Current Challenges in the Development of Open Source Computer Algebra Software

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TU Kaiserslautern

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Algorithmic and Experimental Methods
in Algebra, Geometry, and Number Theory
DFG Priority Project SPP 1489

Some Basic Statements

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Created within SPP 1489

GAP

Powerful language

- General purpose yet ideally suited to algebraic computation;
- rapid implementation of mathematical algorithms;
- intelligent GAP objects and algorithms.

Example

```
gap> grp := PSL(5,3);;
gap> a:=PseudoRandom(grp);; b:=PseudoRandom(grp);;
gap> Size( Group(a,b) );
237783237120 10 msec
```

Parametrizing Rational Curves in SINGULAR

Example

```
> ring R = 0, (x,y,z), dp;
> poly f = x5+10x4y+20x3y2+130x2y3-20xy4+20y5-2x4z-40x3yz-150x2y2z
           -90xy3z-40y4z+x3z2+30x2yz2+110xy2z2+20y3z2;
> LIB "paraplanecurves.lib";
> genus(f); // may require blow-ups
  0
> paraPlaneCurve(f); // requires normalization, integral bases
```

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Remark

Basic workhorse: Buchberger's algorithm for computing Gröbner bases and syzygies.

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```

Remark

Basic workhorse: Buchberger's algorithm for computing Gröbner bases and syzygies.

May require to work over quadratic field extension.

Example

Parametrizing Rational Curves in SINGULAR

Example

We consider the degree-5 curve with equation

$$x^5 + 10x^4y + 20x^3y^2 + 130x^2y^3 - 20xy^4 + 20y^5 - 2x^4z$$
$$- 40x^3yz - 150x^2y^2z - 90xy^3z - 40y^4z + x^3z^2 + 30x^2yz^2$$
$$+ 110xy^2z^2 + 20y^3z^2 = 0.$$

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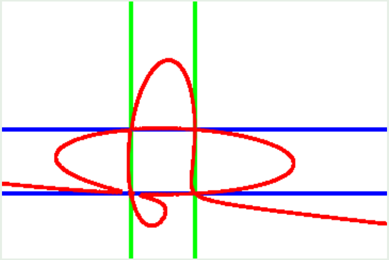

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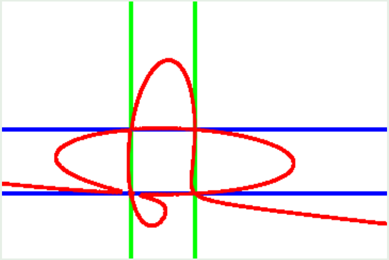

Genus Formula. $p_g(C) = p_a(C) - \delta(C) = p_a(C) - \sum_{P \in \mathrm{Sing}(\Gamma)} \delta_P(C)$

Some Basic Statements

- A decisive feature of current developments is that more and more of the abstract mathematical concepts are made constructive, with interdisciplinary methods playing a significant role.

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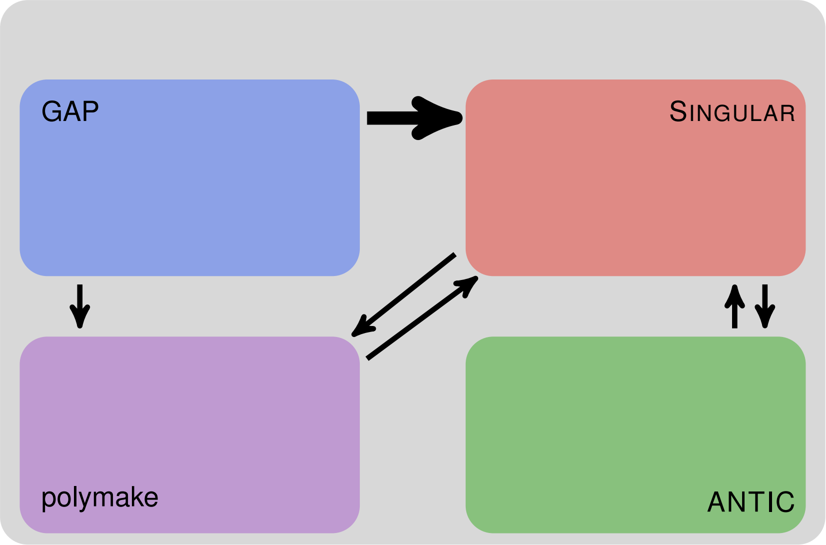
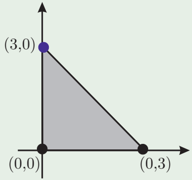
Interfaces created within SPP 1489

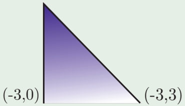


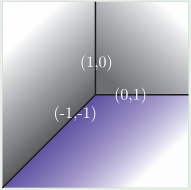
Example: Using POLYMAKE IN SINGULAR

Example

```
> LIB "polymake.so";
   Welcome to polymake
   Copyright (c) 1997-2012
   Ewgenij Gawrilow, Michael Joswig (TU Darmstadt)
   http://www.polymake.org
   // ** loaded polymake.so
> ring r = 0,(x,y),dp; poly g = x3+y3+1;
> polytope p = newtonPolytope(g);
> fan F = normalFan(p); F;
RAYS:
-1 -1 #0
 0  1 #1
 1  0 #2
MAXIMAL_CONES:
{0 1} #Dimension 2
{0 2}
{1 2}
```







- The design and further development of successful open source computer algebra software is always driven by intended applications, irrespective of whether these applications lie within or outside of mathematics.

