Advances in Numerical Algebraic Geometry with Applications

Charles Wampler

General Motors R&D Center

Warren, Michigan, USA

Primary Collaborators

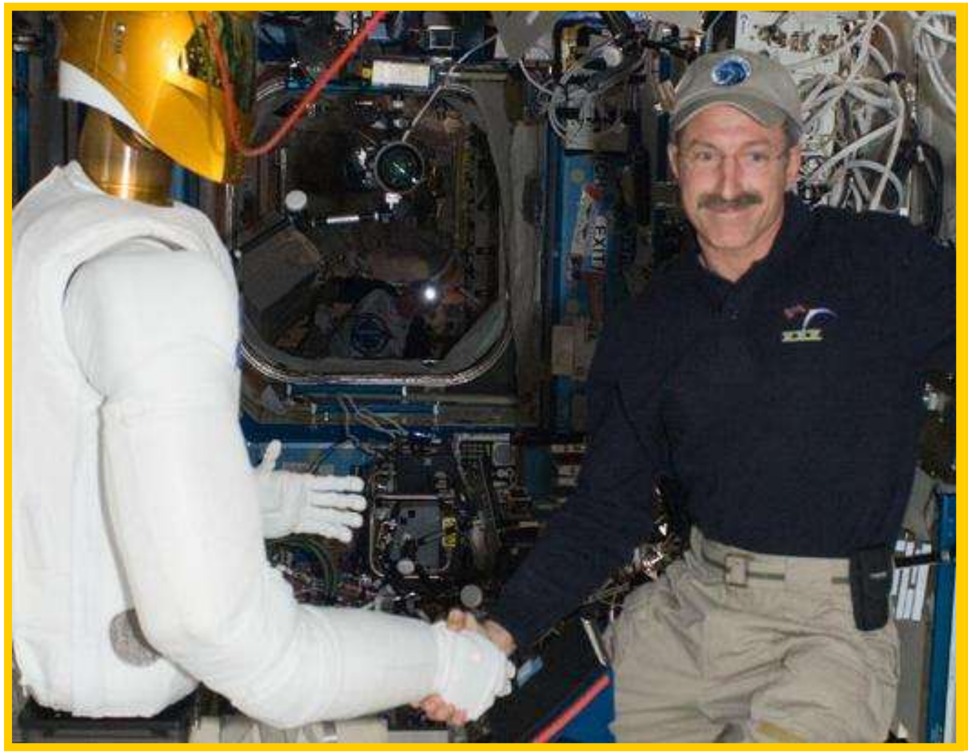
- Numerical Algebraic Geometry (including Bertini software development)
  - Andrew Sommese, Notre Dame
  - Jon Hauenstein, Notre Dame
  - Dan Bates, CSU
- BertiniReal software
  - All of the above
  - Daniel Brake, Notre Dame
  - Wenrui Hao, MBI (Ohio State)
- Applications
  - Mechanism Design: A. Murray, D. Myszka, U. Dayton
  - Sphere Packings: Miranda Holmes-Cerfon, NYU

Outline

- Motivation
- Numerical algebraic geometry
  - Background
  - Intersection of algebraic sets
  - Real algebraic sets
- Applications
  - Mechanism design
  - Sphere packings

MOTIVATION 1: KINEMATICS & ROBOTICS

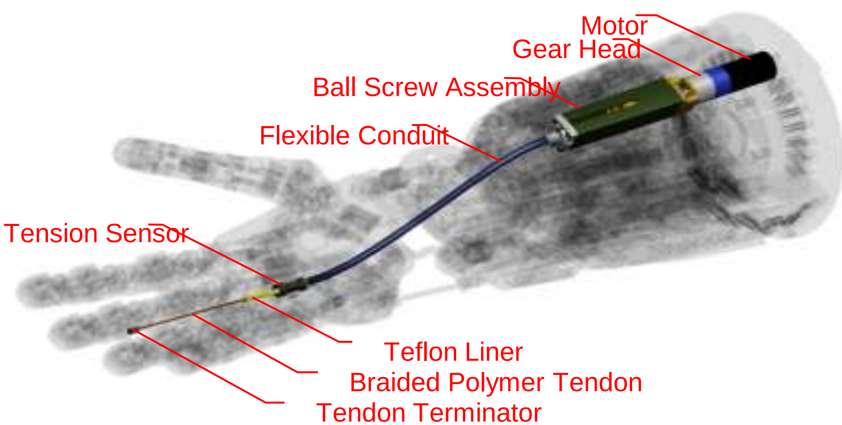
Robonaut 2 on ISS

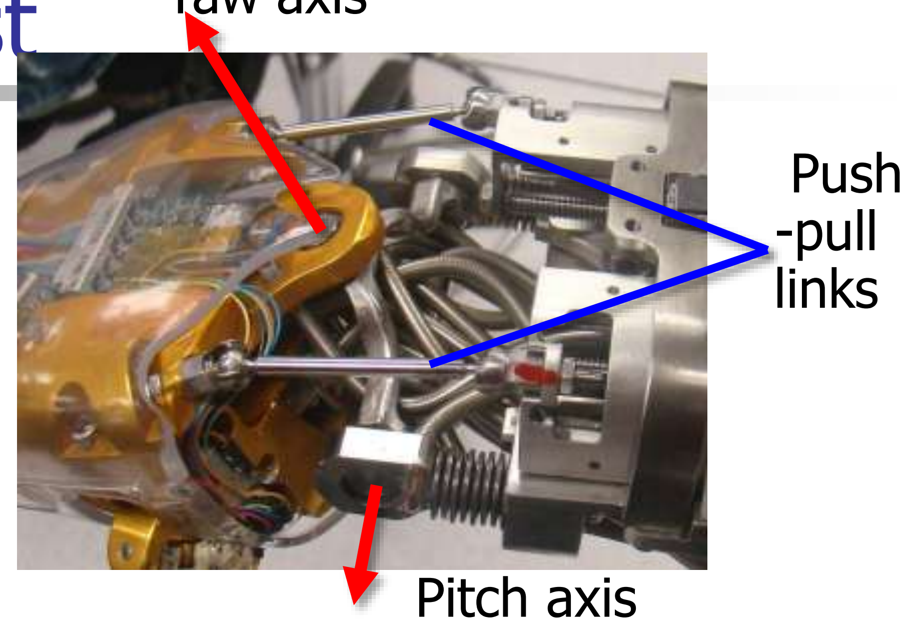


Handshake in space

Working at the task board

R2's Parallel Wrist





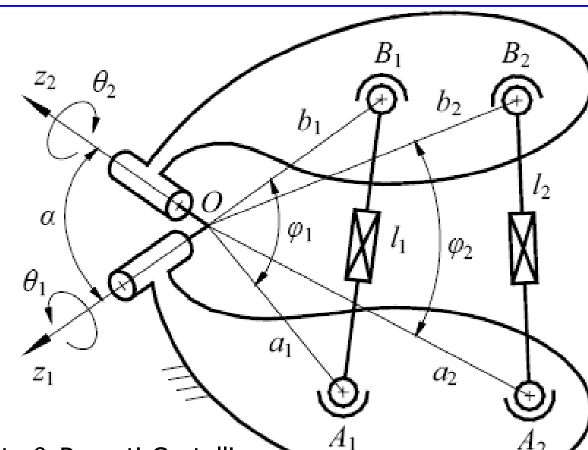
Input: sliders L_1, L_2

Output: angles θ_1, θ_2

System of polynomial equations:

