# What is...computer algebra?

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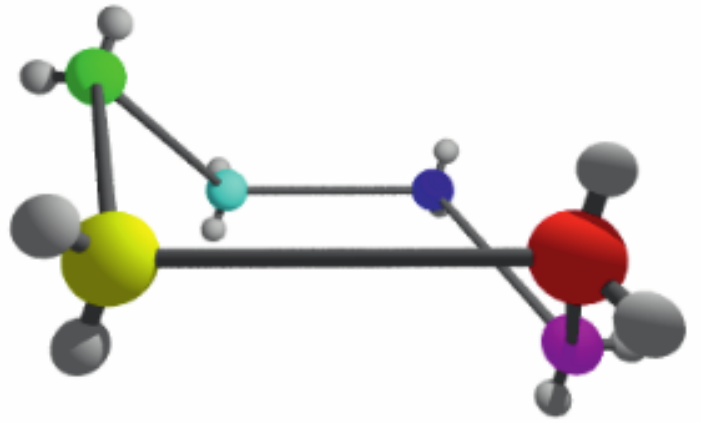
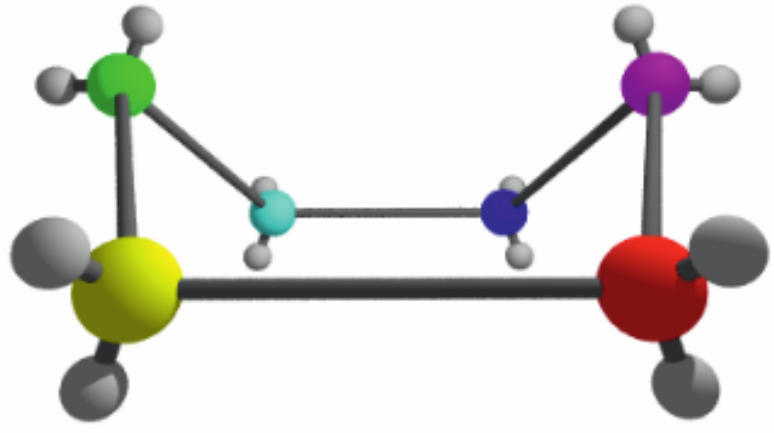
Or: Subfields of mathematics 15

# Chairs and boats

chair:

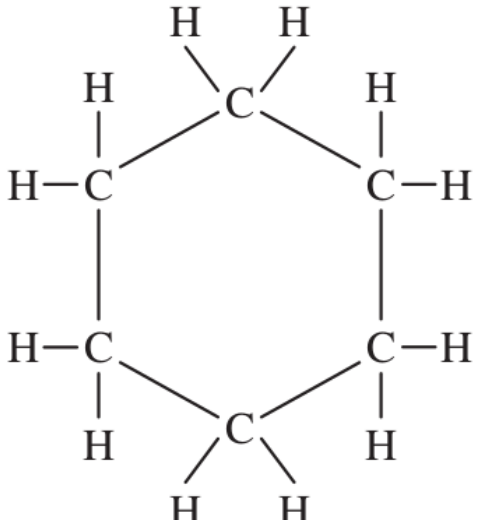


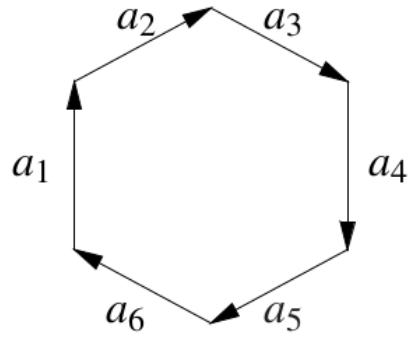
one boat:



- $C_6H_{12}$ occurs in incongruent conformations: chair (one) and boats (many) mod mirrors
- Chair occurs far more frequently than the boats
- Chair is stiff while the boats can twist into one another

# Modeling chairs and boats





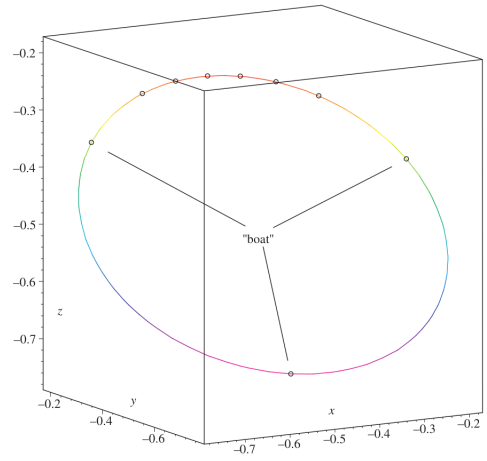

$$a_1 \star a_1 = a_2 \star a_2 = \cdots = a_6 \star a_6 = 1,$$ Length between bonds