A First Motivating Example: Surfaces of General Type With $p_g = 0$

"Can a computer classify all surfaces of general type with $p_g = 0$?"

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Work by Castelnuovo, Enriques, Godeaux, Campedelli, Miyaoka, Reid and students, Beauville, Bauer-Catanese and students, and many more.

A First Motivating Example: Surfaces of General Type With $p_g = 0$

Example (The case $K^2 = 1$: Numerical Godeaux surfaces)

For such a surface X, it is known that $\pi_1(X)^{ab}$ is cyclic of order at most 5, and constructions have been given for each choice of order.

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Joint project with Frank-Olaf Schreyer and Isabel Stenger.

A First Motivating Example: Surfaces of General Type With $p_g = 0$

Why is this computationally hard from the very beginning?

```
> Rextension;
//   characteristic : 0
//   1 parameter    : a
//   minpoly        :
(24873879473832817299558394474990433025260537858429700*a^8
+412197480758832021377448558823165698794277118212212070*a^7
+625366891611244986389942014312773193649951168354090190*a^6
-436561073546512334083477547357856090524552855592558795*a^5
-914947642504230095779800456657440020138074539186145912*a^4
-2227325279423247966617649640155997715235288113299887954*a^3
+2312070077580715288467637707530192772778088469836344950*a^2
+1366053134215201364075122803745127996518986576734818612*a
-1156759915557562158859054495379551857229358735237021536)
//   number of vars : 12
```

- Through computer algebra systems, a large treasure of mathematical knowledge becomes accessible to and can also be applied by non-experts.

Citation Record (data from `https://zbmath.org`)

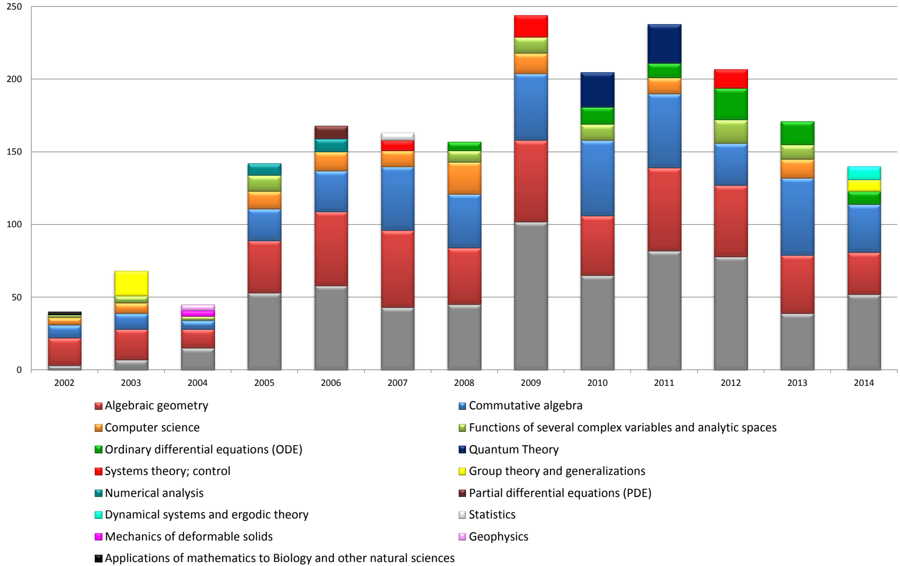
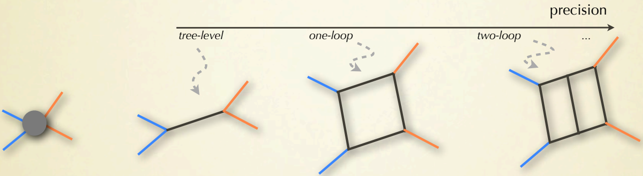
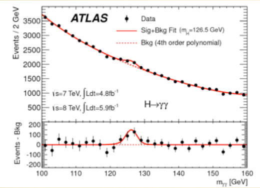
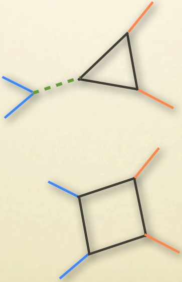