$$F(L_1, L_2, s_{\theta_1}, c_{\theta_1}, s_{\theta_2}, c_{\theta_2})=0$$

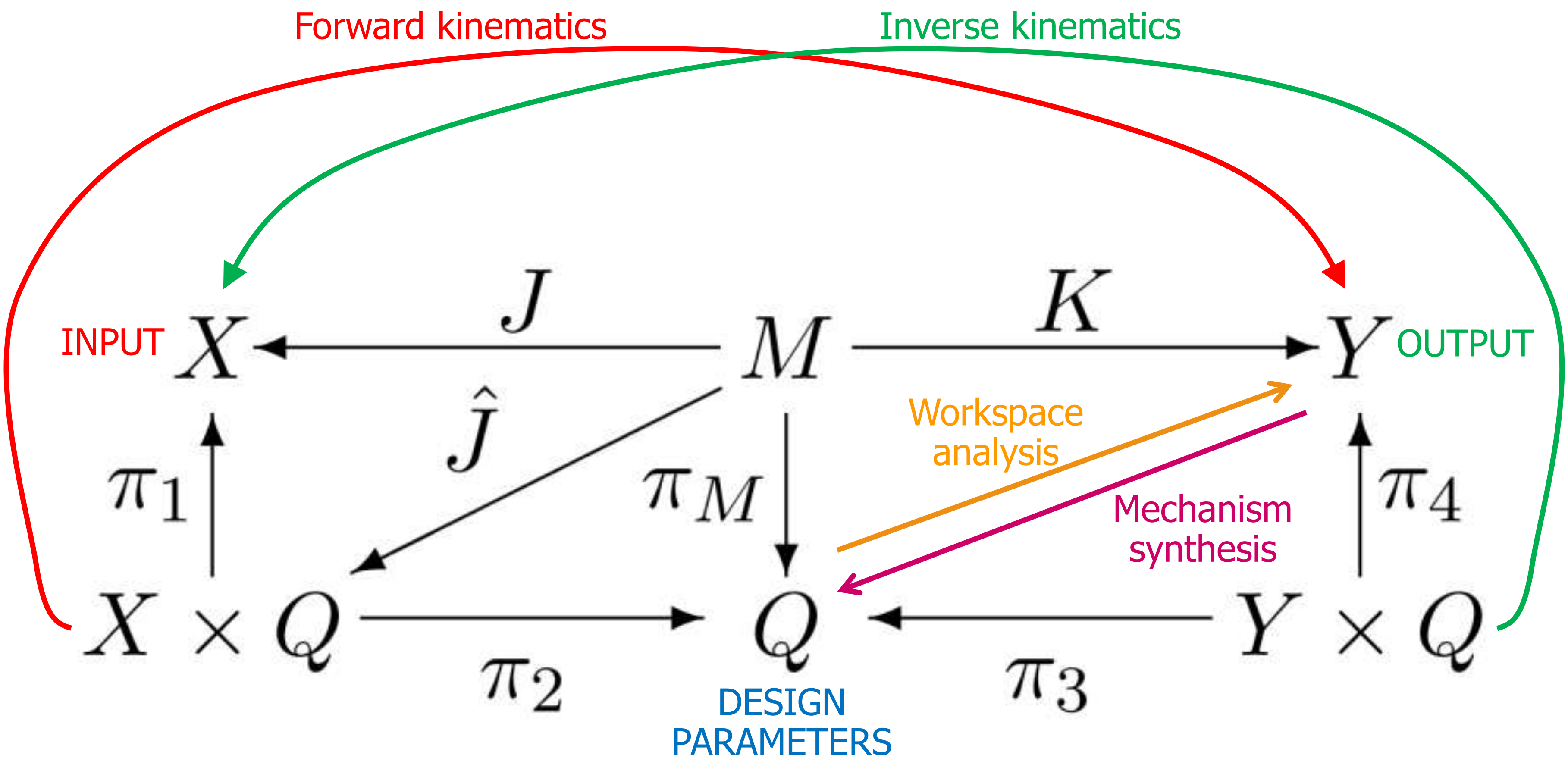
- Inverse problem: $2 \cdot 2 = 4$ solutions
- Forward problem: 8 solutions



Carricato & Parenti-Castelli
IJRR, 2004

Fig. 1. A 2-DoF fully parallel wrist ^almost^ of general geometry.

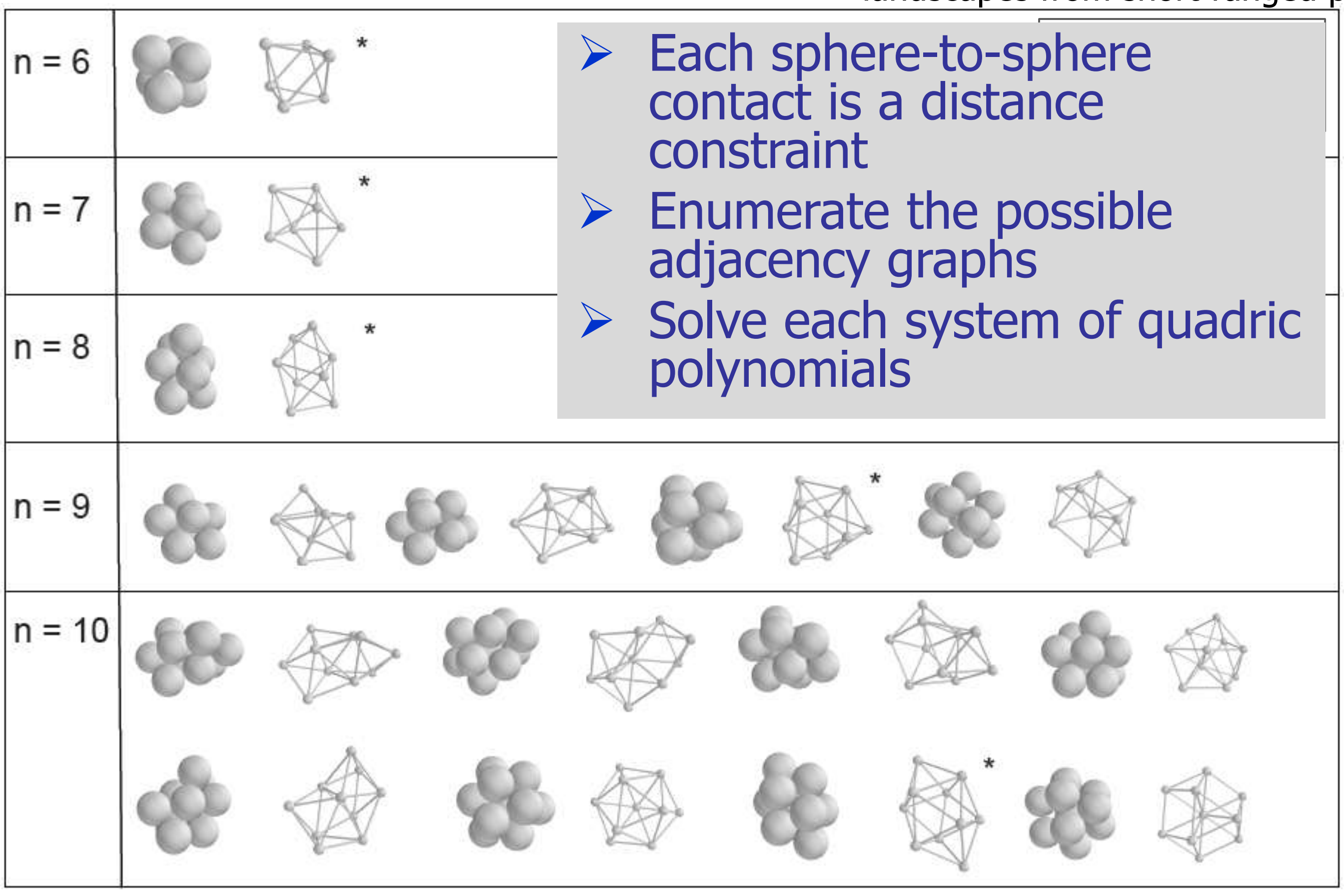
Big Picture


Forward kinematics
Inverse kinematics
INPUT
X
J
M
K
Y
OUTPUT
$\hat{J}$
π_1
π_M
Workspace analysis
Mechanism synthesis
π_4
$X \times Q$
Q
$Y \times Q$
π_2
π_3
DESIGN PARAMETERS

MOTIVATION 2: SPHERE PACKINGS

How do micro-spheres cluster?

