

SINGULAR and Applications

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Department of Mathematics

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A Computer Algebra System for Polynomial Computations
with special emphasize on the needs of algebraic geometry, commutative algebra, and
singularity theory



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The computer is not the philosopher's stone but the philosopher's
whetstone

Hugo Battus, Rekenen op taal 1983

Birth of SINGULAR



● 1984

- rational numbers \mathbb{Q} (characteristic 0)
- finite fields $\mathbb{Z}/p\mathbb{Z}$ ($p \leq 2147483629$)
- finite fields \mathbb{F}_{p^n} ($p^n < 2^{15}$)

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 $K[t]/\text{MinPoly}$
- floating point real and complex numbers

- polynomial rings $K[x_1, \dots, x_n]$
- localizations $K[x_1, \dots, x_n]_M$
 M maximal ideal
- factor rings $K[x_1, \dots, x_n]/J$ oder $K[x_1, \dots, x_n]_M/J$

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- non-commutative G -algebras
 $K\langle x_1, \dots, x_n \mid x_j x_i = C_{ij} x_i x_j + D_{ij} \rangle$
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- tensor products of the rings above

- Standard basis algorithms (Buchberger, SlimGB, factorizing Buchberger, FGLM, Hilbert-driven Buchberger, ...)

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- Characteristic sets (Wu)

Examples for libraries

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dynamic modules

1983

Greuel/Pfister: Exist singularities (not quasi-homogeneous and complete intersection) with exact Poincaré-complex?

1984

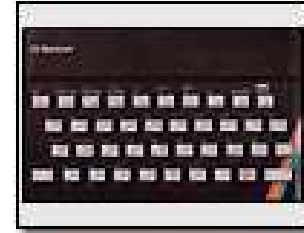
Neuendorf/Pfister: Implementation of the Gröbner basis algorithm in basic at ZX-Spectrum

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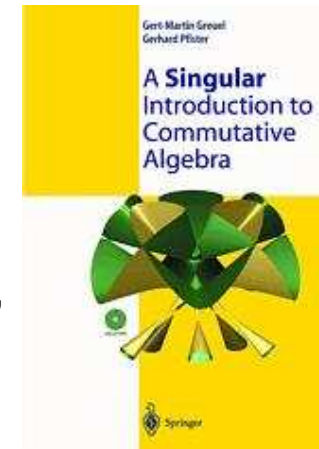
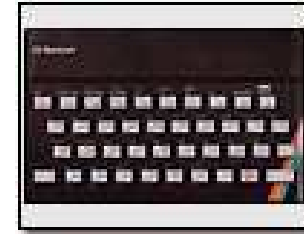
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2002

Book: A SINGULAR Introduction to Commutative Algebra (G.-M. Greuel and G. Pfister, with contributions by O. Bachmann, C. Lossen and H. Schönemann).



2004

Jenks Price

for:

Excellence in Software Engineering
awarded at **ISSAC in Santander**



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- Supported by: Deutsche Forschungsgemeinschaft, Stiftung Rheinland-Pfalz für Innovation, Volkswagen Stiftung
- SINGULAR is free software (Gnu Public Licence)



T. Wichmann, C. Lossen, G.-M. Greuel, H. Schönemann,
W. Pohl, G. Pfister, V. Levandovskyy, E. Westenberger,
A. Frühbis-Krüger, Oscar, K. Krüger



Kaiserslautern
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Theorem (K. Saito 1971): Let $(X, 0)$ be the germ of an isolated hypersurface singularity. The following conditions are equivalent:

- $(X, 0)$ is **quasi-homogeneous**.
- $\mu(X, 0) = \tau(X, 0)$.
- The **Poincaré complex** of $(X, 0)$ is **exact**.

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- The **Poincaré complex** of $(X, 0)$ is **exact**.

We wanted to **generalize** this theorem to the case of **isolated complete intersection singularities**.

Let $(X_{l,k}, 0)$ be the germ of the unimodal space curve singularity $FT_{k,l}$ of the classification of **Terry Wall** defined by the equations

$$\begin{aligned}xy + z^{l-1} &= 0 \\xz + yz^2 + y^{k-1} &= 0\end{aligned}$$

$$4 \leq l \leq k, 5 \leq k.$$

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The **Poincaré complex**

$$0 \longrightarrow \mathbb{C} \longrightarrow \mathcal{O}_{X_{l,k},0} \longrightarrow \Omega_{X_{l,k},0}^1 \longrightarrow \Omega_{X_{l,k},0}^2 \longrightarrow \Omega_{X_{l,k},0}^3 \longrightarrow 0$$

is exact.

But $(X_{l,k}, 0)$ is not quasi-homogeneous:

$$\mu(X, 0) = \tau(X, 0) + 1 = k + l + 2.$$

Let $(X, 0)$ be a germ of a space curve singularity defined by $f = g = 0$, with $f, g \in \mathbb{C}\{x, y, z\}$

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here the M_i are the 2-minors of the Jacobian matrix of f, g .

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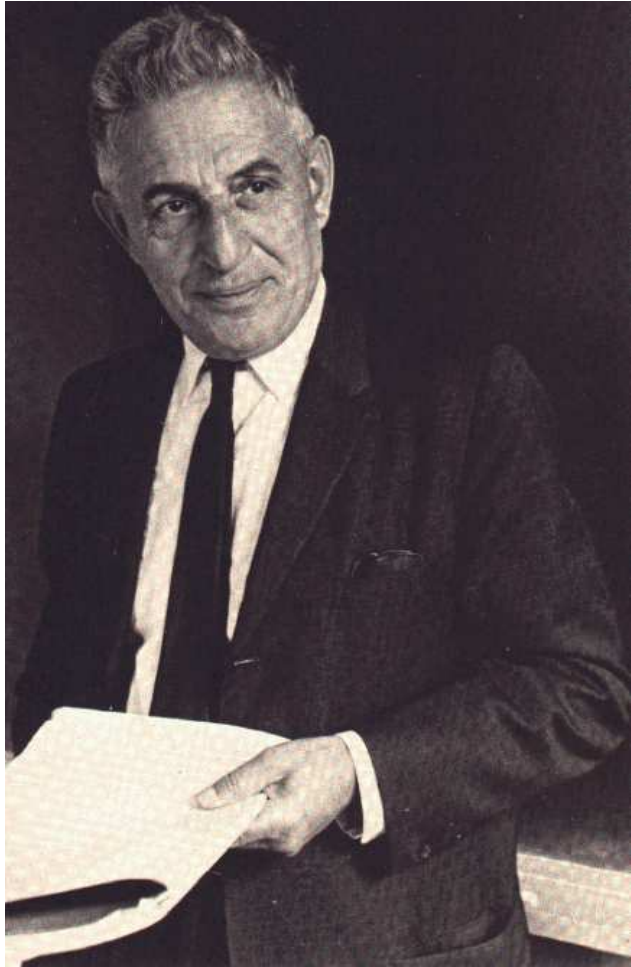
- **Reiffen:** The Poincaré complex is exact if and only if