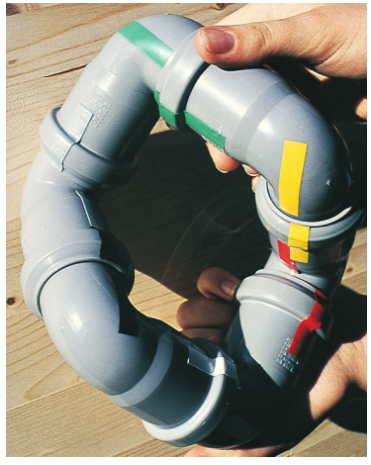
$$a_1 \star a_2 = a_2 \star a_3 = \cdots = a_6 \star a_1 = \frac{1}{3},$$ Angle ≈ 109°

$$a_1 + a_2 + \cdots + a_6 = 0.$$ Cyclic

- Idea Modeled the configurations as vectors $a_i$ and $a_i \star a_j$=inner product
- More Model $S_{ij} = a_i \star a_j$ as variables
- One gets polynomial variables subject to the relations above $\Rightarrow$ get solution via Gröbner bases

# A variety and chemistry



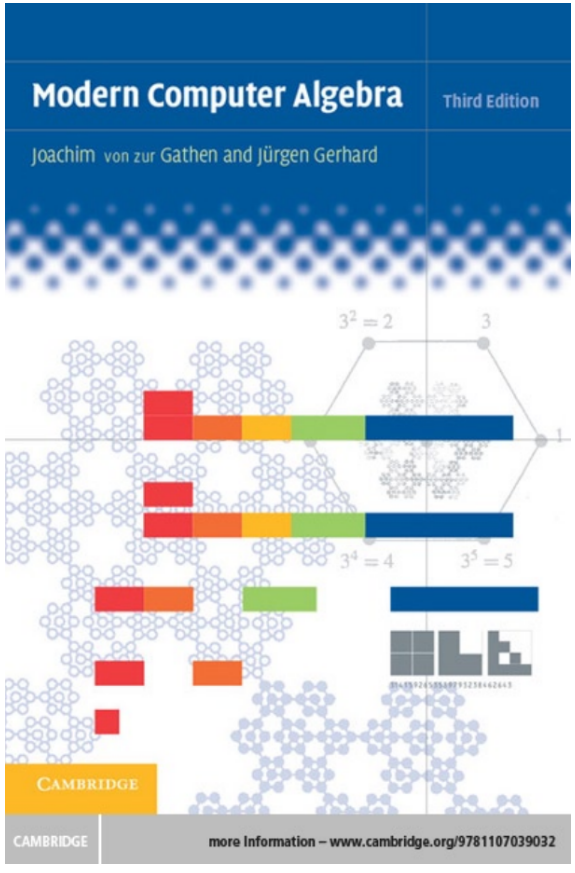



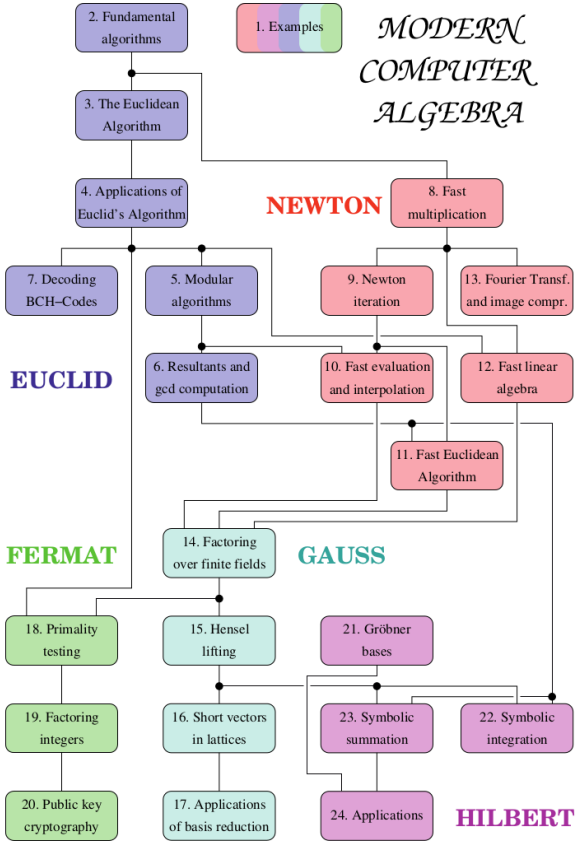
- One gets that the inflexible solution chair is an isolated point
- The boats lie on a curve
- Indeed Chair won't move and boats can be twisted when build from tubes