- Arkus, Manoharan, & Brenner
  - *SIAM Discrete Math* 25(4) 2011
  - "Deriving finite sphere packings"
- Holmes-Cerfon, Gortler, & Brenner, M.P.
  - *Proc. Natl. Acad. Sci.* 110 (1) (2013)
  - "A geometrical approach to computing energy landscapes from short-ranged potentials"



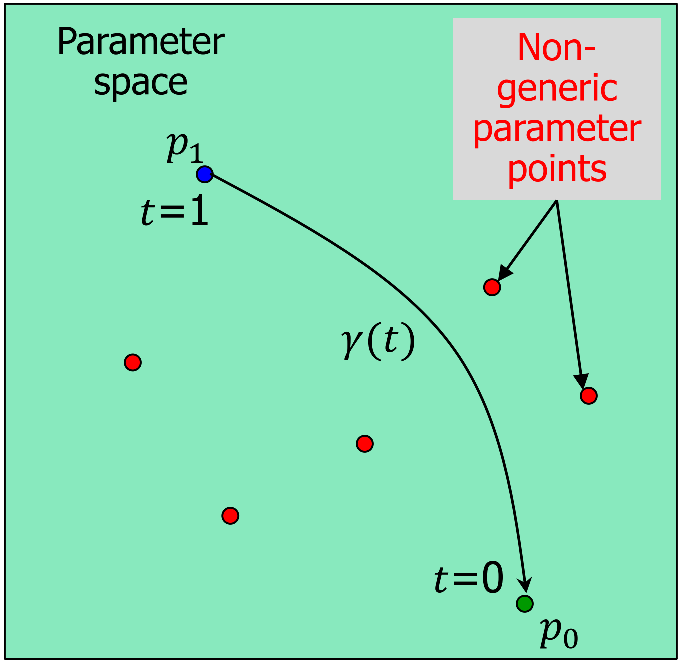
- Each sphere-to-sphere contact is a distance constraint
- Enumerate the possible adjacency graphs
- Solve each system of quadric polynomials

BACKGROUND: NUMERICAL ALGEBRAIC GEOMETRY

Homotopy Algorithms (a.k.a. Continuation)

- Problem 1:
  - Find all **isolated** solutions to a polynomial system
    $$f : \mathbb{C}^N \to \mathbb{C}^N$$
- Approach:
  - Cast $f(x)$ as a member of a parameterized family of systems, say $F(x,p)$, with $F(x,p_0) \equiv f(x)$.
  - Solve a generic member of the family, say $F(x,p_1)$.
    - Isolated solutions are set S.
  - Establish a general continuous path $\gamma(t)$ from p_1 to p_0.
    - $\gamma(1) = p_1,\ \gamma(0) = p_0$.
  - Follow solution paths of the homotopy
    - $H(x,t) \coloneqq F\big(x, \gamma(t)\big)$

    from $x \in S$ at $t = 1$ as $t \to 0$.



Notes:

- Non-generic set is real codimension 2.
- So a randomized path is *general* for $t \in (0,1]$ with **probability 1.**
  - ➢ probability 1 algorithm
- The key is picking a family $F(x,p)$ that
  1. Has a generic p_1 at which $F(x,p_1) = 0$ is easy (enough) to solve.
  2. Has $\#(S)$ as small as possible.
- It's OK if p_0 is not generic.

Basic Total-degree Homotopy

To find all isolated solutions to the polynomial system $\{f_1,\ldots,f_N\}$:

Target system

Start sys.

$$H(x,t) = (1-t)\begin{bmatrix} f_1(x_1,\ldots,x_N) \\ \vdots \\ f_N(x_1,\ldots,x_N) \end{bmatrix} + \gamma t \begin{bmatrix} x_1^{d_1} - 1 \\ \vdots \\ x_N^{d_N} - 1 \end{bmatrix} = 0$$

$d_i = \deg(f_i)$ γ random, complex.

"Probability one" algorithm

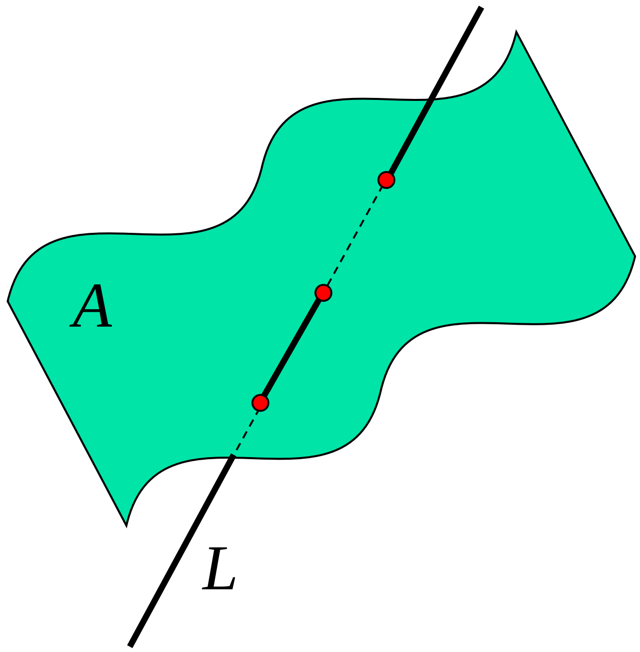
Number of paths to track = $d_1 \cdot d_2 \cdots d_N$

Positive-Dimensional Sets

- Problem 2:
  - Given: polynomial system $f:\mathbb{C}^N \to \mathbb{C}^n$
  - Find: $V(f) := \left\{ x \in \mathbb{C}^N \mid f(x) = 0 \right\}$
- What does this mean when $\dim V(f) > 0$?
  - In numerical algebraic geometry, it means we find **witness sets** for the *irreducible components* of $V(f)$.
  - Reduces Problem 2 to several instances of Problem 1.

Basic Construct: Witness Set

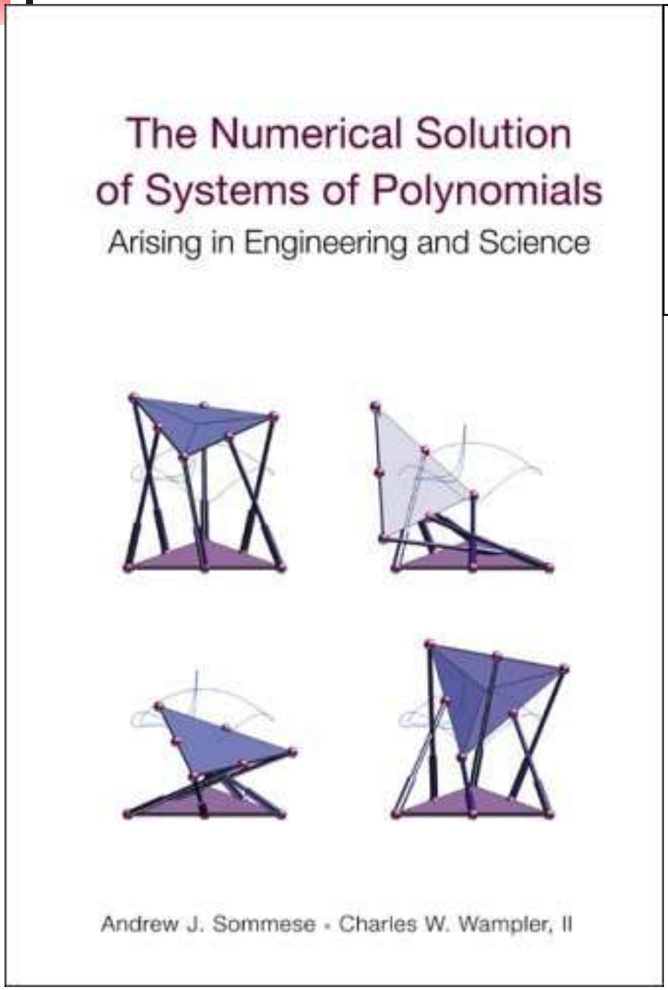
- Witness set for irreducible algebraic set A is $\{F,L,L\cap A\}$
  - F is a polynomial system such that A is an irreducible component of $V(F)$
  - L is a generic linear space of complementary dimension to A
  - $L\cap A$ is the witness point set
    - *d* points on a degree *d* component