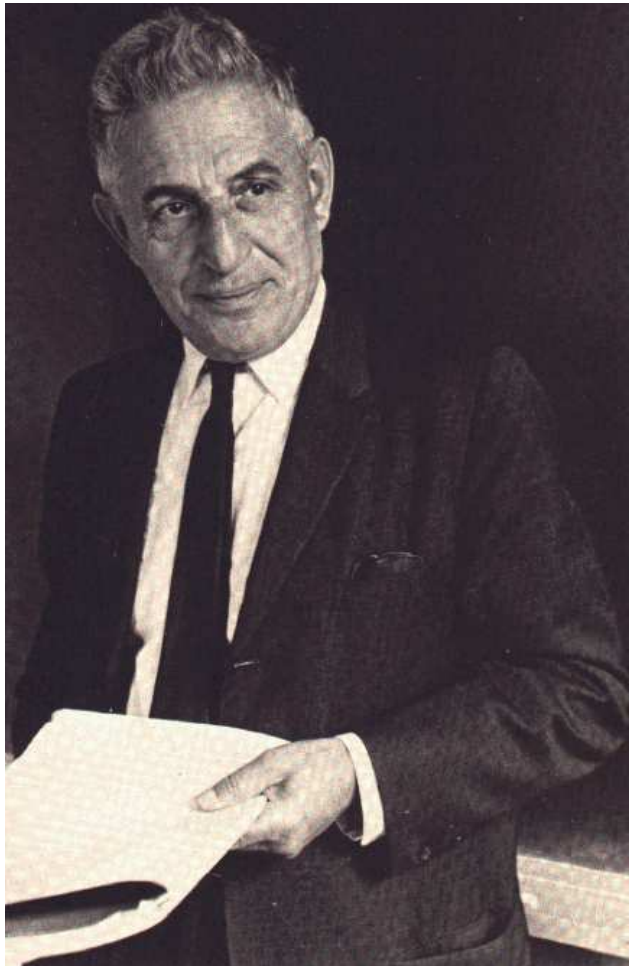
$$\langle f, g \rangle \Omega_{\mathbb{C}^3,0}^3 \subset d(\langle f, g \rangle \Omega_{\mathbb{C}^3,0}^2)$$

and

$$\mu(X, 0) = \dim_{\mathbb{C}}(\Omega_{X,0}^2) - \dim_{\mathbb{C}}(\Omega_{X,0}^3)$$

Zariski's conjecture



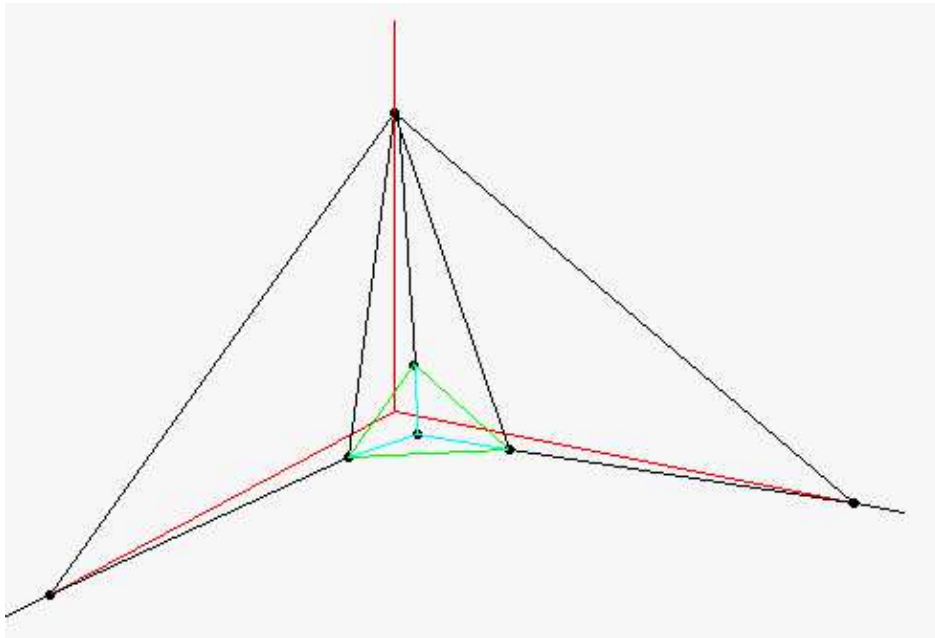


Conjecture (Zariski 1971) :

A μ -constant deformation of an isolated hypersurface singularity is a deformation with constant multiplicity.

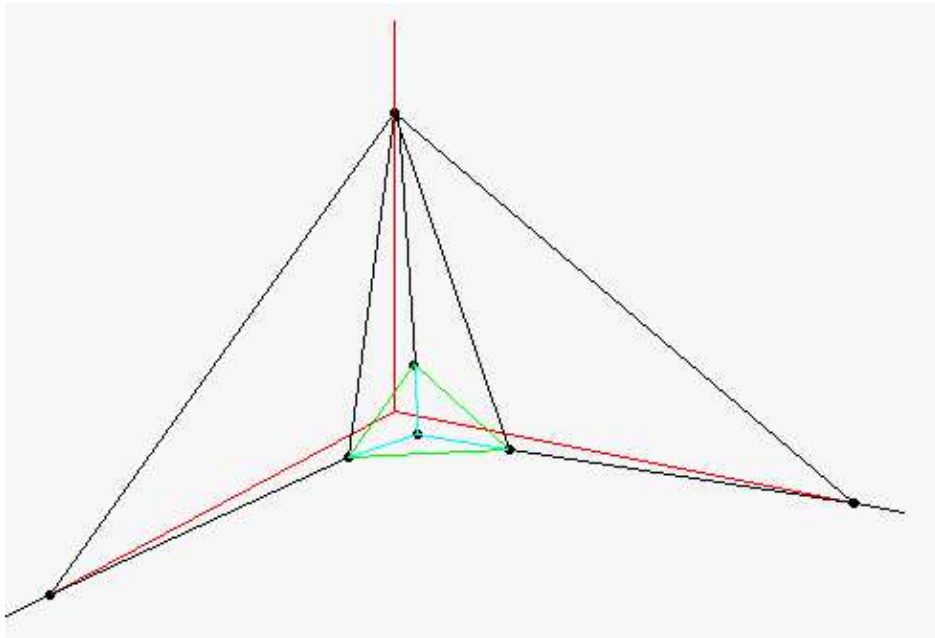
Zariski's conjecture

$$F_t = x^a + y^b + z^{3c} + x^{c+2}y^{c-1} + x^{c-1}y^{c-1}z^3 + x^{c-2}y^c(y^2 + tx)^2$$



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$$(a, b, c) = (40, 30, 8)$$

$$\mu(F_0) = 10661$$

$$\mu(F_t) = 10655$$

- **mathematical**
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 - proving theorems

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- **non-mathematical**
 - engineering (glas melting, robotics, chemical models, analog and digital microelectronics)
 - equilibrian problems in economics
 - theoretical physics

Problem: Characterize the class of finite solvable groups G by 2–variable identities.

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Example:

- G is **abelian** $\Leftrightarrow xy = yx \ \forall x, y \in G$
- (Zorn, 1930) A **finite group** G is **nilpotent** $\Leftrightarrow \exists n \geq 1$, such that
 $v_n(x, y) = 1 \ \forall x, y \in G$
(Engel Identity)

$$v_1 := [x, y] = xyx^{-1}y^{-1} \text{ (commutator)}$$

$$v_{n+1} := [v_n, y]$$

Let G be a finite group

$$G^{(1)} := [G, G] = \langle aba^{-1}b^{-1} \mid a, b \in G \rangle .$$

Let $G^{(i)} := [G^{(i-1)}, G]$, then G is called **nilpotent**, if $G^{(m)} = \{e\}$ for a suitable m .

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- abelian groups are nilpotent.
- if the order of the group is a power of a prime it is nilpotent.
- G is nilpotent \Leftrightarrow it is the direct product of its Sylow groups.
- S_3 is not nilpotent.

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- nilpotente groups are solvable.
- S_3, S_4 are solvable.
- groups of odd order are solvable.
- S_5, A_5 are not solvable.

Theorem (T. Bandman, G.-M. Greuel, F. Grunewald, B. Kunyavsky, G. Pfister, E. Plotkin)

$$U_1 = U_1(x, y) := x^2 y^{-1} x,$$

$$U_{n+1} = U_{n+1}(x, y) = [xU_n x^{-1}, yU_n y^{-1}].$$

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- $U_1(x, y) = 1 \Leftrightarrow y = x^{-1}$
- $U_1(x, y) = U_2(x, y)$
 $\Leftrightarrow x^{-1} y x^{-1} y^{-1} x^2 = y x^{-2} y^{-1} x y^{-1}$
- **Let $x, y \in G$ such that $y \neq x^{-1}$ and $U_1(x, y) = U_2(x, y) \Rightarrow U_n(x, y) \neq 1 \forall n \in \mathbb{N}$.**

G solvable \Rightarrow Identity is true (by definition).

