Parallel Homotopy Algorithms to Solve Polynomial Systems

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Interactive Parallel Computation in Support of Research in Algebra, Geometry and Number Theory MSRI, 29 January - 2 February 2007 Plan of the Talk

• introduction to homotopy algorithms

focus on approximating all isolated solutions

• scheduling path tracking jobs

close to optimal speedup possible

• larger applications can be solved

systems with > 100,000 solutions

Introduction

Polynomial Systems in Applications

What are we solving?

• polynomial systems: format of our input

the study of its solutions = algebraic geometry

• applications: relevance to science & engineering

our application field concerns mechanical design

• benchmarks: test performance of our methods

one goal is to turn applications into benchmarks

About PHCpack

PHC = Polynomial Homotopy Continuation

- Version 1.0 archived as Algorithm 795 by ACM TOMS.
- Pleasingly parallel implementations
 - + Yusong Wang of Pieri homotopies (HPSEC'04);
 - + Anton Leykin of monodromy factorization (HPSEC'05);
 - + Yan Zhuang of polyhedral homotopies (HPSEC'06).
- Some current developments, relevant to this workshop:
 + Yun Guan: PHClab, experiments with MPITB in Octave;
 + Kathy Piret: bindings with SAGE; real path trackers.

Symbolic/Numeric Solving

Consider $f(\mathbf{x}, \lambda) = \mathbf{0}$ a polynomial system in \mathbf{x} with parameter(s) λ .

numeric approach: keep f fixed, design methods to deal with singular situations, e.g.: turning and bifurcation points;

symbolic approach: keep methods fixed,

define families of systems so singular solutions are exceptional.

Typical articificial parameter homotopy:

$$h(\mathbf{x},t) = \gamma(1-t)g(\mathbf{x}) + tf(\mathbf{x}) = \mathbf{0}, \quad t \in [0,1], \quad \gamma \in \mathbb{C}.$$

Except for a finite number of bad choices for γ , all paths $\mathbf{x}(t)$ defined by $h(\mathbf{x}(t), t) = \mathbf{0}$ are regular for all $t \in [0, 1)$.

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Introduction

Product Deformations





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Introduction



Below line A: solving start systems is done automatically.

Above line A: start system has generic values for the parameters.

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Five-Point Path Synthesis

Design a 4-bar linkage = design trajectory of coupler point.

Input: coordinates of points on coupler curve.

Output: lengths of the bars of the linkage.

C.W. Wampler: Isotropic coordinates, circularity and Bezout numbers: planar kinematics from a new perspective.

Proceedings of the 1996 ASME Design Engineering Technical Conference. Irvine, CA, Aug 18–22, 1996.

A.J. Sommese and C.W. Wampler: The Numerical Solution of Systems of Polynomials Arising in Engineering and Science. World Scientific, 2005.

Isotropic Coordinates

- A point $(a, b) \in \mathbb{R}^2$ is mapped to $z = a + ib, i = \sqrt{-1}$.
- $(z, \overline{z}) = (a + ib, a ib) \in \mathbb{C}^2$ are isotropic coordinates.

• Observe
$$z \cdot \overline{z} = a^2 + b^2$$
.

- Rotation around (0,0) through angle θ is multiplication by $e^{i\theta}$. Multiply by $e^{-i\theta}$ to invert the rotation.
- Abbreviate a rotation by $\Theta = e^{i\theta}$, then its inverse $\Theta^{-1} = \overline{\Theta}$, satisfying $\Theta \overline{\Theta} = 1$.

The Loop Equations

Let $A = (a, \bar{a})$ and $B = (b, \bar{b})$ be the fixed base points.

Unknown are (x, \bar{x}) and (y, \bar{y}) , coordinates of the other two points in the 4-bar linkage.