The Bertini Package

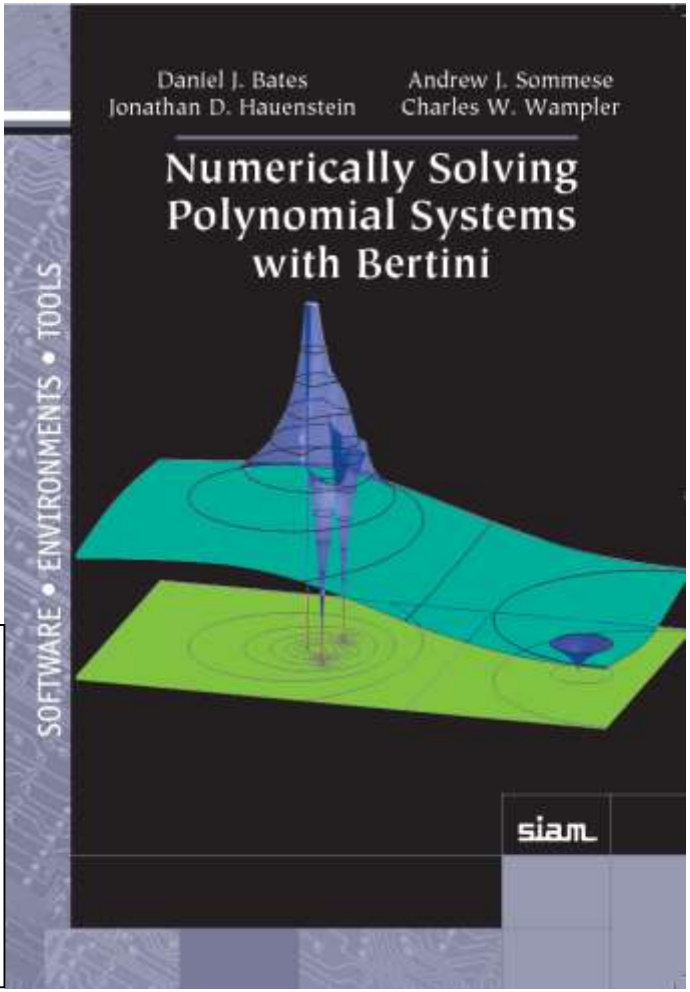
- Procedures available
  - Path tracking
    - Adaptive precision with singular endgame
  - Zero-dimensional solving
    - Multi-homogeneous & regeneration homotopies
    - User-defined & parameter homotopies
  - Positive-dimensional sets
    - Irreducible decomposition
    - Membership test
    - Intersection
- Basic data
  - Written in C, uses GMP & MPFR for multi-precision
  - Executables available for 32 & 64 bit Linux & Windows via Cygwin
  - Version 1.0 released April 2008, current *open-source* version is 1.4
  - Authors: Bates, Hauenstein, Sommese, & Wampler

Further Reading



Sommese & Wampler

World Scientific
2005



Bates, Hauenstein, Sommese & Wampler

SIAM
Nov.2013

COMPUTING INTERSECTIONS

Intersection $A \cap B$

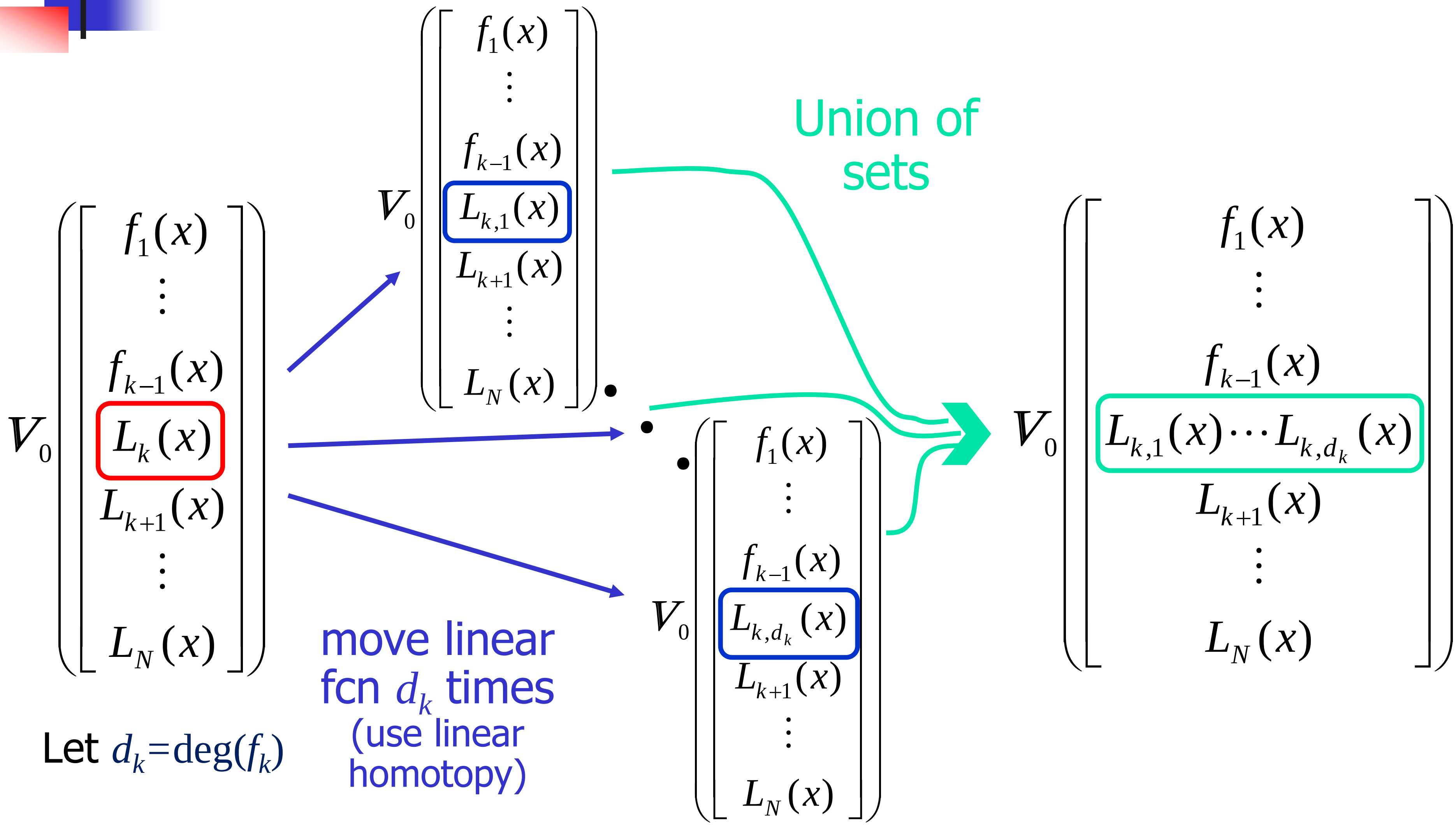
- Suppose irreducible algebraic sets A and B are given by witness sets.
  $$\{f_A, L_A, W_A\}, \{f_B, L_B, W_B\}$$
  - Although $A \cap B \subset V(f_A, f_B)$, it doesn't always suffice to compute the irreducible decomposition of $V(f_A, f_B)$
    - Counterexample is the case $f_A = f_B$
  - Even if that does suffice, it can be very wasteful.
    - Example: $V(f_A)$ can have many irreducible components besides A.
- Intersection methods target $A \cap B$ directly
  - *Diagonal homotopy* finds witness points for $(A \times B) \cap V(x - y)$, where $x \in A, y \in B$.
    - Sommese, Verschelde, W., 2004
  - *Isosingular deflation* completes the witness set when $A \cap B$ is not an irreducible component of $V(f_A, f_B)$.
    - Witness points are *generic* (w/probability 1), so the Jacobian matrix $\begin{bmatrix} Jf_A \\ Jf_B \end{bmatrix}$ evaluated at a witness point has generic rank.
    - When the rank condition is appended to the system & iterated, one obtains a system that completes the witness set.
    - Hauenstein & W., 2013
      - Proof depends on the weak deflation theorem of Leykin, Verscheld, & Zhao 2006.
  - Regeneration allows computation of $A \cap V(f)$ without first decomposing $V(f)$
    - Regeneration: Hauenstein, Sommese, & W. 2011; H&W preprint

Regeneration

- Hauenstein, Sommese, & Wampler
  - "Regeneration homotopies…", Math.Comp. 2011
  - "Regenerative cascades…", Appl.Math.Comp. 2011
- Basic step to find $V_0(f_1, \dots, f_N)$

$$V_0\left(\begin{bmatrix} f_1(x) \\ \vdots \\ f_{k-1}(x) \\ \boxed{L_k(x)} \\ L_{k+1}(x) \\ \vdots \\ L_N(x) \end{bmatrix}\right) \Rightarrow V_0\left(\begin{bmatrix} f_1(x) \\ \vdots \\ f_{k-1}(x) \\ \boxed{f_k(x)} \\ L_{k+1}(x) \\ \vdots \\ L_N(x) \end{bmatrix}\right)$$