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Idea of \Leftarrow

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Let G minimally not solvable. Then G is one of the following groups:

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- **PSL**(2, \mathbb{F}_p), p a prime number ≥ 5

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It is enough to prove (for G in Thompson's list): $\exists x, y \in G$, such that $y \neq x^{-1}$ and $U_1(x, y) = U_2(x, y)$.

Let w be a word in X, Y, X^{-1}, Y^{-1} and

$$U_1 = w$$

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A Computer-search through the 10,000 shortest words in X, X^{-1}, Y, Y^{-1} found the following four words such that the equation $U_1 = U_2$ has a non-trivial solution in $\text{PSL}(2, p)$ for all $p < 1000$:

$$w_1 = X^{-2}Y^{-1}X$$

$$w_2 = X^{-1}YXY^{-1}X$$

$$w_3 = Y^{-2}X^{-1}$$

$$w_4 = XY^{-2}X^{-1}YX^{-1}$$

$$\mathrm{PSL}(2, K) = \mathrm{SL}(2, K) / \left\{ \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \mid a^2 = 1 \right\}$$

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especially

$$\mathrm{PSL}(2, \mathbb{F}_5) = \left\{ \left[\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \right], a_{11}a_{22} - a_{21}a_{12} = 1 \right\}$$

$$\left[\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \right] = \left\{ \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \begin{pmatrix} 4a_{11} & 4a_{12} \\ 4a_{21} & 4a_{22} \end{pmatrix} \right\} .$$

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It holds:

$$\mathrm{PSL}(2, \mathbb{F}_5) \cong \mathrm{PSL}(2, \mathbb{F}_4) \cong A_5$$

Let us consider $G = \mathrm{PSL}(2, \mathbb{F}_p)$, $p \geq 5$

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Consider the matrices

$$x = \begin{pmatrix} t & 1 \\ -1 & 0 \end{pmatrix} \quad y = \begin{pmatrix} 1 & b \\ c & 1 + bc \end{pmatrix}$$

$x^{-1} = \begin{pmatrix} 0 & -1 \\ 1 & t \end{pmatrix}$ implies $y \neq x^{-1}$ for all $(b, c, t) \in \mathbb{F}_p^3$.

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It is enough to prove that the equation

$$U_1(x, y) = U_2(x, y), \text{ i.e.} \\ x^{-1}yx^{-1}y^{-1}x^2 = yx^{-2}y^{-1}xy^{-1}$$

has a solution $(b, c, t) \in \mathbb{F}_p^3$.

The entries of $U_1(x, y) - U_2(x, y)$ are the following polynomials in $\mathbb{Z}[b, c, t]$ Let $I = \langle p_1, \dots, p_4 \rangle$ and $I^{(p)}$ the induced ideal over \mathbb{Z}/p :

$$p_1 = b^3c^2t^2 + b^2c^2t^3 - b^2c^2t^2 - bc^2t^3 - b^3ct + b^2c^2t + b^2ct^2 + 2bc^2t^2 \\ + bct^3 + b^2c^2 + b^2ct + bc^2t - bct^2 - c^2t^2 - ct^3 - b^2t + bct + c^2t \\ + ct^2 + 2bc + c^2 + bt + ct + c + 1$$

$$p_2 = -b^3ct^2 - b^2ct^3 + b^2c^2t + bc^2t^2 + b^3t - b^2ct - 2bct^2 - b^2c + bct \\ + c^2t + ct^2 - bt - ct - b - c - 1$$

$$p_3 = b^3c^3t^2 + b^2c^3t^3 - b^2c^2t^3 - bc^2t^4 - b^3c^2t + b^2c^3t + b^2c^2t^2 \\ + 2bc^3t^2 + bc^2t^3 + b^2c^2t + b^2ct^2 + bc^2t^2 - c^2t^3 - ct^4 - 2b^2ct \\ + bc^2t + c^3t + bct^2 + 2c^2t^2 + ct^3 - b^2c - b^2t + bct + c^2t + bt^2 \\ + 3ct^2 + bc - bt - b - c + 1$$

$$p_4 = -b^3c^2t^2 - b^2c^2t^3 + b^2c^2t^2 + bc^2t^3 + b^3ct - b^2c^2t - b^2ct^2 - 2bc^2t^2 \\ - bct^3 - 2b^2ct + c^2t^2 + ct^3 + b^2t - bct - c^2t - ct^2 + b^2 - bt \\ - 2ct - b - t + 1$$

Theorem von Hasse–Weil (generalized by [Aubry and Perret](#) for
singulare curves):

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Let $C \subseteq \mathbb{A}^n$ be an absolutely irreducible affine curve defined over the finite field \mathbb{F}_q and $\overline{C} \subset \mathbb{P}^n$ its projective closure \Rightarrow

$$\#C(\mathbb{F}_q) \geq q + 1 - 2p_a\sqrt{q} - d$$

($d = \text{degree}$, $p_a = \text{arithmetic genus of } \overline{C}$).

Theorem von Hasse–Weil (generalized by Aubry and Perret for singular curves):

Let $C \subseteq \mathbb{A}^n$ be an absolutely irreducible affine curve defined over the finite field \mathbb{F}_q and $\overline{C} \subset \mathbb{P}^n$ its projective closure \Rightarrow

$$\#C(\mathbb{F}_q) \geq q + 1 - 2p_a\sqrt{q} - d$$

(d = degree, p_a = arithmetic genus of \overline{C}).

The Hilbert–polynomial of \overline{C} , $H(t) = d \cdot t - p_a + 1$, can be computed using the ideal I_h of \overline{C} :

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Since $p + 1 - 24\sqrt{p} - 10 > 0$ if $p > 593$, we obtain the result.

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$$\langle f_1, f_2 \rangle : h^2 = I.$$

$$f_1 = t^2b^4 + (t^4 - 2t^3 - 2t^2)b^3 - (t^5 - 2t^4 - t^2 - 2t - 1)b^2 \\ - (t^5 - 4t^4 + t^3 + 6t^2 + 2t)b + (t^4 - 4t^3 + 2t^2 + 4t + 1)$$

$$f_2 = (t^3 - 2t^2 - t)c + t^2b^3 + (t^4 - 2t^3 - 2t^2)b^2 \\ - (t^5 - 2t^4 - t^2 - 2t - 1)b - (t^5 - 4t^4 + t^3 + 6t^2 + 2t)$$

$$h = t^3 - 2t^2 - t$$

We give explicitly matrices M and N with entries in $\mathbb{Z}[b, c, t]$ such

that
$$M \begin{pmatrix} p_1 \\ \vdots \\ p_4 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \quad \text{and} \quad N \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} h^2 p_1 \\ \vdots \\ h^2 p_4 \end{pmatrix}$$

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We obtain for all fields K

$$IK[b, c, t] = (\langle f_1, f_2 \rangle K[b, c, t]) : h^2 .$$

f_2 is linear in c , it is enough to show, that f_1 is absolutely irreducibel.

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- $IK[b, c, t]$ is prime
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- f_1 irreducible in $K(t)[b]$ resp. in $K[t, b]$.

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- $IK[b, c, t]$ is prime
- $\langle f_1, f_2 \rangle K(t)[b, c]$ prime
- f_1 irreducible in $K(t)[b]$ resp. in $K[t, b]$.

geometrically:

Curve $V(I)$ is irreducible, if the projection to the b, t -plane is irreducible.

Let $P(x) := t^2 J[1]|_{b=x/t}$ then P is monic of degree 4.

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$$x^4 + (t^3 - 2t^2 - 2t)x^3 - (t^5 - 2t^4 - t^2 - 2t - 1)x^2 - \\ (t^6 - 4t^5 + t^4 + 6t^3 + 2t^2)x + (t^6 - 4t^5 + 2t^4 + 4t^3 + t^2).$$

We prove, that the induced polynomial $P \in \mathbb{F}_p[t, x]$ is absolutely irreducible for all primes $p \geq 2$.

(Using the lemma of Gauß this is equivalent to P being irreducible in $\overline{\mathbb{F}_p}(t)[x]$.)