Figure: Top five MSC areas for SINGULAR per year, remaining areas in grey

Scattering ~ Feynman Diagrams







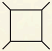
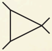
- same signature in the experiment
- only one of them contributes to the little bump
- precision calculation to distinguish them:

  signal vs background analysis

A Second Motivating Example: High Energy Physics

One-Loop Scattering Amplitudes

- n-particle Scattering: $1+2 \to 3+4+\ldots+n$
- Reduction to a Scalar-Integral Basis Passarino-Veltman

$$= \sum_{10^2-10^3} \int d^D\ell \, \frac{\ell^\mu \ell^\nu \ell^\rho \ldots}{D_1 D_2 \ldots D_n} = c_4$$  $$+ c_3$$  $$+ c_2$$  $$+ c_1$$ 

- Known: Master Integrals

 $= \int d^D\ell \, \frac{1}{D_1 D_2 D_3 D_4}$,  $= \int d^D\ell \, \frac{1}{D_1 D_2 D_3}$,  $= \int d^D\ell \, \frac{1}{D_1 D_2}$,  $= \int d^D\ell \, \frac{1}{D_1}$

- Unknowns: c_i are rational functions of external kinematic invariants

A Second Motivating Example: High Energy Physics

Example

```
> ring R = (0,p11,p12,p22,e34,m1,m2,m3), (x1,x2,x3,x4), dp;
> poly D1 = 2*x3*x4*e34+x1*(p11*x1+p12*x2)
.            +(x1*p12+p22*x2)*x2-m1;
> poly D2 = -m2+2*x3*x4*e34-2*p11*x1+p11+x1*(p11*x1+p12*x2)
.            +(x1*p12+p22*x2)*x2-2*p12*x2;
> poly D3 = 2*x3*x4*e34+2*x1*p12-m3+x1*(p11*x1+p12*x2)+p22
.            +(x1*p12+p22*x2)*x2+2*p22*x2;
> ideal I = D1, D2, D3;
> ideal GI = groebner(I);
```

Joint project with Pierpaolo Mastrolia, Tiziano Peraro, and Janko Böhm.

First Challenge: Efficiency of Fundamental Algorithms

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- normalization: algorithms of de Jong, Greuel-Laplagne-Seelisch.
- means to analyse singularities: Hamburger-Noether expansions, blow-ups, resolution of singularities, and more.

Example

- Dereje Kifle Boku, Wolfram Decker, Claus Fieker, Andreas Steenpass: *Gröbner Bases over Algebraic Number Fields.* Proceedings of the 2015 International Workshop on Parallel Symbolic Computation. PASCO 15. Bath, United Kingdom: ACM, 2015, 1624.

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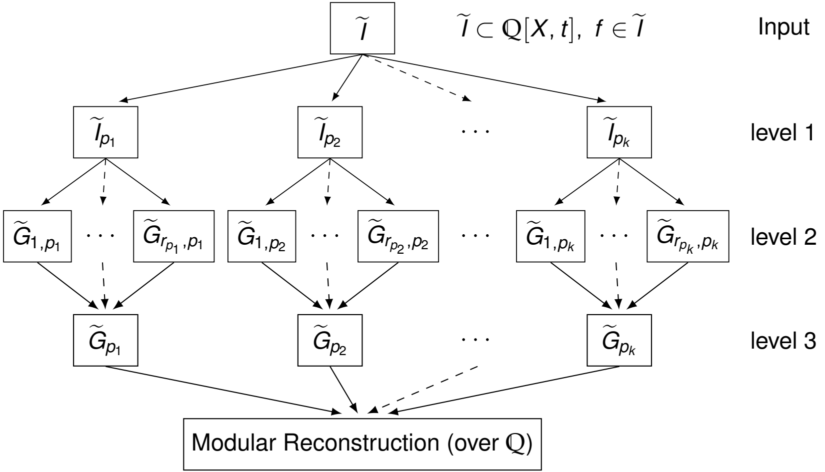
- Burcin Eröcal, Oleksandr Motsak, Frank-Olaf Schreyer, Andreas Steenpass: *Refined Algorithms to Compute Syzygies.* J. Symb. Comput. 74 (2016), 308327.

Ongoing work: Gröbner bases over rational function fields, various approaches to computing syzygies.

Example: Gröbner Bases over Number Fields



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Computer science point of view

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The latter requires, for example, to make the memory management of the CAS thread-safe in an effective way.