Regeneration: Step 1



Regeneration: Step 2

$$V_0\left(\begin{bmatrix} f_1(x) \\ \vdots \\ f_{k-1}(x) \\ L_{k,1}(x)\cdots L_{k,d_k}(x) \\ L_{k+1}(x) \\ \vdots \\ L_N(x) \end{bmatrix}\right) \xrightarrow{\text{Linear homotopy}} V_0\left(\begin{bmatrix} f_1(x) \\ \vdots \\ f_{k-1}(x) \\ f_k(x) \\ L_{k+1}(x) \\ \vdots \\ L_N(x) \end{bmatrix}\right)$$

Repeat for k+1,k+2,…,N

New Method for $(A \times B) \cap V(f)$

Note: $(A \times B \times C) \cap V(f)$, etc., similar

- Generalization of the diagonal homotopy for

$$A \cap B \equiv (A \times B) \cap V(x - y)$$

  - Replaces the diagonal $V(x-y)$ with $V(f)$
  - Notes:
    - f can involve new variables
    - $(A \times B \times C) \cap V(f)$, etc., are treated similarly
    - $A \cap V(x - x_0)$ is the homotopy membership test to answer "Is $x_0 \in A$?"
- Procedure
  - Step 1: use witness sets for A, B to get a witness set for $A \times B \times \mathbb{C}^N$
  - Step 2: use the linear equations to regenerate a randomization of f equation-by-equation
  - Step 3: use isosingular deflation, as necessary, to get a witness system
  - Step 4: (optional) decompose into irreducible components.

GM

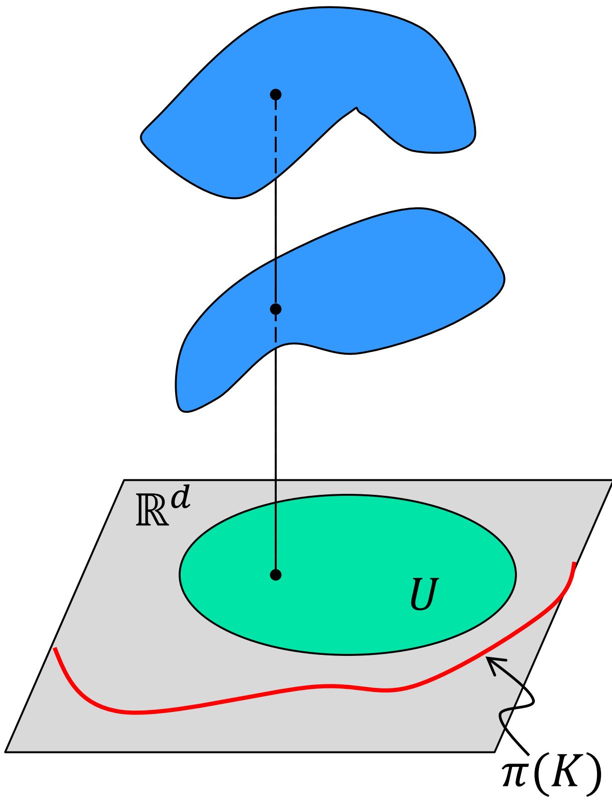
COMPUTING
REAL ALGEBRAIC SETS

Projections and Cell Decomposition

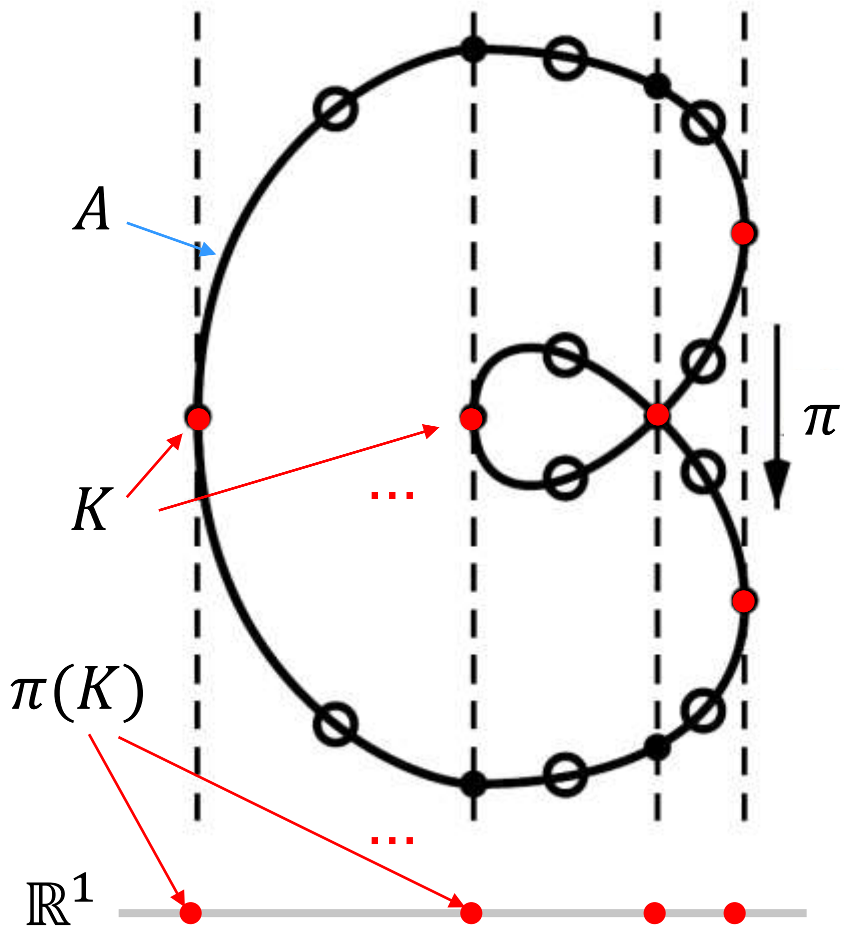
- Let $A \subset \mathbb{C}^N$ be an irreducible algebraic set of dimension d and multiplicity 1
  - If $\mathrm{mult}(A) > 1$, replace A by $\mathrm{iso}(A)$
  - Let $\{f_A, L_A, W_A\}$ be a witness set for A. We assume f_A is real.
  - We want to find $A \cap \mathbb{R}^N$
- Let $\pi: \mathbb{C}^N \to \mathbb{C}^d$ be a generic linear projection
  - For x in a Zariski-open subset of $\mathbb{C}^d$, $A \cap \pi^{-1}(x)$ consists of $\deg(A)$ isolated, nonsingular points.
- This still holds for generic $\pi: \mathbb{R}^N \to \mathbb{R}^d$
  - We have $\deg(A)$ points in $\mathbb{C}^N$, of which $\leq \deg(A)$ are in $\mathbb{R}^N$.
  - Define the *critical set* of A with respect to π as

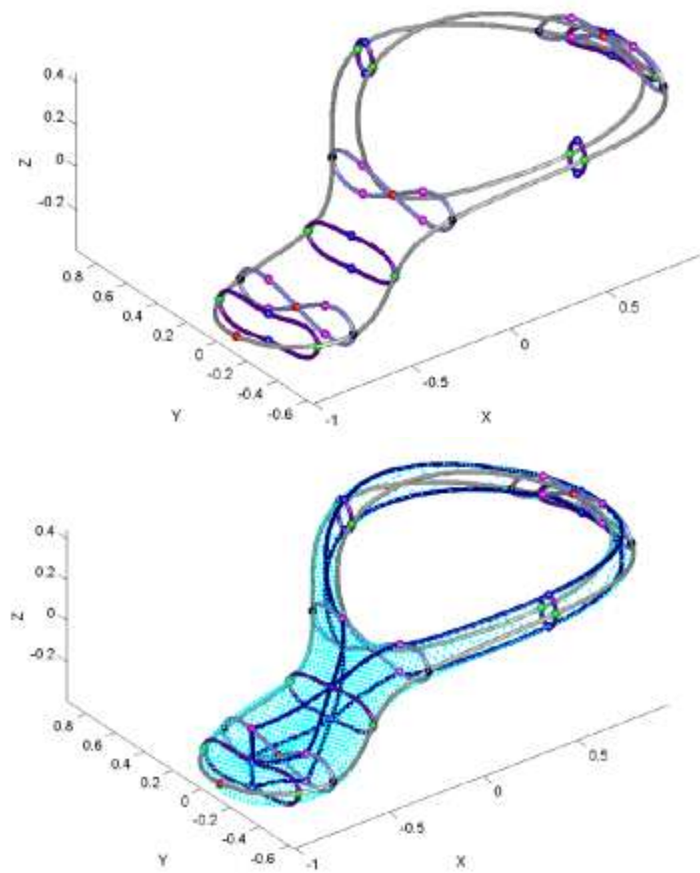
$$K \coloneqq crit_\pi(A) = A \cap V\left(\det\begin{bmatrix} Jf_A \\ J\pi \end{bmatrix}\right) \cap \mathbb{R}^N$$