Ansatz

$$(*) \quad P = (x^2 + ax + b)(x^2 + gx + d)$$

a, b, g, d polynomials in t with variable coefficients

$$a(i), b(i), g(i), d(i).$$

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a, b, g, d polynomials in t with variable coefficients

$$a(i), b(i), g(i), d(i).$$

The decomposition $(*)$ with $a(i), b(i), g(i), d(i) \in \overline{\mathbb{F}}_p$ does not exist iff the ideal \mathbb{C} generated by the coefficients with respect to x, t of $P - (x^2 + ax + b)(x^2 + gx + d)$ has no solution in $\overline{\mathbb{F}}_p$. This is equivalent to the fact that $1 \in \mathbb{C}$.

The ideal of the coefficients of C :

$$C[1] = -b(5) * d(3)$$

$$C[2] = -b(5) * g(2)$$

$$C[3] = -b(4) * d(3) - b(5) * d(2)$$

$$C[4] = -b(4) * g(2) - b(5) * g(1) - d(3) - 1$$

$$C[5] = -b(3) * d(3) - b(4) * d(2) - b(5) * d(1) + 1$$

$$C[6] = -b(5) - g(2) - 1$$

$$C[7] = a(0) * b(5) - a(2) * d(3) - b(3) * g(2) - b(4) * g(1) - d(2) + 4$$

$$C[8] = -a(0)^2 * b(5) + b(0) * b(5) - b(2) * d(3) - b(3) * d(2) - b(4) * d(1) - b(5) - 4$$

$$C[9] = -a(2) * g(2) - b(4) - g(1) + 2$$

$$C[10] = a(0) * b(4) - a(1) * d(3) - a(2) * d(2) - b(2) * g(2) - b(3) * g(1) - d(1) - 1$$

$$C[11] = -a(0)^2 * b(4) + b(0) * b(4) - b(1) * d(3) - b(2) * d(2) - b(3) * d(1) - b(4) + 2$$

$$C[12] = a(0) - a(1) * g(2) - a(2) * g(1) - b(3) - d(3)$$

$$C[13] = -a(0)^2 + a(0) * b(3) - a(0) * d(3) - a(1) * d(2) - a(2) * d(1) + b(0) - b(1) * g(2) - b(2) * g(1) - 7$$

$$C[14] = -a(0)^2 * b(3) + b(0) * b(3) - b(0) * d(3) - b(1) * d(2) - b(2) * d(1) - b(3) + 4$$

$$C[15] = -a(2) - g(2) - 2$$

$$C[16] = a(0) * a(2) - a(0) * g(2) - a(1) * g(1) - b(2) - d(2) + 1$$

$$C[17] = -a(0)^2 * a(2) + a(0) * b(2) - a(0) * d(2) - a(1) * d(1) + a(2) * b(0) - a(2) - b(0) * g(2) - b(1) * g(1) - 2$$

$$C[18] = -a(0)^2 * b(2) + b(0) * b(2) - b(0) * d(2) - b(1) * d(1) - b(2) + 1$$

$$C[19] = -a(1) - g(1) - 2$$

$$C[20] = a(0) * a(1) - a(0) * g(1) - b(1) - d(1) + 2$$

$$C[21] = -a(0)^2 * a(1) + a(0) * b(1) - a(0) * d(1) + a(1) * b(0) - a(1) - b(0) * g(1)$$

$$C[22] = -a(0)^2 * b(1) + b(0) * b(1) - b(0) * d(1) - b(1)$$

$$C[23] = -a(0)^3 + 2 * a(0) * b(0) - a(0)$$

$$C[24] = -a(0)^2 * b(0) + b(0)^2 - b(0)$$

Using SINGULAR, one shows that over
 $\mathbb{Z}[\{a(i)\}, \{b(i)\}, \{g(i)\}, \{d(i)\}]$

$$4 = \sum_{i=1}^{24} M_i C[i].$$

This case is much more complicated.
We have to prove that on a surface U any odd power of a certain endomorphism θ has fixed points.

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We have to prove that on a surface U any odd power of a certain endomorphism θ has fixed points.

Here we use the **Lefschetz–Weil–Grothendieck trace formulae** generalized by [Deligne–Lusztig](#), [Th. Zink](#), [Pink](#), [Katz](#) and [Adolphson–Sperber](#):

$$2^n - b_1(U) \cdot 2^{\frac{3}{4}n} - b_2(U) \cdot 2^{\frac{1}{2}n} \leq \# \text{Fix}(\theta^n, U)$$

for n sufficiently large.

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General problem:

- Study a computer model of a national economy
- especially study equilibria

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General problem:

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Mathematical problem:

Find the positive real roots of a given system of polynomial equations

A small example

This example could be solved by the economists themselves

```
ring R= 0,x(1..8),dp;
ideal I =
  -1024+x(1)^5*x(3)*x(7),
  -1+x(2)^5*x(3)*x(8),
  -1+x(4)^5*x(6)*x(7),
  -1024+x(5)^5*x(6)*x(8),
  x(1)*x(7)+x(2)*x(8)-12*x(7)-x(8),
  x(1)+x(4)-13,
  x(2)+x(5)-13,
  x(7)+x(8)-1;
ideal J=std(I);
vdim(J);
// 25   there are 25 zeros
list L=solve(J,100,0,100);size(L);
// 25   the zeros are simple
```

A hard example

```
ring R = 0,x(1..22),dp;
ideal I =
-1+x(1)^5*x(4)*x(13),-1+x(2)^5*x(4)*x(14),
-1+x(3)^5*x(4)*x(15),-1+x(5)^3*x(8)*x(13),
-1+x(6)^3*x(8)*x(14),-1+x(7)^3*x(8)*x(15),
-1+x(9)^4*x(12)*x(13),-1+x(10)^4*x(12)*x(14),
-1+x(11)^4*x(12)*x(15),
5+2*x(16)-x(1)*x(13)-x(2)*x(14)-x(3)*x(15),
3+5*x(16)-x(5)*x(13)-x(6)*x(14)-x(7)*x(15),
(x(1)+x(5)+x(9))^3-x(17)^2*x(18),
(x(2)+x(6)+x(10))^2-x(19)*x(20),
(x(3)+x(7)+x(11))^2-4*x(21)*x(22),
x(17)+x(19)+x(21)-10,x(18)+x(20)+x(22)-10,
8*x(13)^3*x(18)-27*x(16)^3*x(17),
x(13)^3*x(17)^2-27*x(18)^2,
x(14)^2*x(20)-4*x(16)^2*x(19),x(14)^2*x(19)-4*x(20),
x(15)^2*x(22)-x(16)^2*x(21),x(15)^2*x(21)-x(22);
```

A hard example

Problem:

- a purely numerical approach was not successful
- automatical symbolical preprocessing was not successful

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- a purely numerical approach was not successful
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Computer-Human solution:

- using factorization to split the problem
- Substitution of variables
- choose suitable field extensions to simplify the problem

