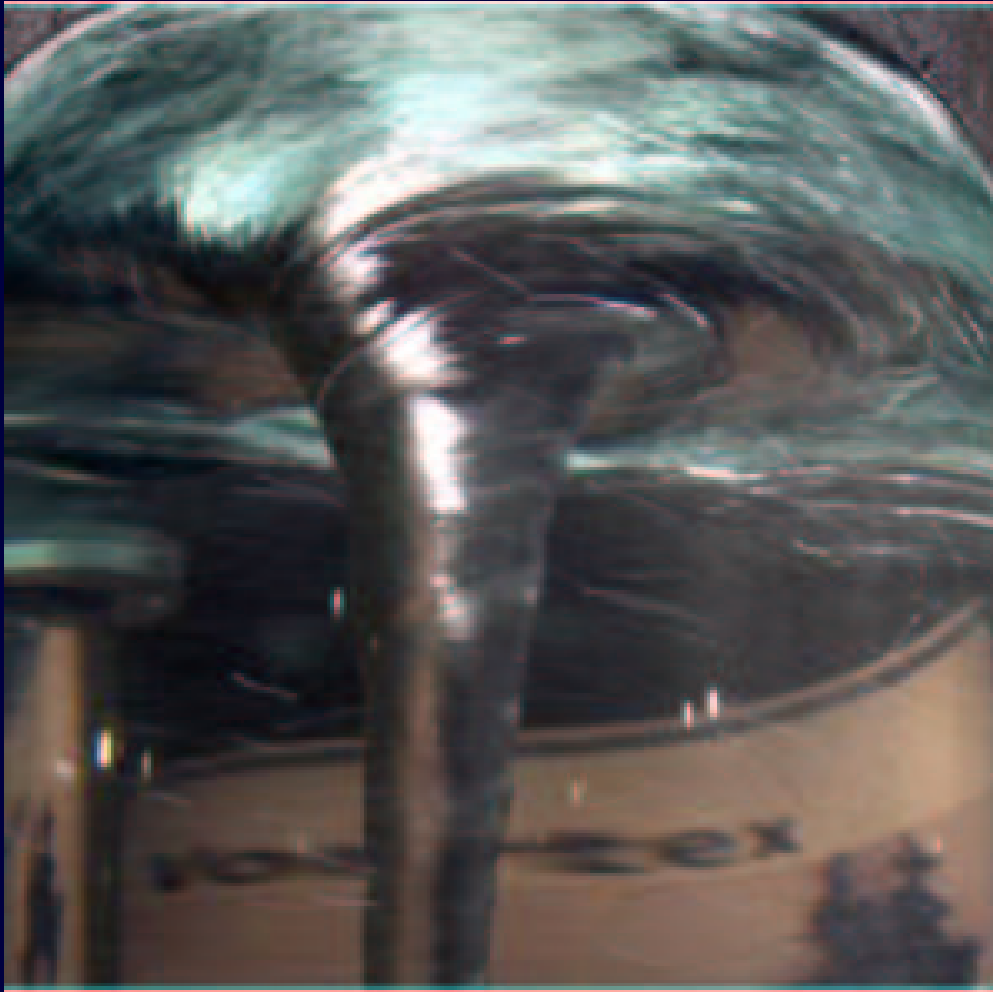
M. D. Anderson Cancer Center

June 27, 2003

ROBOTS AND EQUATIONS



CAUCHY'S THEOREM



ONE DIMENSIONAL RESIDUES

For **analytic** functions f_1, \dots, f_n in n variables, you can count the **number of roots (with multiplicities)** lying in a domain $U \subseteq \mathbb{C}^n$ as follows...

$$n=1: \frac{1}{2\pi i} \int_{\partial U} \frac{f_1'(z) dz}{f_1(z)} = \dots = \frac{1}{4\pi} \sum_{i=1}^N \text{ArcSin} \left(\text{Im} \left(\frac{\bar{f}_1(u(\frac{i-1}{N})) f_1(u(\frac{i}{N}))}{f_1(u(\frac{i-1}{N})) \bar{f}_1(u(\frac{i}{N}))} \right) \right),$$

where $u([0, 1]) = \partial U$.