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Example

```
> LIB("parallel.lib","random.lib");
> ring R = 0,x(1..4),dp;
> ideal I = randomid(maxideal(3),3,100);
```

Example

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> LIB("parallel.lib","random.lib");
> ring R = 0,x(1..4),dp;
> ideal I = randomid(maxideal(3),3,100);
> proc sizeStd(ideal I, string monord){
      def R = basering; list RL = ringlist(R);
      RL[3][1][1] = monord; def S = ring(RL); setring(S);
      return(size(std(imap(R,I))));}
```

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> list commands = "sizeStd","sizeStd";
> list args = list(I,"lp"),list(I,"dp");
```

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> list commands = "sizeStd","sizeStd";
> list args = list(I,"lp"),list(I,"dp");
> parallelWaitFirst(commands, args);
  [1] empty list
  [2] 11
```

Coarse Grained Parallelism in SINGULAR by Example

Example

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> list args = list(I,"lp"),list(I,"dp");
> parallelWaitFirst(commands, args);
  [1] empty list
  [2] 11
> parallelWaitAll(commands, args);
  [1] 55
  [2] 11
```

Second Challenge: Parallelization

Mathematical point of view

- There are many algorithms whose basic strategy is sequential in nature. The systematic design of parallel algorithms in areas where no such algorithms exist is a tremendous task. For computations over the rationals, it is important to identify algorithms which allow parallelization via modular methods. Here, mathematical ideas are needed to design the final verification steps.

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- A prominent example of an approach which is inherently parallel is Villamayor's constructive version of Hironaka's desingularization theorem.

Example: Resolution of Singularities

Theorem (Hironaka, 1964)

For every algebraic variety over a field K with $\operatorname{char} K = 0$ *a desingularization can be obtained by a finite sequence of blow-ups along smooth centers.*

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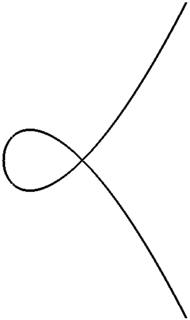
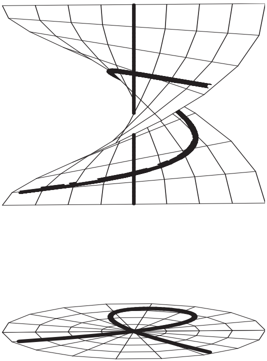
For example, resolve the

node



by one blow-up



which replaces the singular point inside the plane by a line, hence separating the two branches of the curve intersecting in the singularity.

Example: Resolution of Singularities

Working with blow-ups means to work with different charts.

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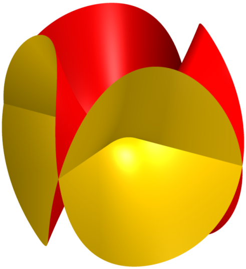

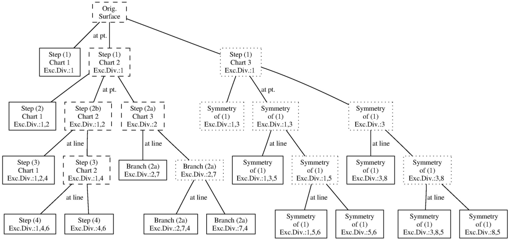

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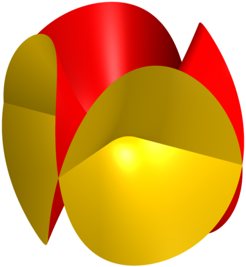

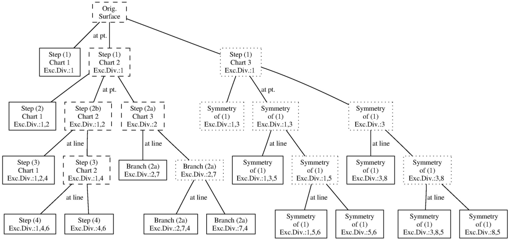

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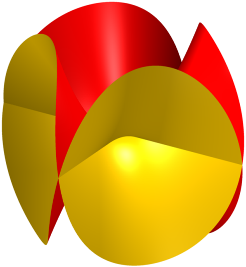

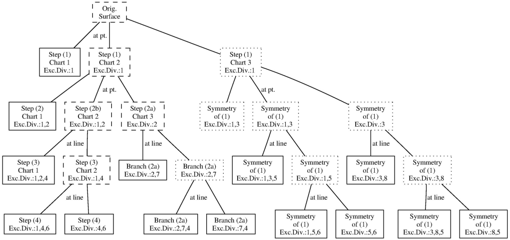

The implementation of a massively parallel general framework for Hironaka-type resolution algorithms may help to find evidence on the resolution of singularities in characteristic p. Use the GPI-Space framework by Fraunhofer ITWM at Kaiserslautern.

Third Challenge: Make More and More of the Abstract Concepts of Pure Mathematics Constructive

Example: Cohomology

Typical applications of Gröbner Bases and Syzygies in the non-commutative case:

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Use the Weyl algebra to compute the de Rham cohomology of complements of affine varieties. Algorithm by Uli Walther, implemented by Cornelia Rottner in SINGULAR.

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Example (Sheaf cohomology)

Use the exterior algebra to compute the cohomology of coherent sheaves on projective space via the constructive version of the Bernstein-Gel'fand-Gel'fand (BGG) correspondence by Eisenbud-Fløystad-Schreyer.

Notation

Let V be a vector space of dimension $n+1$ over a field K with dual space $W = V^*$, and with fixed dual bases $e_0, \ldots, e_n$ and $x_0, \ldots, x_n$.