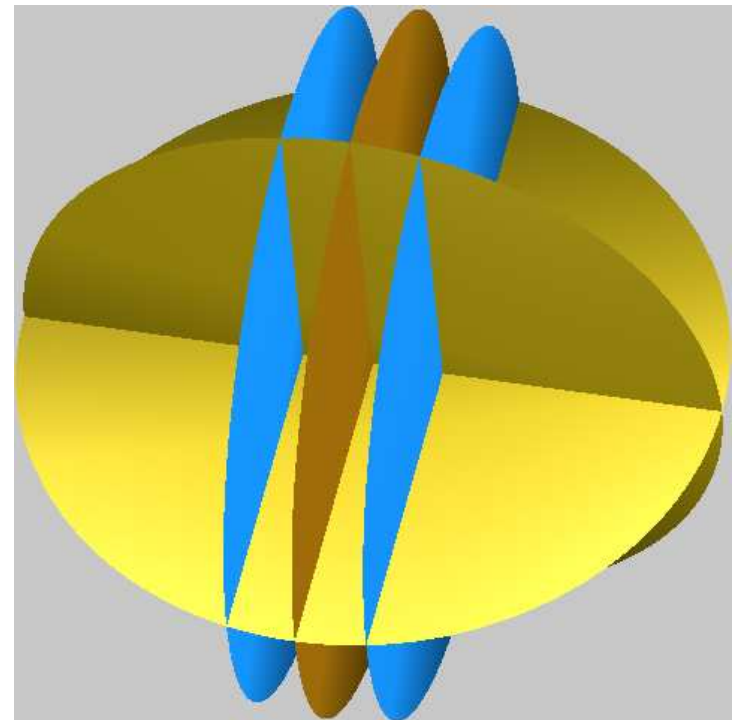
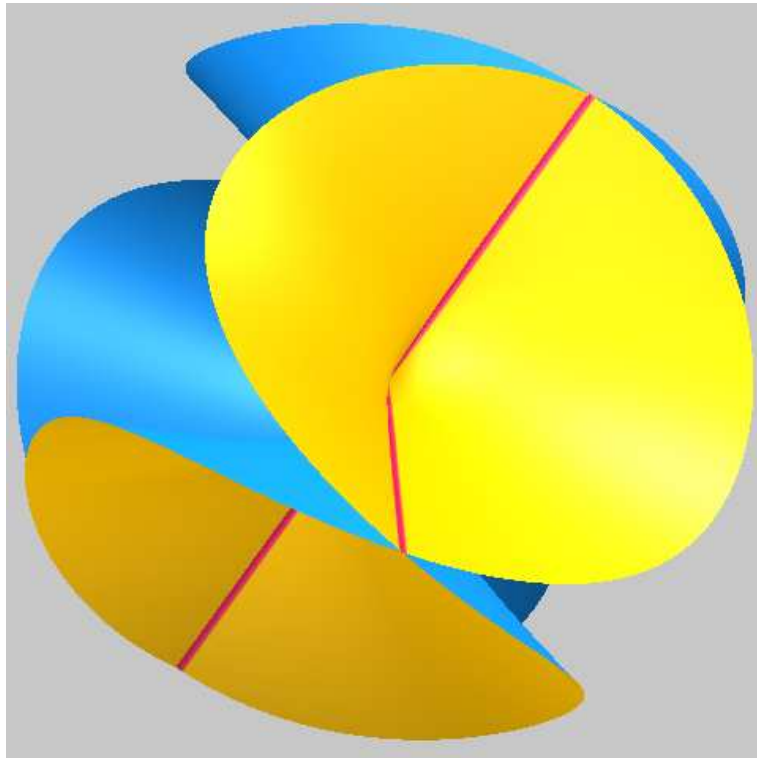
A degenerate example

```
int i;
ring R=0,x,dp;
poly p=x+1;
for(i=2;i<=20;i++){p=p*(x+i);}
p=p+1/2^23*x19;

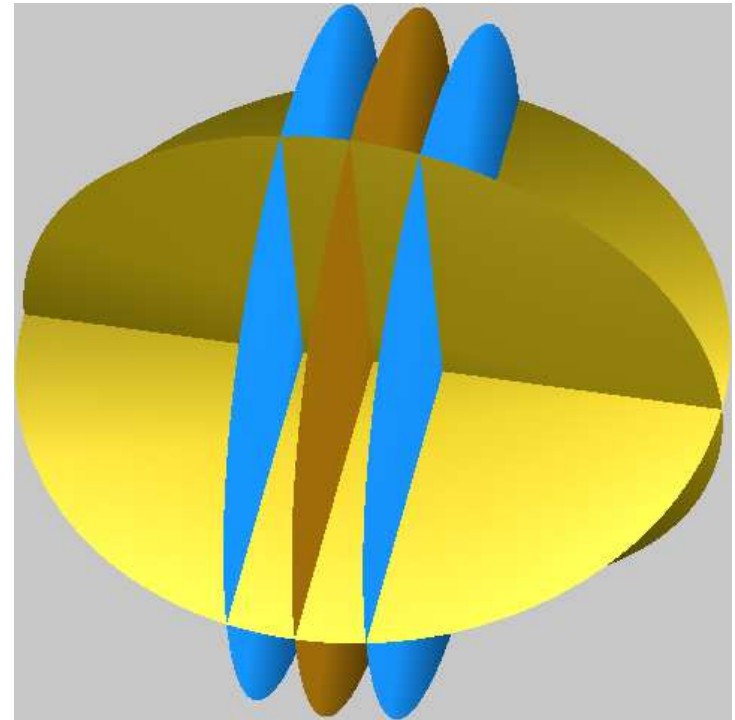
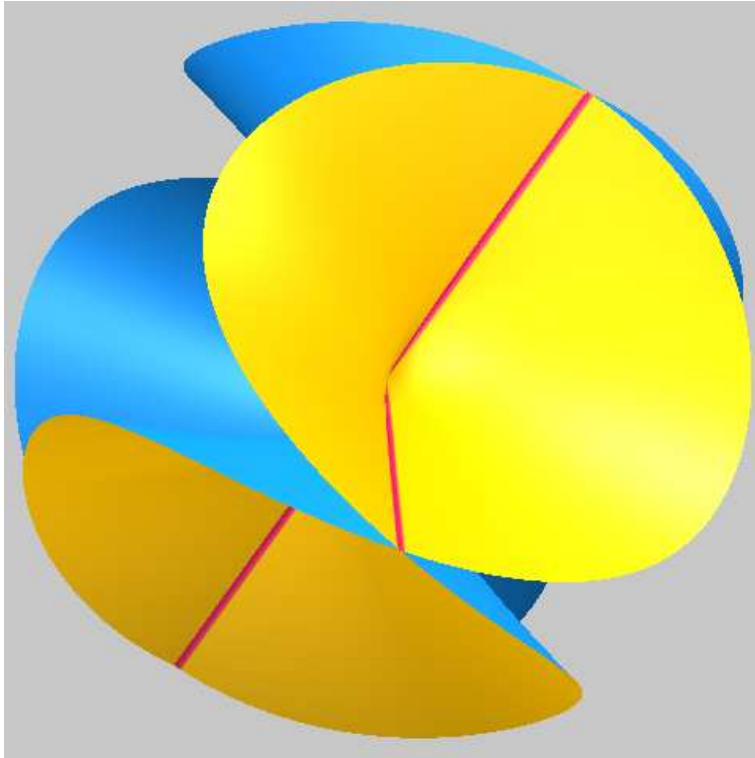
x20+1761607681/8388608x19+20615x18+1256850x17+53327946x16+1672280820x15
+40171771630x14+756111184500x13+11310276995381x12+135585182899530x11
+1307535010540395x10+10142299865511450x9+63030812099294896x8
+311333643161390640x7+1206647803780373360x6+3599979517947607200x5
+8037811822645051776x4+12870931245150988800x3+13803759753640704000x2
+8752948036761600000x+2432902008176640000

LIB"solve.lib";
list L=solve(p,1000,0,1000,"nodisplay");
LIB "rootsur.lib";
nrroots(p);
```

Resolution of $X = V(z^2 - x^2y^2) \subset K^3$



Resolution of $X = V(z^2 - x^2y^2) \subset K^3$



 resolve.lib

- Let $S = \mathbb{K}[x_0, \dots, x_n]$ and M be a finitely generated graded S -module.
We want to compute