  - This is a necessary condition for the real root count to change.
  - In any continuous subset $U \subset \mathbb{R}^d$ with $U \cap \pi(K) = \emptyset$, $\pi^{-1}(U) \cap A$ is a collection of nonsingular d-dimensional sheets
  - Coordinates on U define coordinate patches on A.
  - We can track paths on the sheets of A by continuation.
- To describe $A \cap \mathbb{R}^N$, it suffices to decompose $\mathbb{R}^d \setminus \pi(K)$ into cells and use continuation to determine:
  - How the real sheets meet each other, and
  - How the real sheets meet K.
  - Note: some pieces of K might have no sheets meeting them.
    - These are lower-dimensional pieces of $A \cap \mathbb{R}^N$.
    - Ex: isolated singular points, Whitney umbrella handle.



Real curves and surfaces



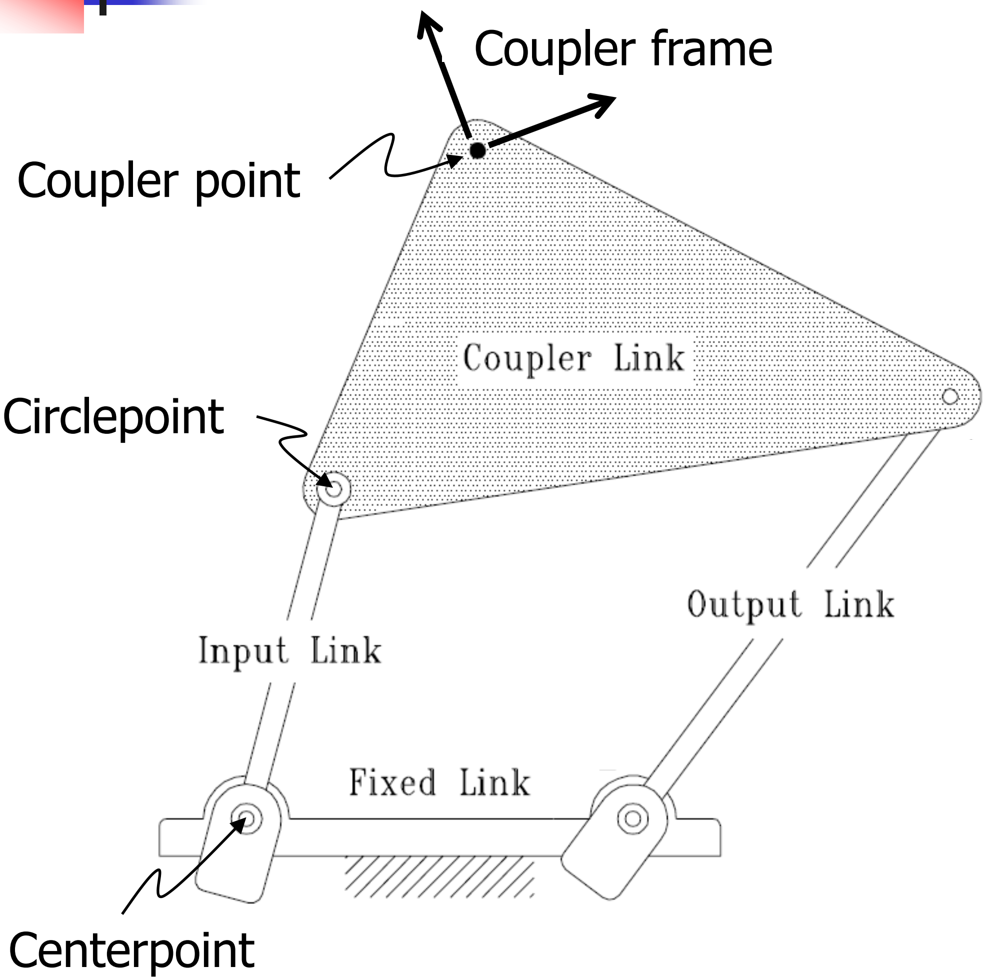


Real Cell Decomposition

- Steps
  - Find a witness set for critical set K in $\mathbb{C}^N$.
    - Use an intersection algorithm: $(A \times P^N) \cap V\left(\begin{bmatrix} Jf_A \\ J\pi \end{bmatrix} v\right)$
  - Find a real cell decomposition of K.
    - If A is a curve, then K is just a set of points.
      - The real points in K are the endpoints of the cell decomposition.
    - If A is a surface, then K is a curve, and we have to apply cell decomposition to K.
      - Computing $crit_{\pi_1}(crit_{\pi_2}(A))$ is the bottleneck
    - The situation will be even worse for 3-folds and up.
  - Use homotopies to connect all the patches.
- History
    - Curve case: Lu, Bates, Sommese, & W., 2007
    - Surface case: Besana, DiRocco, Hauenstein, Sommese, & W., 2013
      - Restricted to "almost smooth" surfaces
    - BertiniReal project: Brake, Hao, B,H,S,&W, preprint
      - Software. Curves & surfaces. No theoretical restrictions.
- Daniel Brake's talk will give more details.

APPLICATIONS

Four-Bar Design: Burmester Problems



- "Body guidance"
  - Specify precision poses for the coupler frame to attain.
  - Classic Burmester problem, 1888
- "Path generation"
  - Specify precision points for the coupler curve to interpolate
    - Orientation ignored
  - Alt's 9-point problem, 1923
- "Mixed Burmester"
  - Specify some poses and some positions
  - Tong, Murray & Myszka, 2013

Mixed Burmester family of problems

- Let m=# poses, n=# points
- Generic dimension of solution set is

$$D = 10 - 2m - n$$

# poses	# points 0	1	2	3	4	5	6	7	8
1	8	7	6	5	4	3	2	1	0
2	6	5	4	3	2	1	0		
3	4	3	2	1	0				
4	2	1	0						
5	0								

Alt's 9-point problem. Posed 1923. Solved 1992.

Burmester's problems 1888

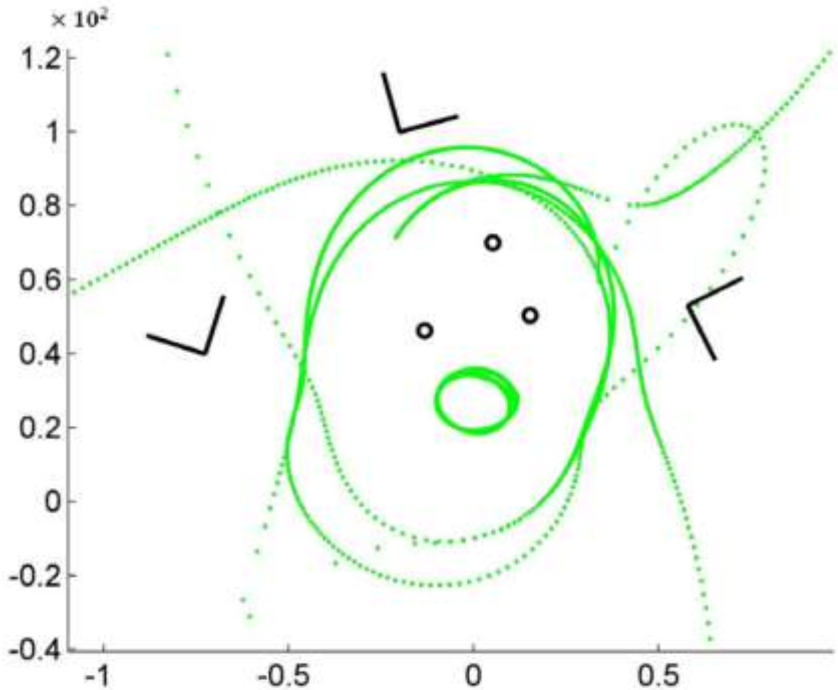
Degree of Solution Set

	# points								
# poses	0	1	2	3	4	5	6	7	8
1	1	7	43	234	1108	3832	8716	10858	8652
2	2·2=4	24	134	552	1554	2388	2224		
3	4·4=16	64	194	362	402*				
4	4·4=16	48	60*						
5	4·4=16								