For given precision points (p_j, \bar{p}_j) , assuming $\theta_0 = 1$,

$$\begin{cases} (p_j + x\theta_j + a)(\bar{p}_j + \bar{x}\bar{\theta}_j + \bar{a}) = (p_0 + x + a)(\bar{p}_0 + \bar{x} + \bar{a}) \\ (p_j + y\theta_j + b)(\bar{p}_j + \bar{y}\bar{\theta}_j + \bar{b}) = (p_0 + y + b)(\bar{p}_0 + \bar{y} + \bar{b}) \end{cases}$$

Since the angle θ_j corresponding to each (p_j, \bar{p}_j) is unknown, five precision points are needed to determine the linkage uniquely. Adding $\theta_j \bar{\theta}_j = 1$ to the system leads to 12 equations in 12 unknowns: $(x, \bar{x}), (y, \bar{y}), \text{ and } (\theta_j, \bar{\theta}_j), \text{ for } j = 1, 2, 3, 4.$

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theta[1]*Theta[1]-1;

theta[2]*Theta[2]-1;

theta[3]*Theta[3]-1;

theta[4]*Theta[4]-1;

-.4091256991*x*theta[1]-1.061607555*I*x*theta[1]+1.157260179-.3374636810*X+.1524877812*I*X -.3374636810*x-.1524877812*I*x-.4091256991*X*Theta[1]+1.061607555*I*X*Theta[1]; .4011300738*x*theta[2]-1.146477955*I*x*theta[2]+1.338182778-.3374636810*X+.1524877812*I*X -.3374636810*x-.1524877812*I*x+.4011300738*X*Theta[2]+1.146477955*I*X*Theta[2]; .3705985316*x*theta[3]-1.454067014*I*x*theta[3]+2.114519894-.3374636810*X+.1524877812*I*X -.3374636810*x-.1524877812*I*x+.3705985316*X*Theta[3]+1.454067014*I*X*Theta[3]; .3188425748*x*theta[4]-.850446965*I*x*theta[4]+.6877863684-.3374636810*X+.1524877812*I*X -.3374636810*x-.1524877812*I*x+.3188425748*X*Theta[4]+.850446965*I*X*Theta[4]; -1.742137552*y*theta[1]-.3932004150*I*y*theta[1]+1.524665181+.9955481716*Y+.8208949212*I*Y +.9955481716*y-.8208949212*I*y-1.742137552*Y*Theta[1]+.3932004150*I*Y*Theta[1]; -.9318817788*y*theta[2]-.4780708150*I*y*theta[2]-.5680292799+.9955481716*Y+.8208949212*I*Y +.9955481716*y-.8208949212*I*y-.9318817788*Y*Theta[2]+.4780708150*I*Y*Theta[2]; -.9624133210*y*theta[3]-.7856598740*I*y*theta[3]-.1214837957+.9955481716*Y+.8208949212*I*Y +.9955481716*y-.8208949212*I*y-.9624133210*Y*Theta[3]+.7856598740*I*Y*Theta[3]; -1.014169278*y*theta[4]-.1820398250*I*y*theta[4]-.6033068118+.9955481716*Y+.8208949212*I*Y +.9955481716*y-.8208949212*I*y-1.014169278*Y*Theta[4]+.1820398250*I*Y*Theta[4];

Output of phc -b on 5-Point Synthesis Problem

```
total degree : 4096
6-homogeneous Bezout number : 96
general linear-product Bezout number : 96
mixed volume : 36
solution 36 : start residual : 1.672E-15 #iterations : 1 success
t : 1.00000000000000E+00 0.000000000000E+00
m : 1
the solution for t :
 theta[1] : 3.04923062675137E+00 -1.36666126486689E+01
 Theta[1] : 1.55514190369546E-02 6.97012611150467E-02
 theta[2] : 1.94158500874355E-01 -1.70861689159530E+00
. . .
Y : 7.72626833143914E-01 -4.06259823401552E-01
== err : 7.607E-14 = rco : 3.915E-04 = res : 1.439E-15 = complex regu
```