The BGG Correspondence

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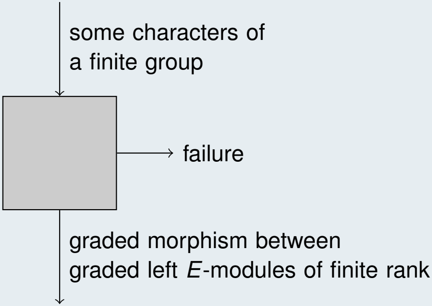
The BGG correspondence relates bounded complexes of coherent sheaves on $\mathbb{P}^n$ and minimal doubly infinite free resolutions over E. In particular, it associates to each finitely generated graded S-module M a so-called *Tate resolution* which only depends on the sheafification $\widetilde{M}$ and which “reflects” the cohomology of $\widetilde{M}$ and all its twists.

A `homalg` Example: From Groups to Vector Bundles

A homalg Example: From Groups to Vector Bundles

Mohamed Barakat’s dream to construct low rank vecor bundles on projective space using homalg



A homalg Example: From Groups to Vector Bundles

```
gap> LoadPackage( "repsn" );;
gap> LoadPackage( "GradedModules" );;
gap> G := SmallGroup( 1000, 93 );
<pc group of size 1000 with 6 generators>
gap> Display( StructureDescription( G ) );
((C5 x C5) : C5) : Q8

gap> V := Irr( G )[6];; Degree( V );
5
gap> T0 := Irr( G )[5];; Degree( T0 );
2
gap> T1 := Irr( G )[8];; Degree( T1 );
5
gap> mu0 := ConstructTateMap( V, T0, T1, 2 );
<A homomorphism of graded left modules>
```

A homalg Example:: From groups to Vector Bundles

```
gap> A := HomalgRing( mu0 );
Q{e0,e1,e2,e3,e4}
(weights: [ -1, -1, -1, -1, -1 ])
gap> M:=GuessModuleOfGlobalSectionsFromATateMap(2, mu0);;
gap> ByASmallerPresentation( M );
<A graded non-zero module presented by 92
  relations for 19 generators>

gap> S := HomalgRing( M );
Q[x0,x1,x2,x3,x4]
(weights: [ 1, 1, 1, 1, 1 ])
gap> ChernPolynomial( M );
( 2 | 1-h+4*h^2 ) -> P^4
gap> tate := TateResolution( M, -5, 5 );;
```

```
gap> Display( BettiTable( tate ) );
total:   100  37  14  10   5   2   5  10  14  37 100   ?   ?   ?   ?
----------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
    4:   100  35   4   .   .   .   .   .   .   .   .   0   0   0   0
    3:     *   .   2  10  10   5   .   .   .   .   .   .   0   0   0
    2:     *   *   .   .   .   .   .   2   .   .   .   .   .   0   0
    1:     *   *   *   .   .   .   .   .   .   5  10  10   2   .   0
    0:     *   *   *   *   .   .   .   .   .   .   .   .   4  35 100
----------|---|---|---|---|---|---|---|---|---|---|---|---|---|---S
twist:    -9  -8  -7  -6  -5  -4  -3  -2  -1   0   1   2   3   4   5
---------------------------------------------------------------------
Euler:   100  35   2 -10 -10  -5   0   2   0  -5 -10 -10   2  35 100
```

Third Challenge: Make More and More of the Abstract Concepts of Pure Mathematics Constructive

Exploit derived equivalences in computer algebra

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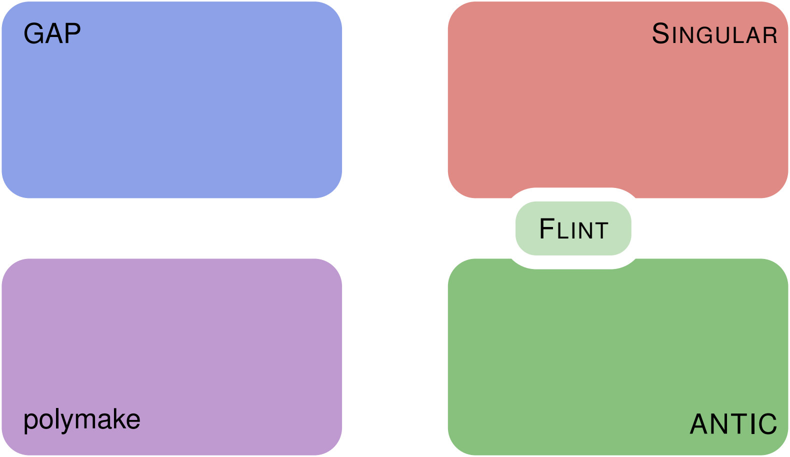
The Cornerstone Systems Rely on Packages