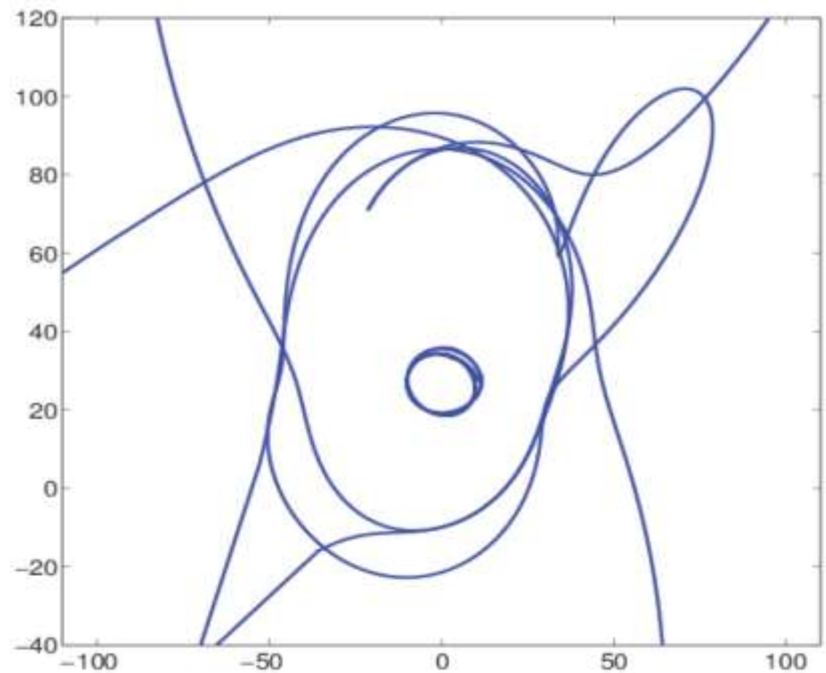
*Tong had 156 & 3116 for the 4-2 and 3-4 cases, resp., but this included degenerate singular solutions.

Case 3-3: Curve of degree 362

- Plots show centerpoint curve (a projection): degree 128
- Generic # of critical points = 1440 nonsingular + 144 singular

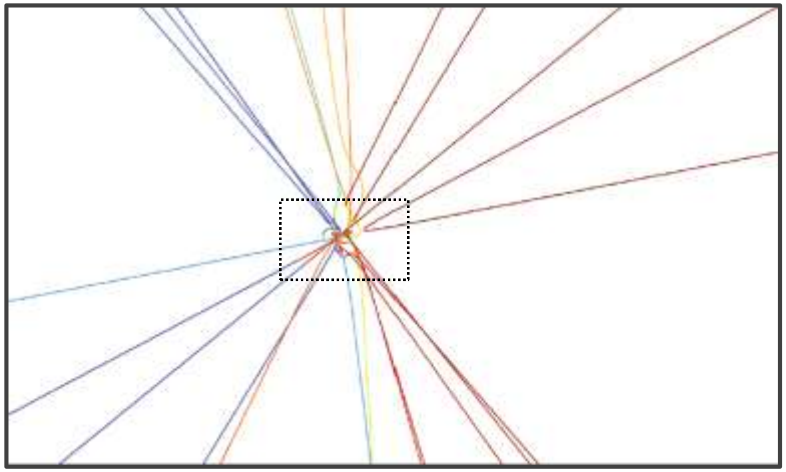


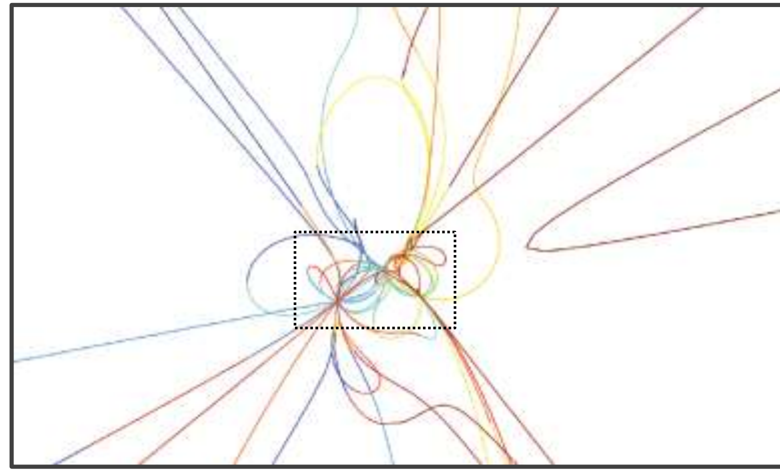
Curve as sampled by Tong, Murray, & Myszka, 2013