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Summary of Output of phc -b

== err : 7.607E-14 = rco : 3.915E-04 = res : 1.439E-15 = complex regu Frequency tables for correction, residual, condition, and distances : FreqCorr : 0 0 0 0 0 0 0 0 0 0 0 1 8 17 0 10 : 36 FreqResi : 0 0 0 0 0 0 0 0 0 0 0 0 0 3 0 33 : 36 FreqCond : 0 10 15 9 0 2 0 0 0 0 0 0 0 0 0 0 0 : 36 FreqDist : 36 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 : 36 Small correction terms and residuals counted to the right. Well conditioned and distinct roots counted to the left.

	root	counts		start	system		continuation		total time	
	Oh Om	4s910ms		Oh Om	7s570ms		Oh Om 8s 60ms		0h 0m20s720ms	

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Parallel PHCpack

- PHCpack builds phc, user should not compile to use it.
- Most of the code in PHCpack is in Ada, compiles with gcc.
- The parallel path trackers follow manager-worker protocol.
- The main parallel program is written in C, using MPI. Also all routines which handle job scheduling are written in C.
- The C interface uses PHCpack as a state machine:
 - 1. Feed data into machine and select methods;
 - 2. Compute with given data and selected methods;
 - 3. Extract the results from the machine.

The C user is unaware of the data structures and algorithms.

Other Parallel Homotopy Solvers

T. Gunji, S. Kim, K. Fujisawa, and M. Kojima: PHoMpara – parallel implementation of the Polyhedral <u>Homotopy continuation Method for polynomial systems</u>. Computing 77(4):387–411, 2006.

H.-J. Su, J.M. McCarthy, M. Sosonkina, and L.T. Watson: Algorithm 857: POLSYS_GLP: A parallel general linear product homotopy code for solving polynomial systems of equations. ACM Trans. Math. Softw. 32(4):561–579, 2006.

Numerical Algebraic Geometry

A.J. Sommese and C.W. Wampler: The Numerical Solution of Systems of Polynomials Arising in Engineering and Science. World Scientific Press, Singapore, 2005.

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design of phc as a toolbox

Roughly, there are three stages when solving a polynomial system using polynomial homotopy continuation:



Usually stage III is most time consuming.

But if millions of start solutions, memory gets too full...

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Applying Program Inversion to Homotopy Solver

$$h(\mathbf{x},t) = \gamma(1-t)g(\mathbf{x}) + tf(\mathbf{x}) = \mathbf{0}, \quad \gamma \in \mathbb{C}, \quad t \in [0,1].$$



Applying Program Inversion to Homotopy Solver

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Jumpstarting Homotopies

Problem: huge # paths (e.g.: > 100,000),

undesirable to store all start solutions in main memory.

Solution:

(assume manager/worker protocol)

- 1. The manager reads start solution from file "just in time" whenever a worker needs another path tracking job.
- 2. For total degree and linear-product start systems, it is **simple to compute** the solutions whenever needed.
- 3. As soon as worker reports the end of a solution path back to the manager, the solution is **written to file**.

Indexing Start Solutions

The start system
$$\begin{cases} x_1^4 - 1 = 0 \\ x_2^5 - 1 = 0 \\ x_3^3 - 1 = 0 \end{cases}$$
 has $4 \times 5 \times 3 = 60$ solutions.

Get 25th solution via decomposition: $24 = 1(5 \times 3) + 3(3) + 0$. Verify via lexicographic enumeration:

 $000 \rightarrow 001 \rightarrow 002 \rightarrow 010 \rightarrow 011 \rightarrow 012 \rightarrow 020 \rightarrow 021 \rightarrow 022 \rightarrow 030 \rightarrow 031 \rightarrow 032 \rightarrow 040 \rightarrow 041 \rightarrow 042$ $100 \rightarrow 101 \rightarrow 102 \rightarrow 110 \rightarrow 111 \rightarrow 112 \rightarrow 120 \rightarrow 121 \rightarrow 122 \rightarrow \boxed{130} \rightarrow 131 \rightarrow 132 \rightarrow 140 \rightarrow 141 \rightarrow 142$ $200 \rightarrow 201 \rightarrow 202 \rightarrow 210 \rightarrow 211 \rightarrow 212 \rightarrow 220 \rightarrow 221 \rightarrow 222 \rightarrow 230 \rightarrow 231 \rightarrow 232 \rightarrow 240 \rightarrow 241 \rightarrow 242$ $300 \rightarrow 301 \rightarrow 302 \rightarrow 310 \rightarrow 311 \rightarrow 312 \rightarrow 320 \rightarrow 321 \rightarrow 322 \rightarrow 330 \rightarrow 331 \rightarrow 332 \rightarrow 340 \rightarrow 341 \rightarrow 342$