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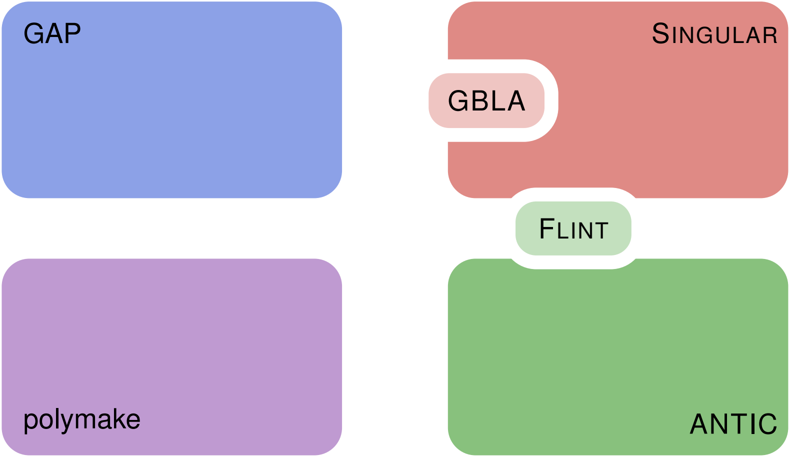

Software for Number Theory

- FLINT (Bill Hart, Fredrik Johansson, et. al.) provides specific *highly optimized* implementations in C of arithmetic with numbers, polynomials, power series and matrices over many base rings;
- ANTIC (Claus Fieker, Bill Hart, Tommy Hofmann): Fastest known library for number field arithmetic; written in a mixture of C and JULIA;

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- NEMO (Bill Hart, Tommy Hofmann, Fredrik Johansson, Oleksandr Motsak): Implementation of recursive, generic rings in JULIA;
- HECKE (Claus Fieker, Tommy Hofmann): Class groups and much more; written in JULIA.

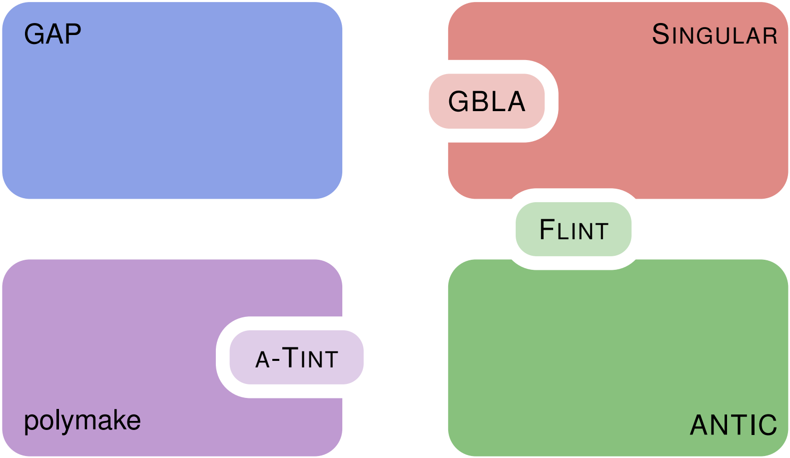
Resultant benchmark: NEMO

```
R = GF(17^11)
S = R[y]
T = S/(y^3 + 3x*y + 1)
U = T[z]
f = T(3y^2 + y + x)*z^2 + T((x + 2)*y^2 + x + 1)*z + T(4x*y + 3)
g = T(7y^2 - y + 2x + 7)*z^2 + T(3y^2 + 4x + 1)*z + T((2x + 1)*y + 1)
s = f^12
t = (s + g)^12
time r = resultant(s, t)
```

This benchmark is designed to test generics and computation of the resultant.

SageMath 6.8	Magma V2.21-4	Nemo-0.3
179907s	82s	2s

Other Packages Rely on the Cornerstones



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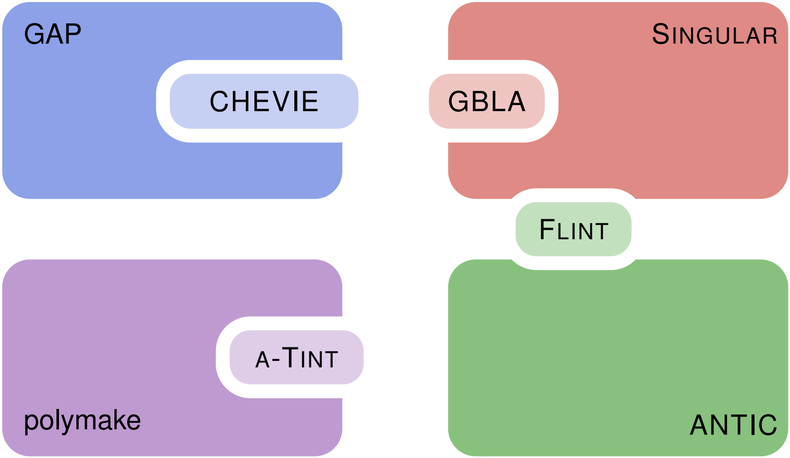