MULTIDIMENSIONAL RESIDUES

$n = 2$ (and beyond):

$$\frac{1}{(2\pi i)^2} \int_{\partial U} \frac{\text{DetJac}(F)(z_1, z_2) dz_1 \wedge dz_2}{f_1(z_1, z_2) f_2(z_1, z_2)}$$

$$\dots \approx \frac{1}{32\pi^2} \sum_{\text{cells}} \text{of } \frac{\pm 1}{f_\ell^2(u(a, b, c)) \bar{f}_\ell^2(u(a, b, c))} \times \dots$$

$u([a, a'] \times [b, b'] \times [c, c'])$
of a subdivision of ∂U

$$\text{Det} \begin{bmatrix} \text{ArcSin} \left(\text{Im} \left(\frac{\bar{f}_\ell(u(a, b, c)) f_\ell(u(a', b, c))}{f_\ell(u(a, b, c)) \bar{f}_\ell(u(a', b, c))} \right) \right) & \text{Re}(f_{3-\ell}^2(u(a', b, c)) - f_{3-\ell}^2(u(a, b, c))) & \text{Im}(f_{3-\ell}^2(u(a', b, c)) - f_{3-\ell}^2(u(a, b, c))) \\ \text{ArcSin} \left(\text{Im} \left(\frac{\bar{f}_\ell(u(a, b, c)) f_\ell(u(a, b', c))}{f_\ell(u(a, b, c)) \bar{f}_\ell(u(a, b', c))} \right) \right) & \text{Re}(f_{3-\ell}^2(u(a, b', c)) - f_{3-\ell}^2(u(a, b, c))) & \text{Im}(f_{3-\ell}^2(u(a, b', c)) - f_{3-\ell}^2(u(a, b, c))) \\ \text{ArcSin} \left(\text{Im} \left(\frac{\bar{f}_\ell(u(a, b, c)) f_\ell(u(a, b, c'))}{f_\ell(u(a, b, c)) \bar{f}_\ell(u(a, b, c'))} \right) \right) & \text{Re}(f_{3-\ell}^2(u(a, b, c')) - f_{3-\ell}^2(u(a, b, c))) & \text{Im}(f_{3-\ell}^2(u(a, b, c')) - f_{3-\ell}^2(u(a, b, c))) \end{bmatrix},$$

where $f_\ell(\cdot)$ has maximal norm.

OLDER APPROACHES INADEQUATE!

For key 9×9 example...

Gröbner Bases: Too slow!: About $(198,359,290,368)^3$ arithmetic ops! And don't think about the coefficient swell!

Toric Resultants: Still too slow!: About $\gg (185,794,560)^3$ arithmetic ops!

Polyhedral Homotopy: Too slow as well!: About $> (185,794,560)^3$ arithmetic ops, followed by a slow iteration!

Hermite's Method: Assumes only finitely complex roots and that something close to a Gröbner basis is available!

ALGORITHMIC SPEED-UP!

Monomials to Bernstein Basis: Shows promise, but numerical stability not clear. Also, root isolation not guaranteed. But $> (177147)^2$ arithmetic operations, followed by $2^? \times (177147)^2$ more...

Mollified Winding Numbers: Much greater numerical stability and guaranteed root isolation! Furthermore, with high probability, about $(262144)^2$ arithmetic operations total [Malajovich-Rojas, 2003; Rojas, 2003].

Finish off by **Newton's Method Certified by α -Theory...**

♡ THANKS TO KEENER AND MOGILNER!



James!



Alex!

QUESTIONS?

♡ Thank you for listening!

email:

- Rojas: rojas@math.tamu.edu
- Zhang: ming@odin.mdacc.tmc.edu