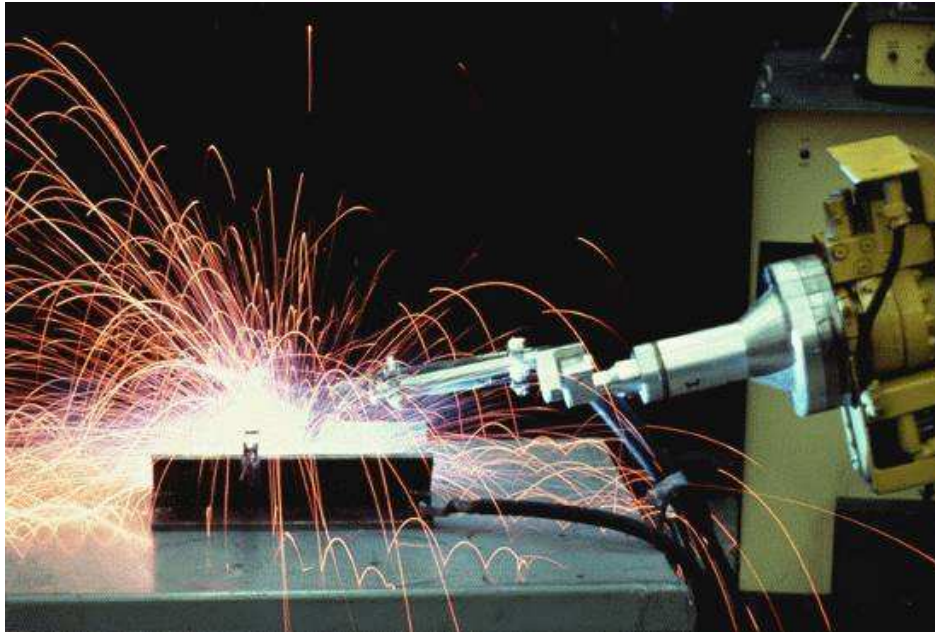
$$H^j(\widetilde{M}(k))$$

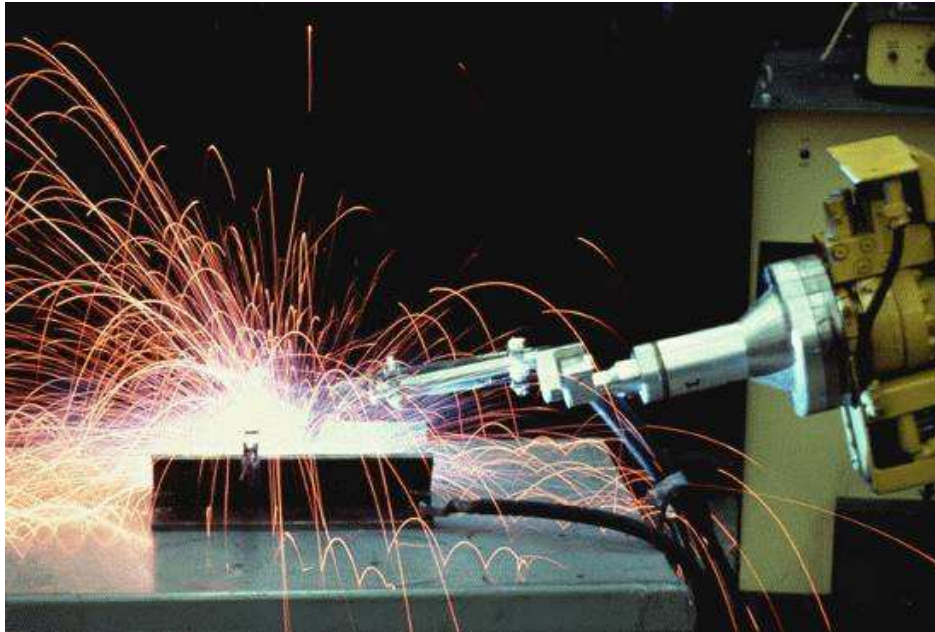
- Let $S = \mathbb{K}[x_0, \dots, x_n]$ and M be a finitely generated graded S -module.
We want to compute

$$H^j(\widetilde{M}(k))$$

- Using non-commutative methods will be 50 times faster than the direct (commutative) approach.

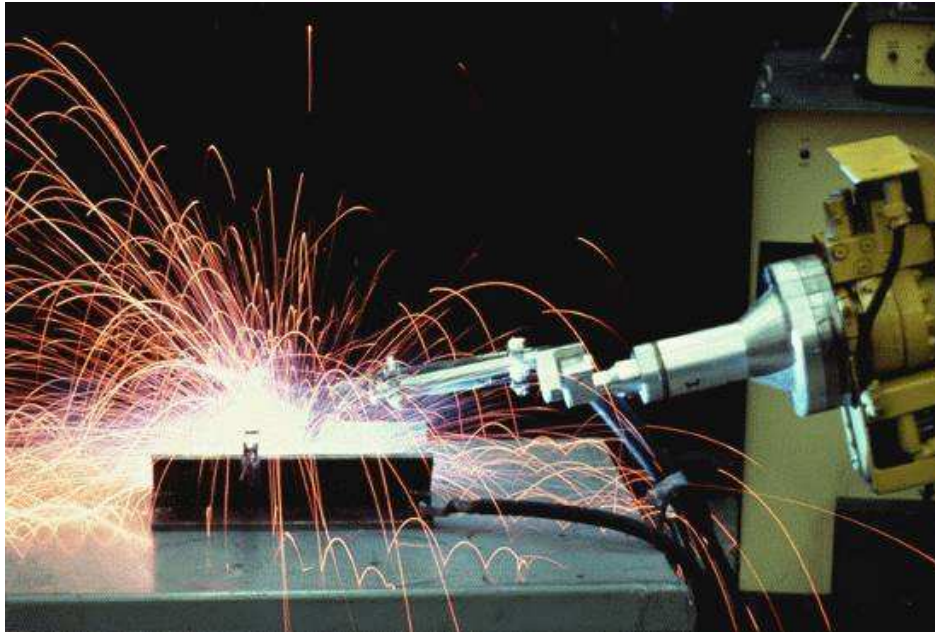
Robotics and the Cycloheptane Molecule



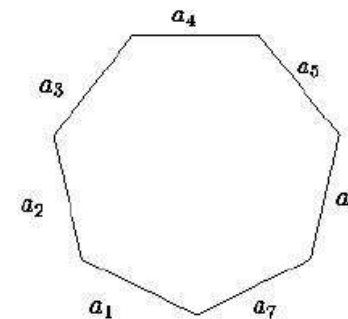
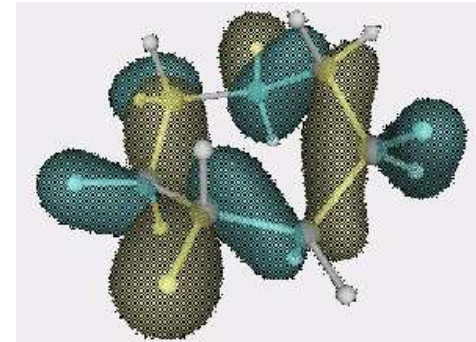