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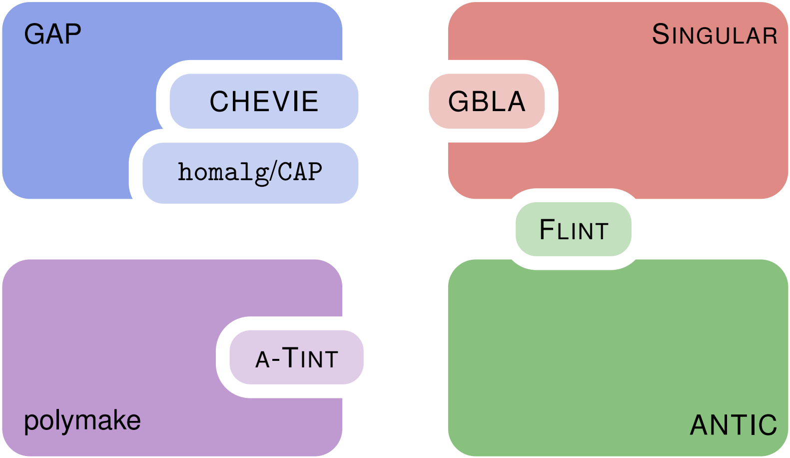

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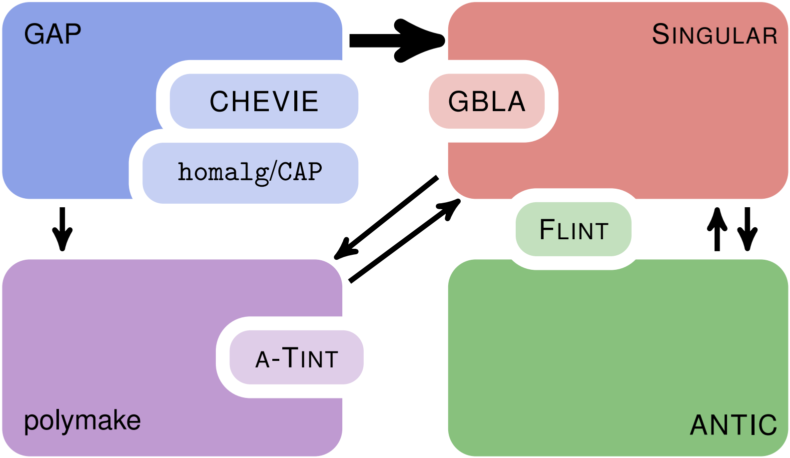
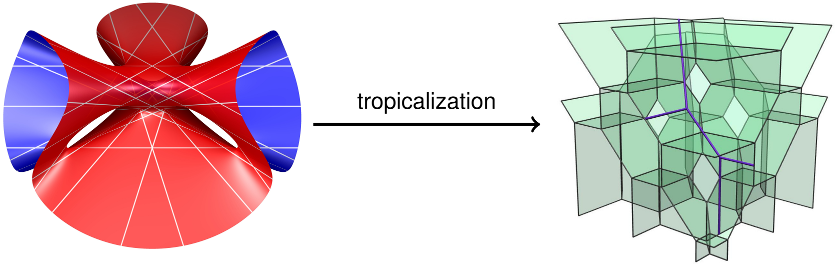


What is tropical geometry?

- Tropical geometry is a piece-vise linear version of algebraic geometry.
- Algebraic objects become discrete / polyhedral objects. Tropical varieties are polyhedral complexes.



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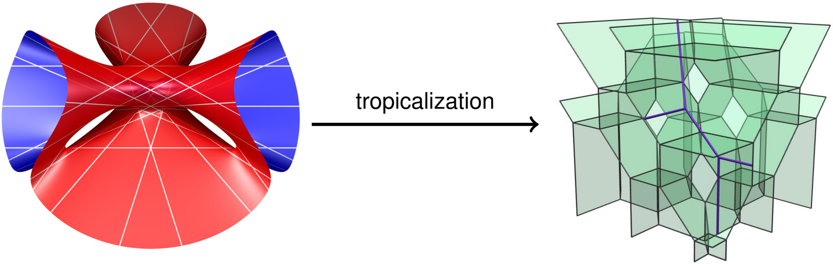
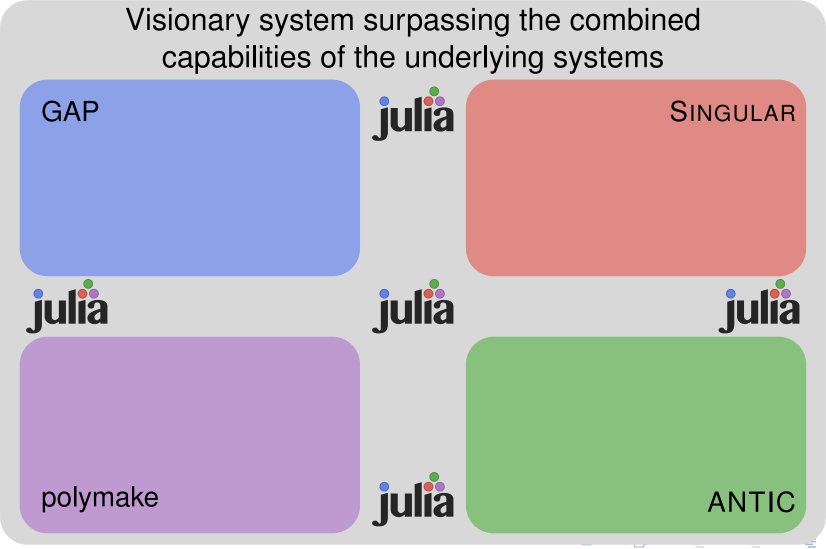