# Enter, the theorem

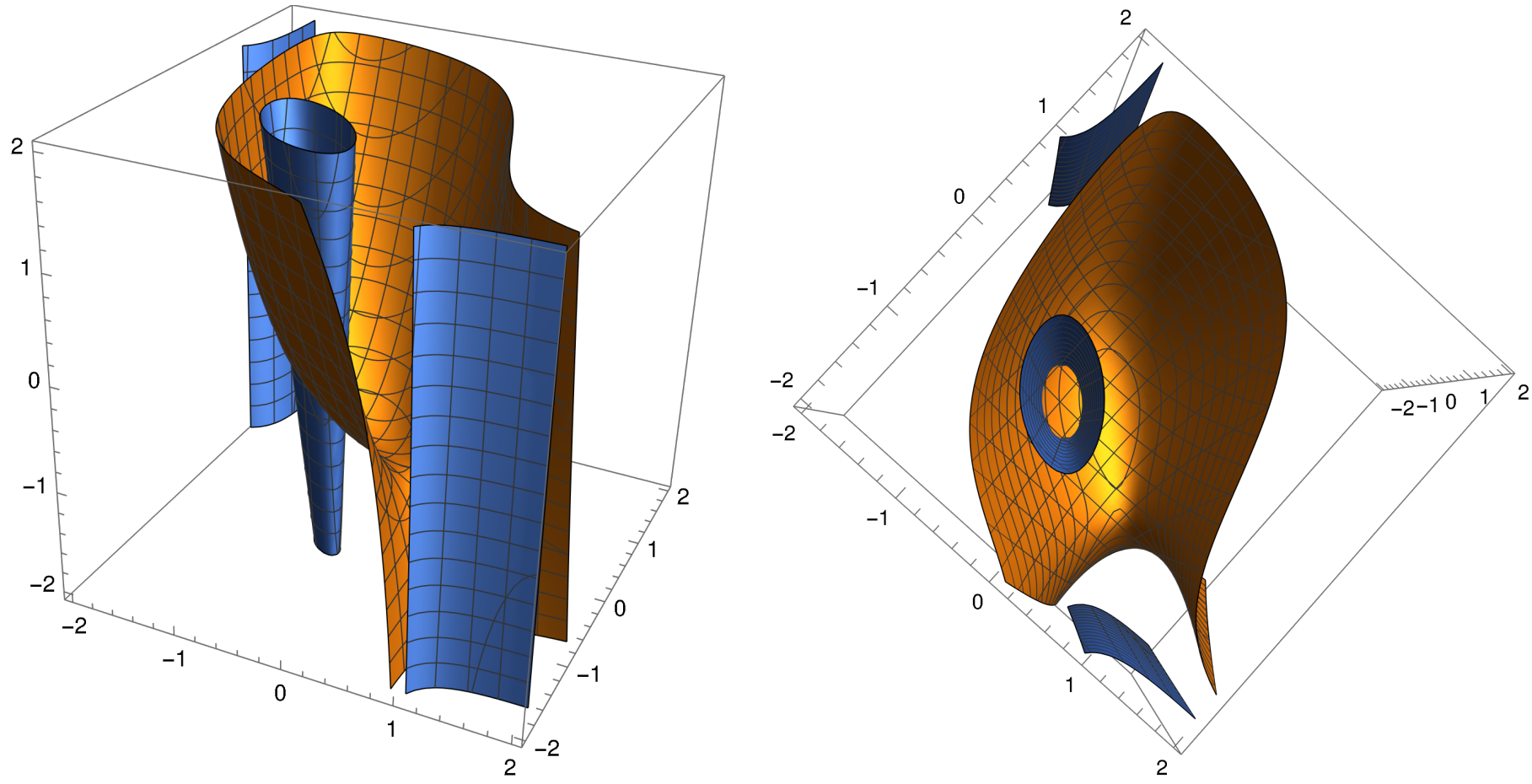
Gröbner bases can be computed in $O(d^{2^n})$

- Here $d$ = degree, $n$ = number of variables
- Computer algebra answers similar questions!



# More on chairs and boats




- Above Plots of the variety (excluding chair) for the chemistry problem
- Using Gröbner bases one can show that the solution set has:
  - Two (mirrors) isolated solutions $\leftrightsquigarrow$ chair
  - A circle of solutions $\leftrightsquigarrow$ boats

**Thank you for your attention!**

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I hope that was of some help.