A.H.M. Levelt

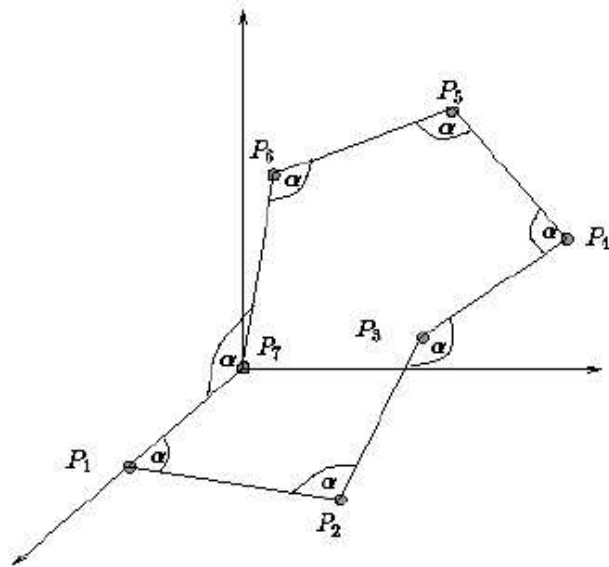
Robotics and the Cycloheptane Molecule



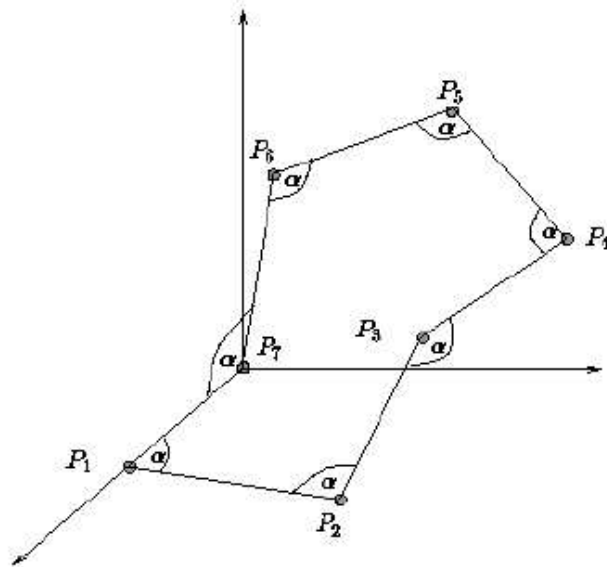
A.H.M. Levelt



The Heptagon



The Heptagon

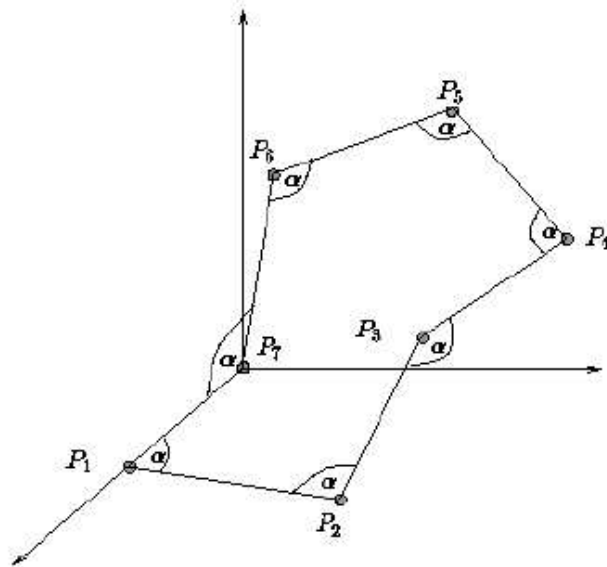


Equations for the vectors:

- $(a_1, a_2) = (a_2, a_3) = \dots = (a_7, a_1) = c$
- $(a_1, a_1) = (a_2, a_2) = \dots = (a_7, a_7) = 1$
- $a_1 + a_2 + \dots + a_7 = 0$

$c = \cos(\alpha)$ and $(,)$ is the scalar product.

The Heptagon



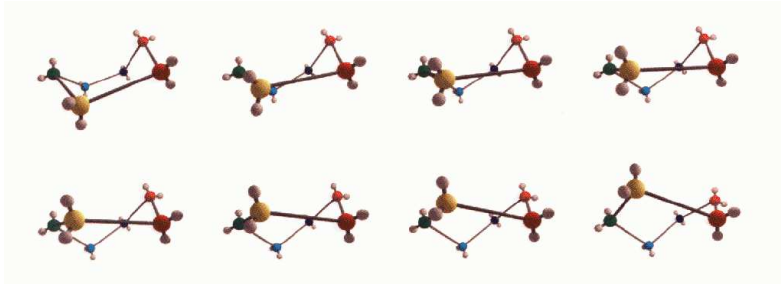
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- $a_1 + a_2 + \dots + a_7 = 0$

$c = \cos(\alpha)$ and $(,)$ is the scalar product.

- For $c = 0$: equations for the configuration space of a robot
- For $c = \frac{1}{3}$: equations for the configurations space of a molecule

Equations for the configuration space (in SINGULAR):



ring $R=0, (v, w, x, y, z), dp;$

ideal $I=$

$81y^2z^2 - 54wyz + 54y^2z + 54yz^2 - 72w^2 + 198wy - 207y^2 + 198wz - 225yz - 207z^2 + 114w - 141y - 141z + 10,$

$81w^2x^2 + 54w^2x + 54wx^2 - 54wxz - 207w^2 - 225wx - 207x^2 + 198wz + 198xz - 72z^2 - 141w - 141x + 114z + 10,$

$324vw^2x + 432vw^2 + 540vwx + 432w^2x - 432wxy - 432vwz + 324wyz + 180vw + 846w^2 - 576vx + 180wx -$

$306wy + 144xy + 144vz - 306wz - 36yz + 12v + 585w + 12x - 318y - 318z - 79,$

$81v^2w^2 + 54v^2w + 54vw^2 - 54vwy - 207v^2 - 225vw - 207w^2 + 198vy + 198wy - 72y^2 - 141v - 141w + 114y + 10;$

The Projection

The equations describe a **curve in \mathbb{R}^5** . The **projection** to the w, x -plane is difficult to compute:

The Projection

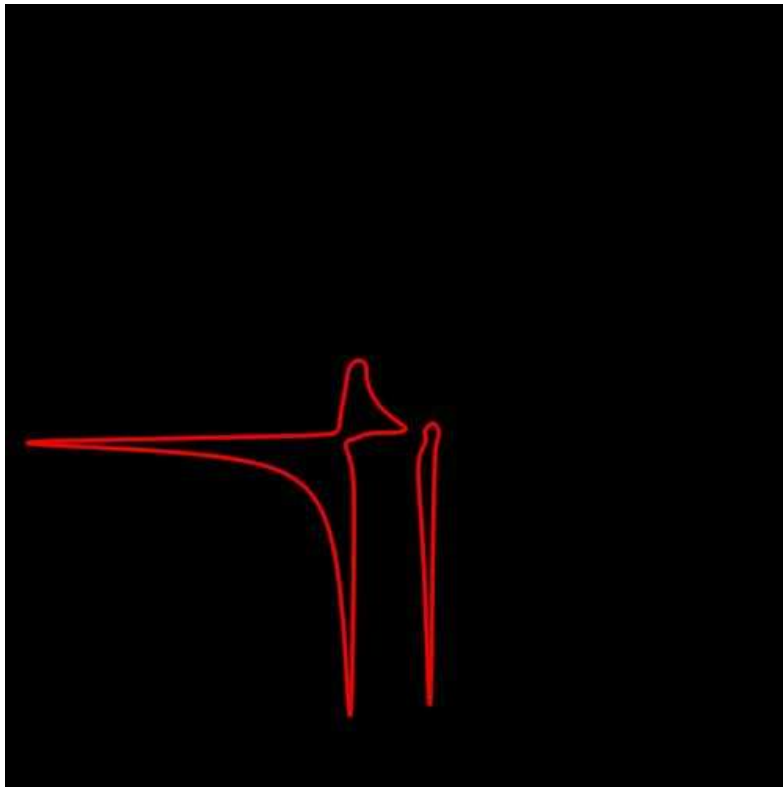
The equations describe a **curve in \mathbb{R}^5** . The **projection** to the w, x -plane is difficult to compute:

$$\begin{aligned} &13343098629642274643741505w^{20}x^{16}+18458805154059402163602552w^{20}x^{15} \\ &+12528539096440613433050772w^{19}x^{16}-307469543636682571308498792w^{20}x^{14} \\ &-308745089273555811810514188w^{19}x^{15}-335770469789305978523636514w^{18}x^{16} \end{aligned}$$