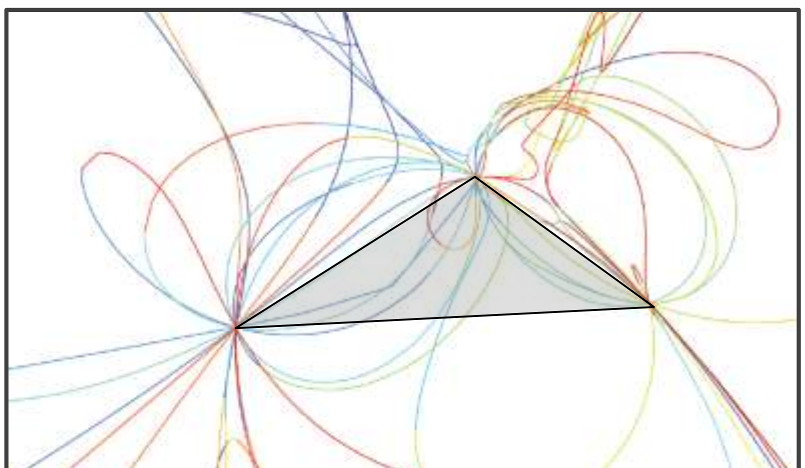
Curve as decomposed by Hauenstein, 2014

Another 3-3 Burmester curve

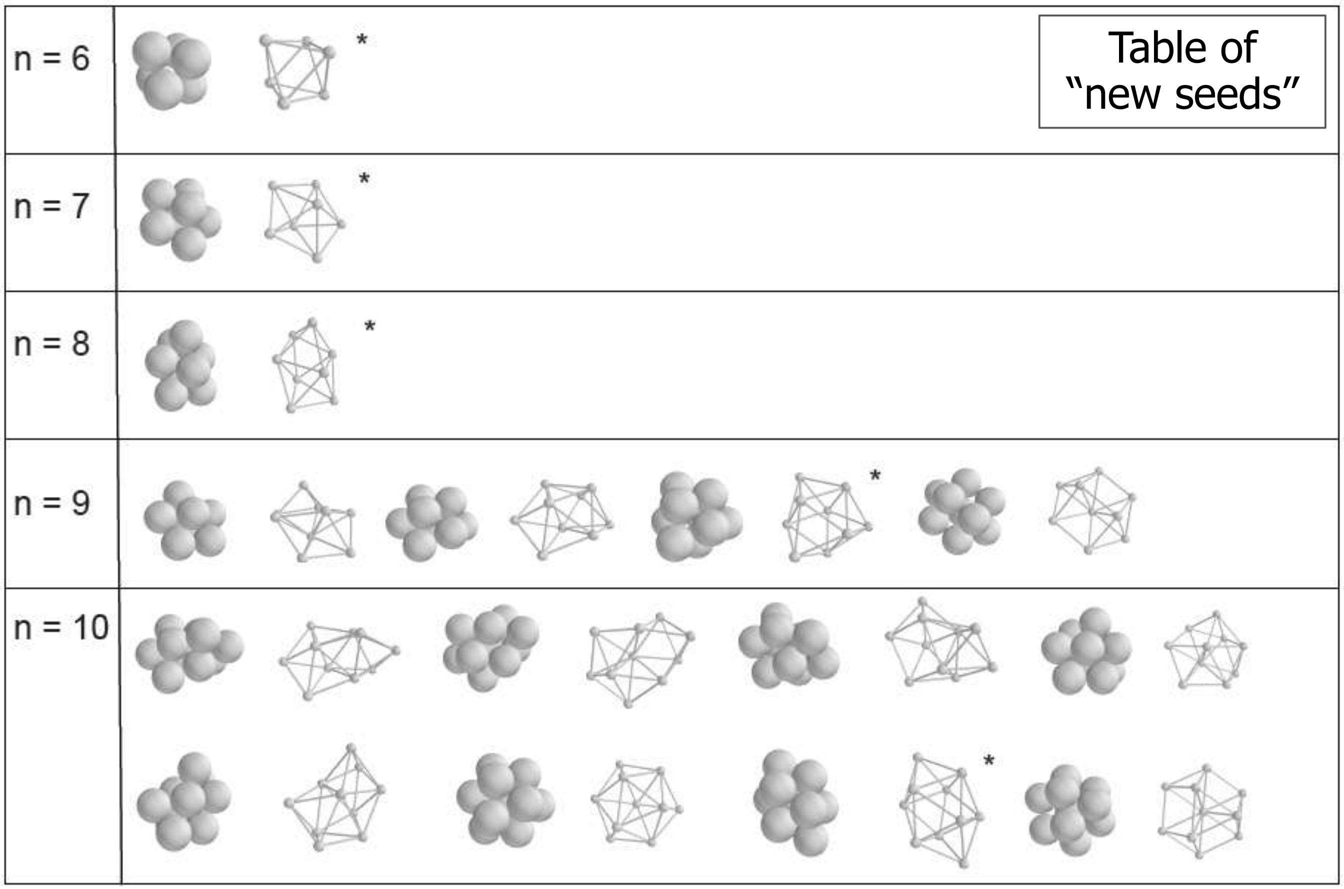




An irreducible curve of degree 362



Sphere Packings



- Arkus, Manoharan, & Brenner
  - *SIAM Discrete Math* 25(4) 2011
  - “Deriving finite sphere packings”

Sphere Packings

- Problem:
  - determine all rigid packings of N or fewer identical spheres
- Why is it interesting?
  - Models how spheres immersed in a liquid form into colloidal mixtures of particle clusters.
    - Hard spheres with short-range attraction
  - Knowing the complete list of packings allows determination of energies and predictions of cluster distribution.
  - Manoharan (Harvard) runs experiments with microspheres.
    - Uses diffraction imaging to analyze the clusters.
  - Possibility of designing colloids or micro-manufacturing desired clusters by mixing spheres with different DNA coatings
- Determining all packings of size $\leq N$:
  - Enumerate all non-isomorphic, minimally-rigid, adjacency matrices, A.
    - $A_{ij} = \{1, \text{if } S_i \text{ touches } S_j; 0, \text{else.}\}$
    - Minimally-rigid = exactly $3N - 6$ contacts for N spheres.
    - Prune by impossibility rules
      - Example: if a touches b, at most 5 spheres can touch a&b.
  - For each A, solve the system of distance equations.
    - Find all isolated real roots – not necessarily unique!
    - Cull out any with interpenetrating spheres.
    - Detect chiral pairs.

bad packing

good packing

Solving Packings

- Packings do not need to be solved from scratch
  - They can be decomposed into a series of previously solved sub-problems.
    - We call these "packing rules"
    - Each is a parameterized polynomial system
    - After solving a rule for generic parameters, subsequent appearances of the rule can be solved via *parameter continuation*.
- Packing rules can be represented by a kinematic type graph
  - Graphs composed from
    - 2 types of nodes:
      - P = point
      - R = rigid body
    - 3 types of edges:
      - c = Simple contact – points have only this kind
      - v = Shared vertex (spherical joint)
      - e = Shared edge (hinge joint)
  - Minimally rigid: $3P + 6R - c - 3v - 5e = 6$

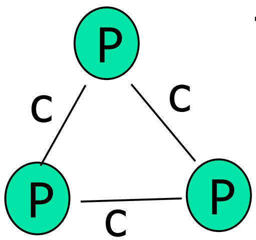
Combinatorics of packings

n	$\mathcal{A}$'s	Non-Isomorphic $\mathcal{A}$'s	Minimally rigid $\mathcal{A}$'s	Iterative $\mathcal{A}$'s	Non-Iterative $\mathcal{A}$'s
1	1	1	1	1	0
2	2	2	1	1	0
3	8	4	1	1	0
4	64	11	1	1	0
5	1,024	34	1	1	0
6	32,768	156	4	3	1
7	2,097,152	1,044	29	26	3
8	268,435,456	12,346	438	437	1
9	$6.8719 \cdot 10^{10}$	274,668	13,828	13,823	5
10	$3.5184 \cdot 10^{13}$	12,005,168	750,352	750,258	94

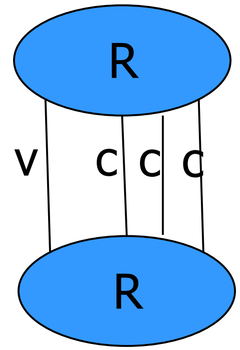
TABLE 1. **The Growth of Adjacency Matrices with n.**

- From Arkus, Manoharan, & Brenner
- Here, "Iterative" means solvable with
  - Tetrahedron rule applied to $n - 1$; or
  - Gluing rigid bodies at shared faces.
- A bigger set of rules will tamp down the combinatorial explosion

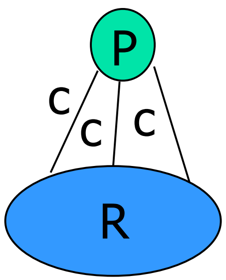
Some Packing Rules



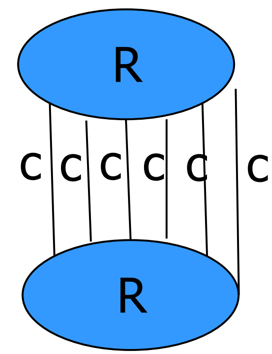
Triangle.
1 Root.

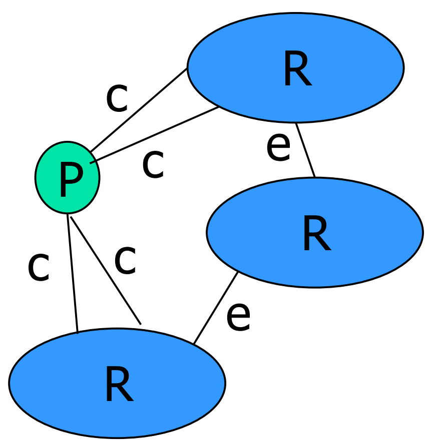


Spherical pentad.
6 Roots.



Tetrahedron.
2 Roots.





4 Revolute robot.
4 Roots.

Stewart-Gough platform.
40 Roots.

Building with rules

- Each rule gives (one or more) solutions, each a rigid packing.
- These can be a rigid body that is a subset of a bigger packing.
- The vast majority of big N packings have at least one rigid sub-packing.
- Rules can be deployed as:
  - Elimination-type solutions for easy cases
  - Parameter-continuation solutions for harder ones.
    - M. Holmes-Cerfon is using Bertini
  - 2 caveats:
    - Singular solutions occur. First is at $N = 9$.
    - Numerical error propagates, so one may need to solve the sub-problems more accurately than the final problem.
      - Use endpoint refinement algorithms.

Wrap-up

- Numerical algebraic geometry
  - Witness sets are the fundamental construct
  - Irreducible decomposition is key.
  - Software: Bertini
    - Open source, free.
- Intersection algorithms
  - Enable further investigations of sets represented by witness sets
  - Regeneration approach is the most effective at present
  - Isosingular theory enables treatment of singular cases
- Cell decomposition of real algebraic sets
  - Builds a complete topological map of the real set
  - Uses intersection and isosingular deflation
  - Limited at present to curves and surfaces
- Applications
  - Robot and mechanism kinematics lead to interesting polynomial systems
    - Mechanism design problems are especially challenging
    - Real solutions are desirable.
    - BertiniReal can decompose high degree curves from this class.
  - Sphere packing problems
    - Intersection algorithms can solve the packing rules as parameterized families
    - Deploying the rules effectively should push the envelope on # of spheres.