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a problem from electromagnetics

- posed by Shigetoshi Katsura to PoSSo in 1994: a family of n - 1 quadrics and one linear equation; #solutions is 2^{n-1} (= Bézout bound).
- n = 21: **32 hours and 44 minutes** to track 2^{20} paths by 13 workers at 2.4Ghz, producing output file of 1.3Gb.

tracking about 546 paths/minute.

verification of output:

- 1. parsing 1.3Gb file into memory takes 400Mb and 4 minutes;
- 2. data compression to quadtree of 58Mb takes 7 seconds.

Using Linear-Product Start Systems Efficiently

• Store start systems in their linear-product product form, e.g.:

$$g(\mathbf{x}) = \begin{cases} (x_1 + c_{11}) \times (x_2 + c_{12}x_3 + c_{13}) \times (x_2 + c_{14}x_3 + c_{15}) = 0\\ (x_2 + c_{21}) \times (x_1 + c_{22}x_3 + c_{23}) \times (x_1 + c_{24}x_3 + c_{25}) = 0\\ (x_3 + c_{31}) \times (x_1 + c_{32}x_2 + c_{33}) \times (x_1 + c_{34}x_2 + c_{35}) = 0 \end{cases}$$

- Lexicographic enumeration of start solutions,
 → as many candidates as the total degree.
- Store results of incremental LU factorization.
 - \rightarrow prune in the tree of combinations.

Nine-Point Path Synthesis

H. Alt: Über die Erzeugung gegebener Kurven mit Hilfe des Gelenkvierseits. Zeitschrift für angewandte Mathematik und Mechanik 3:13–19, 1923.

Find all four-bar linkages whose coupler curve passes through nine precision points.

C.W. Wampler, A.P. Morgan, A.J. Sommese: Complete Solution of the Nine-Point Path Synthesis Problem for Four-Bar Linkages. Transactions of the ASME. Journal of Mechanical Design 114(1): 153–159, 1992.

Formulation into Polynomial System

The 9-point problem was translated into

- a system of 4 quadrics and 8 quartics in 12 unknowns.
- Its total degree equals $2^4 4^8 = 2^{20}$.
- A 2-homogeneous Bézout number equals 286,720.
- Exploiting a 2-way symmetry leads to 143,360 solution paths.

At that time – early nineties – this was the largest polynomial system solved using numerical continuation methods.

Timings – Past and Present

Back Then: Tracking 143,360 solution paths in 12 variables took 331.9 hours of CPU time (about two weeks) on a IBM 3081 at the University of Notre Dame.

1,442 four-bar linkages were found

Computing various instances of the parameters with coefficient-parameter polynomial continuation requires only 1,442 paths to track. The number of real meaningful linkages ranged between 21 and 120.

Present: Using a personal cluster computer of 13 workers and one manager at 2.4 Ghz, running Linux, tracking 286,720 paths of a formulation in 20 variables takes about 14.1 hours.

The Theorems of Bernshtein

- Theorem A: The number of roots of a generic system equals the mixed volume of its Newton polytopes.
- Theorem B: Solutions at infinity are solutions of systems supported on faces of the Newton polytopes.
- D.N. Bernshtein: The number of roots of a system of equations. Functional Anal. Appl., 9(3):183–185, 1975.
- Structure of proofs: First show Theorem B, looking at power series expansions of diverging paths defined by a linear homotopy starting at a generic system. Then show Theorem A, using Theorem B with a homotopy defined by *lifting* the polytopes.