Some Software

GFAN (Anders Jensen), SINGULAR (Yue Ren, Thomas Markwig), A-TINT (Simon Hampe)

Fourth Challenge: Integration and Interaction of the Computer Algebra Systems and Libraries Involved



Fourth Challenge: Integration and Interaction of the Computer Algebra Systems and Libraries Involved

Visionary system surpassing the combined capabilities of the underlying systems

GAP

julia

SINGULAR

... we can much easier implement:

- Multigraded equivariant Cox rings of toric varieties over number fields

julia

julia

polymake

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ANTIC

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- Gröbner complexes over fields with a discrete valuation

julia

julia

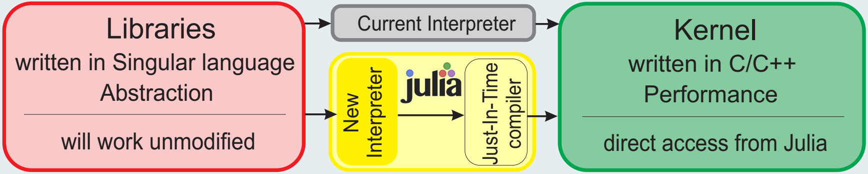
polymake

julia

ANTIC

Fifth Challenge: A Convenient Hierarchy of Languages

System design of SINGULAR



Sixth Challenge: Create and Integrate Data Bases Relevant to Research

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Developing generic concepts to make mathematical data easy to access by the mathematical community, providing both a human interface for browsing and a computer interface to feed the data directly into the computer algebra systems for further studies, is another challenge.

Seventh Challenge: Easy Access

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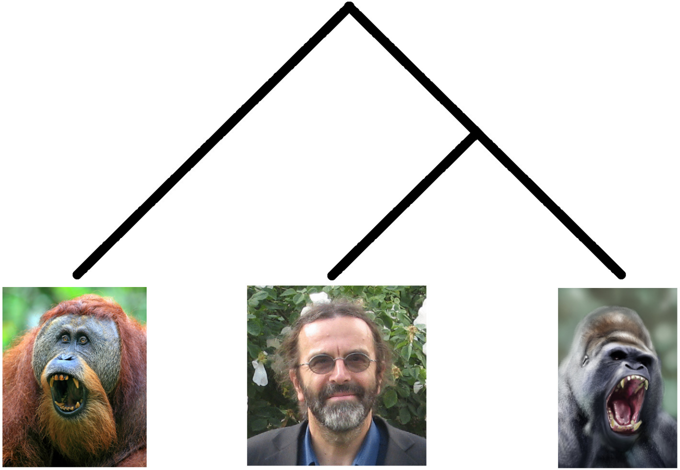
An Example From Phylogenetics

Mathematical Models of DNA Mutation



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The Horizon 2020 European Research Infrastructures project OPENDREAMKIT centers around this problem. It aims in particular at providing DOCKER images resp. creating JUPYTER notebooks for the use of the systems.

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Using DOCKER, starting GAP with connection to POLYMAKE and SINGULAR gets as easy as

```
docker run -it sppcomputeralgebra/sppdocker gap
```

Seventh Challenge: Easy Access

jupyter Demo Last Checkpoint: 4 minutes ago (autosaved)

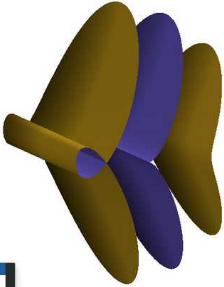
File Edit View Insert Cell Kernel Help | Singular

Code Cell Toolbar: None

```
In [5]: poly logo = ((x+3)^3 + 2*(x+3)^2 - y^2)*(x^3 - y^2)*((x-3)^3-2*(x-3)^2-y^2);

In [6]: LIB "surf_jupyter.lib";
Out[6]: // ** loaded /usr/local/bin/../share/singular/LIB/surf_jupyter.lib (0.0.0.1,Jan_2016)

In [7]: plot_jupyter(logo);
```



```
In [8]: (logo);
In [ ]: st
```

st
status
std
stdfglm
stdhilb
string