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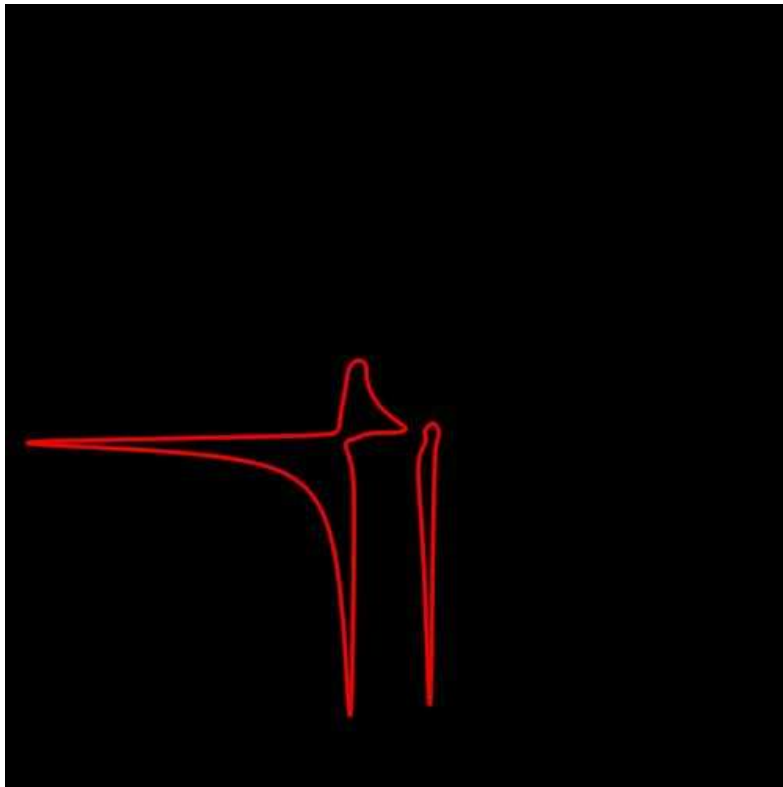
$$\begin{aligned} &-57603722394732542788396875000w^2x-56209703485755917382271875000wx^2 \\ &-29459059311819369252628125000x^3-3456386878638867977468750000w^2 \\ &-388065077492910629437500000wx-3500955605594366547468750000x^2 \\ &+1264097844032306972500000000w+1126578705265908772500000000x \\ &+240658492841196850000000000 \end{aligned}$$

Projection of the curve to the w, x -plane



```
ideal K = eliminate(I,vyz);  
LIB''surf.lib'';  
plot(K[1]);
```


Projection of the curve to the w, x -plane



```
ideal K = eliminate(I,vyz);  
LIB''surf.lib'';  
plot(K[1]);
```

The curve shows the possible w, x -coordinates of the molecule.

The sizing leads to the following system of equations:

```
ring R=(0,VCC,vLF,p,VBE1,IB1,VCE1,IC1,VBE2,IB2,VCE2,IC2,vHF),
    (V_Vin, V_C1, V_BE_Q1, V_CE_Q1, V_R1, V_R2, V_R3, V_C3, V_R4, V_R5,
    V_R6, V_R7, V_R8, V_BE_Q2, V_CE_Q2, V_C2, V_VCC, I_Vin, I_C1,
    I_BE_Q1, I_CE_Q1, I_R1, I_R2, I_R3, I_C3, I_R4, I_R5, I_R6, I_R7,
    I_R8, I_BE_Q2, I_CE_Q2, I_C2, I_VCC,
    R1,R2,R3,R4,R5,R6,R7,R8,C3),lp;

ideal I=
    V_BE_Q1 + V_C1 + V_R1 - V_Vin,
    V_C3 - V_R2 + V_R3,
    -V_CE_Q1 - V_R2 - V_R4 + V_R5,
    V_C1 - V_R7 + V_R8 - V_Vin,
    V_BE_Q1 + V_BE_Q2 - V_CE_Q1 + V_R6 + V_R7,
    V_BE_Q1 + V_CE_Q2 + V_R2 + V_R6 + V_R7,
    V_C1 + V_C2 - V_R6 - V_R7 - V_Vin,
    .
    .
    .
    -R2 + R1*vLF,
    -R2*R3 + R1*(R2 + R3)*vHF,1 + C3*p*(R2 + R3),
    -VCC + 3*V_R5,R6 - R8;
```

Elimination of variables: The resistors R_1, \dots, R_8 and the capacities C_3 in terms of currents and voltages:.

```
option(redSB);
ideal J=std(I);
J=J[1..9];
simplify(J,1);
==>
_[1]=C3+(3*vLF*IB1+3*vLF*IC1-3*IB1*vHF-3*IC1*vHF)/(2*VCC*vLF^2*p-
3*vLF^2*p*VCE1+3*vLF^2*p*VBE2-3*vLF^2*p*VCE2-3*vLF*p*VCE1+3*vLF*p*VBE2-
3*vLF*p*VCE2)
.
.
.
_[6]=R4+(-VCC+3*VBE2-3*VCE2)/(3*IC1+3*IB2)
.
.
R6 = -(2*VCC-3*VCE2)/(3*IB1-6*IB2-6*IC2).
```

$$\mathcal{D} = K[\partial_1, \dots, \partial_n] \quad R \in \mathcal{D}^{g \times q} \quad \mathcal{A} = \mathcal{C}^\infty(\mathbb{R}^n, K)$$

$$\mathcal{B} = \text{Ker}(R) = \{\omega \in \mathcal{A}^q \mid R\omega = 0\}$$

$$\mathcal{D} = K[\partial_1, \dots, \partial_n] \quad R \in \mathcal{D}^{g \times q} \quad \mathcal{A} = \mathcal{C}^\infty(\mathbb{R}^n, K)$$

$$\mathcal{B} = \text{Ker}(R) = \{\omega \in \mathcal{A}^q \mid R\omega = 0\}$$

$$\mathcal{B} \text{ controllable} \iff \mathcal{B} = \text{im}(M) \text{ for some } M \in \mathcal{D}^{q \times l}$$

$$\text{system module } \mathcal{M} = \mathcal{D}^q / \mathcal{D}^g R, \mathcal{N} = \mathcal{D}^g / R\mathcal{D}^q$$

the transposed one

$$\mathcal{B} \text{ controllable} \iff \mathcal{M} \text{ torsion free}$$
$$\iff \text{Ext}_{\mathcal{D}}^1(\mathcal{N}, \mathcal{D}) = 0$$

- Let C be a projective curve, and let $H_C(t) = d(C)t - p_a(C) + 1$ be its Hilbert polynomial, then
 - $d(C) =:$ degree of the curve C
 - $p_a(C) =:$ arithmetic genus of the curve.
- The geometric genus $g(C)$ is the arithmetic genus of the normalization C_n of C :
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- The geometric genus $g(C)$ is the arithmetic genus of the normalization C_n of C :
 - $g(C) := p_a(C_n)$
- If we are able to compute the normalization, we can compute the geometric genus. But this is very time consuming.

The procedure we implemented is based on the following knowledge:

- $p_a(C) = g(C) + \delta(C)$, where $\delta(C)$ is the sum over the local δ -invariants in the singular points.
- There exist a projection $C \longrightarrow D$ to a plane curve D with degree $d(D) = d(C)$, such that $C_n = D_n$. Then
 - $g(C) = p_a(C_n) = p_a(D_n) = g(D)$.
 - Almost every projection has this property.

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 - $g(C) = p_a(C_n) = p_a(D_n) = g(D)$.
 - Almost every projection has this property.
- Let C be a plane projective curve. We compute the geometric genus by a local analysis of the singularities.

Assume the plane curve C is defined by $f=0$.

We know:

- the ideal $Sing(f) := \langle f, f_x, f_y \rangle$ defines the singular locus
- the ideal $Sing(Sing(f)) := \langle f, f_x, f_y, det(Hess(f)) \rangle$ defines the non-nodal locus
- the ideal $S := Sing(Sing(Sing(f)))$ defines the non-nodal-cuspidal locus
- $\delta(C, x) = 1$ in nodal or cuspidal singularities, so we just have to count them.

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- $\delta(C, x) = 1$ in nodal or cuspidal singularities, so we just have to count them.
- the singular points different from cusps and nodes are obtained by a **primary decomposition** of S .
- The primary decomposition is done over \mathbb{Q} . To obtain the points, we have to **extend the field**.

We know:

- $\mu(f) = \dim(\mathbb{C}[[x, y]] / \langle f_x, f_y \rangle) = 2\delta - \text{number of branches} + 1,$
- To compute the number of (local) branches, we proceed as follows:
 - Test for A_k - and D_k -singularities.
 - Compute the Newton Polygon.
 - If the Newton Polygon is non-degenerate, then the number of branches can be computed combinatorially from the faces.
 - If the Newton Polygon is degenerate and has more than one face, then f can be splitted (modulo analytic equivalence) into a product.
 - If the Newton Polygon is degenerate and has only one face, then we use the Puiseux expansion to compute the number of branches.

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- Needs:
 - Puiseux expansion
 - Primary decomposition
 - Field extensions
 - Newton polygon.