Some References on Polyhedral Methods

- I.M. Gel'fand, M.M. Kapranov, and A.V. Zelevinsky: **Discriminants**, **Resultants and Multidimensional Determinants**. Birkhäuser, 1994.
- B. Huber and B. Sturmfels: A polyhedral method for solving sparse polynomial systems. *Math. Comp.* 64(212):1541–1555, 1995.
- T.Y. Li.: Numerical solution of polynomial systems by homotopy continuation methods. In F. Cucker, editor, Handbook of Numerical Analysis. Volume XI. Special Volume: Foundations of Computational Mathematics, pages 209–304. North-Holland, 2003.
- T. Gao and T.Y. Li and M. Wu: Algorithm 846: MixedVol: a software package for mixed-volume computation. ACM Trans. Math. Softw. 31(4):555–560, 2005.
- T. Gunji, S. Kim, M. Kojima, A. Takeda, K. Fujisawa, and T. Mizutani:
 PHoM a polyhedral homotopy continuation method for polynomial systems. Computing 73(4): 55–77, 2004.
- T. Mizutani, A. Takeda, and M. Kojima: **Dynamic enumeration of all mixed cells**. *Discrete Comput. Geom.* to appear.

3 stages to solve a polynomial system $f(\mathbf{x}) = \mathbf{0}$

- 1. Compute the mixed volume (aka the BKK bound) of the Newton polytopes spanned by the supports A of f via a regular mixed-cell configuration Δ_{ω} .
- 2. Given Δ_{ω} , solve a generic system $g(\mathbf{x}) = \mathbf{0}$, using polyhedral homotopies. Every cell $C \in \Delta_{\omega}$ defines one homotopy

$$h_C(\mathbf{x},s) = \sum_{\mathbf{a}\in C} c_{\mathbf{a}} \mathbf{x}^{\mathbf{a}} + \sum_{\mathbf{a}\in A\setminus C} c_{\mathbf{a}} \mathbf{x}^{\mathbf{a}} s^{\nu_{\mathbf{a}}}, \quad \nu_{\mathbf{a}} > 0,$$

tracking as many paths as the mixed volume of the cell C, as s goes from 0 to 1.

3. Use $(1-t)g(\mathbf{x}) + tf(\mathbf{x}) = \mathbf{0}$ to solve $f(\mathbf{x}) = \mathbf{0}$.

Stages 2 and 3 are computationally most intensive $(1 \ll 2 < 3)$.

A Static Distribution of the Workload

manager	worker 1	worker 2	worker 3
Vol(cell 1) = 5	#paths(cell 1) : 5		
Vol(cell 2) = 4	# paths(cell 2): 4		
Vol(cell 3) = 4	# paths(cell 3): 4		
Vol(cell 4) = 6	# paths(cell 4): 1	# paths(cell 4): 5	
Vol(cell 5) = 7		# paths(cell 5):7	
Vol(cell 6) = 3		# paths(cell 6): 2	# paths(cell 6): 1
Vol(cell 7) = 4			# paths(cell 7): 4
Vol(cell 8) = 8			# paths(cell 8): 8
total $\#$ paths : 41	#paths : 14	#paths : 14	#paths : 13

Since polyhedral homotopies solve a **generic** system $g(\mathbf{x}) = \mathbf{0}$, we **expect** every path to take the same amount of work...

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An academic Benchmark: cyclic *n*-roots

The system

$$f(\mathbf{x}) = \begin{cases} f_i = \sum_{j=0}^{n=1} \prod_{k=1}^{i} x_{(k+j) \mod n} = 0, & i = 1, 2, \dots, n-1 \\ f_n = x_0 x_1 x_2 \cdots x_{n-1} - 1 = 0 \end{cases}$$

appeared in

G. Björck: Functions of modulus one on Z_p whose Fourier transforms have constant modulus In Proceedings of the Alfred Haar Memorial Conference, Budapest, pages 193–197, 1985.

very sparse, well suited for polyhedral methods

Results on the cyclic *n***-roots problem**

Problem	#Paths	CPU Time	
cyclic 5-roots	70	0.13m	
cyclic 6-roots	156	$0.19\mathrm{m}$	
cyclic 7-roots	924	$0.30\mathrm{m}$	
cyclic 8-roots	$2,\!560$	$0.78\mathrm{m}$	
cyclic 9-roots	$11,\!016$	$3.64\mathrm{m}$	
cyclic 10-roots	$35,\!940$	$21.33\mathrm{m}$	
cyclic 11-roots	184,756	2h $39m$	
cyclic 12-roots	$500,\!352$	24h 36m	

Wall time for start systems to solve the cyclic n-roots problems, using 13 workers, with static load distribution.

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Dynamic versus Static Workload Distribution

	Static	versus Dyn	Dynamic on argo			
#workers	Static	Speedup	Dynamic	Speedup	Dynamic	Speedup
1	50.7021	—	53.0707	_	29.2389	_
2	24.5172	2.1	25.3852	2.1	15.5455	1.9
3	18.3850	2.8	17.6367	3.0	10.8063	2.7
4	14.6994	3.4	12.4157	4.2	7.9660	3.7
5	11.6913	4.3	10.3054	5.1	6.2054	4.7
6	10.3779	4.9	9.3411	5.7	5.0996	5.7
7	9.6877	5.2	8.4180	6.3	4.2603	6.9
8	7.8157	6.5	7.4337	7.1	3.8528	7.6
9	7.5133	6.8	6.8029	7.8	3.6010	8.1
10	6.9154	7.3	5.7883	9.2	3.2075	9.1
11	6.5668	7.7	5.3014	10.0	2.8427	10.3
12	6.4407	7.9	4.8232	11.0	2.5873	11.3
13	5.1462	9.8	4.6894	11.3	2.3224	12.6

Wall time in seconds to solve a start system for the cyclic 7-roots problem.

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Figure 4.4: The elliptic cylinder reachable by a PRS serial chain.

H.J. Su. Computer-Aided Constrained Robot Design Using Mechanism Synthesis Theory. PhD thesis, University of California, Irvine, 2004.

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Design of Serial Chains II



Figure 4.7: The circular torus traced by the wrist center of a "right" RRS serial chain.

H.J. Su. Computer-Aided Constrained Robot Design Using Mechanism Synthesis Theory. PhD thesis, University of California, Irvine, 2004.

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Design of Serial Chains III



Figure 4.8: The general torus reachable by the wrist center of an RRS serial chain.

H.J. Su. Computer-Aided Constrained Robot Design Using Mechanism Synthesis Theory. PhD thesis, University of California, Irvine, 2004.

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For more about these problems:

- H.-J. Su and J.M. McCarthy: Kinematic synthesis of RPS serial chains. In the Proceedings of the ASME Design Engineering Technical Conferences (CDROM), Chicago, IL, Sep 2-6, 2003.
- H.-J. Su, C.W. Wampler, and J.M. McCarthy: Geometric
 design of cylindric PRS serial chains.
 ASME Journal of Mechanical Design 126(2):269–277, 2004.
- H.-J. Su, J.M. McCarthy, and L.T. Watson: Generalized linear product homotopy algorithms and the computation of reachable surfaces. ASME Journal of Information and Computer Sciences in Engineering 4(3):226–234, 2004.

Results on Mechanical Design Problems

Bézout vs Bernshteĭn

	Bounds	on #Sol	Wall Time		
Surface	D	В	V	our cluster	on argo
elliptic cylinder	2,097,152	247,968	125,888	11h 33m	6h 12m
circular torus	2,097,152	868,352	474,112	7h 17m	4h 3m
general torus	4,194,304	448,702	226,512	14h 15m	6h 36m

D =total degree; B =generalized Bézout bound; V =mixed volume

Wall time for mechanism design problems on our cluster and argo.

- Compared to the linear-product bound, polyhedral homotopies cut the #paths about in half.
- The second example is easier (despite the larger #paths) because of increased sparsity, and thus lower evaluation cost.
Conclusions

- To solve large polynomial systems in parallel we had to rethink the design of the original program.
- Scheduling of path tracking jobs leads to an almost optimal speedup, using dynamic load balancing.
- Still much work left to develop tools to process and certify the results, we need to consider also "quality up".