The long and winding road between theory and practice
Symbolic Computation

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Universidad de Cantabria

OUTLINE

- Definitions.
- The past.
- From the past to the future.
- The future.
- The future: “getting closer” examples.
- The future: some opportunities.
- The long and winding road.

Symbolic computation practicioners argue that our field of research has a wide and huge number of potential applications

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Computer Algebra is that part of Computer Science and/or Mathematics which designs, analyzes, implements and applies algebraic algorithms.

Compared with other algorithms, algebraic algorithms have simple formal specifications, have proofs of correctness and asymptotic time bounds which can be stablished on the base of a well developed mathematical theory.

Furthermore, algebraic objects can be represented exactly in the memory of a computer so that algebraic computations can be performed without loss of precision and significance. Usually, algebraic algorithms are implemented in software systems allowing input and output in the symbolic notation of algebra.

Rüdiger Loos en:
Computer Algebra
Editores: B. Buchberger, G. E. Collins y R. Loos
Computing Suplementum 4, Springer Verlag, 1982.

Applications

Inside Mathematics?

Inside Computer Science?

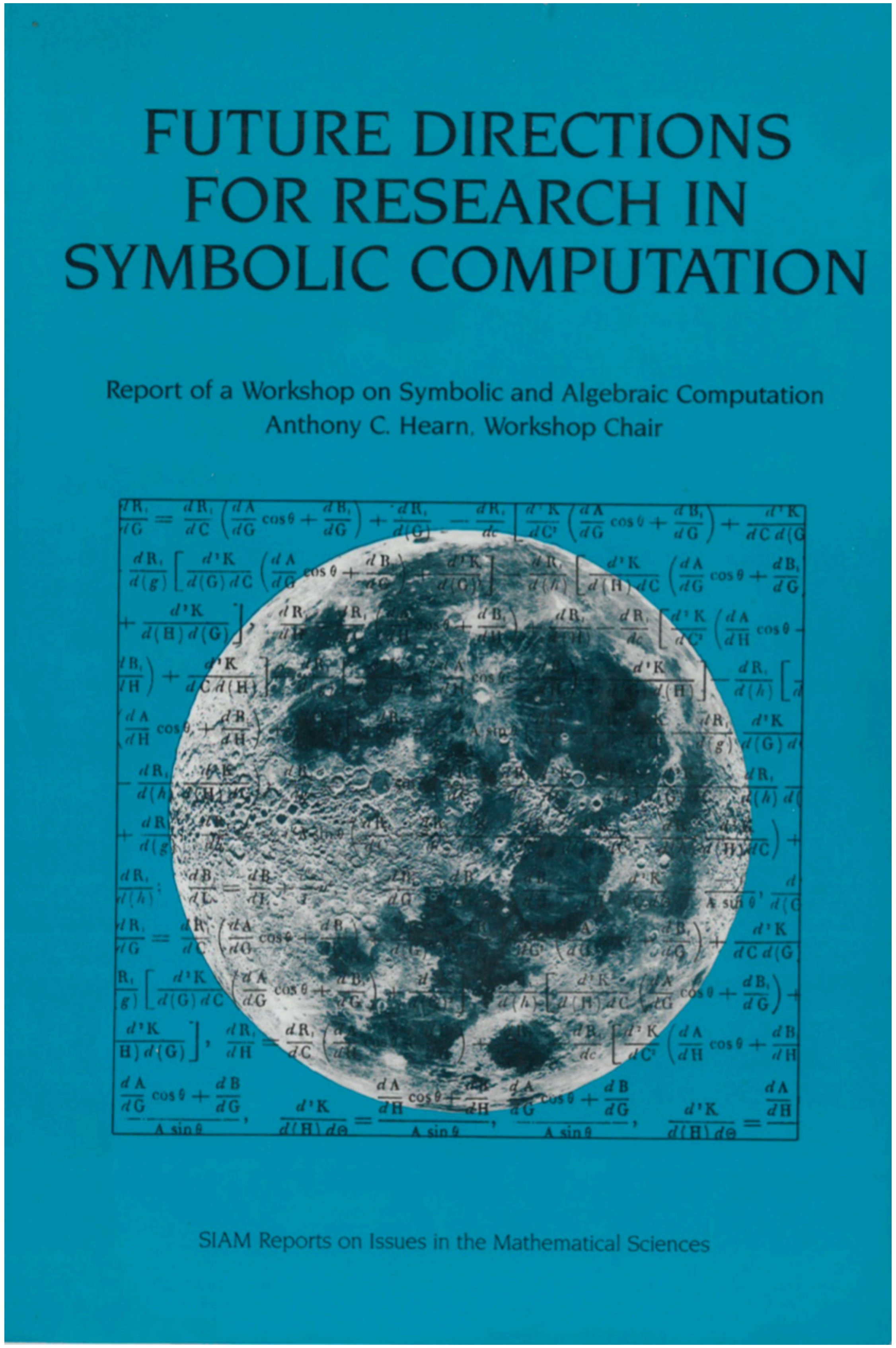
Inside Academia (Science & Technology)?

Outside Academia (Engineering)?

Outside Academia (Industry)?

Symbolic computation practicioners argue that our field of research has a wide and huge number of potential applications

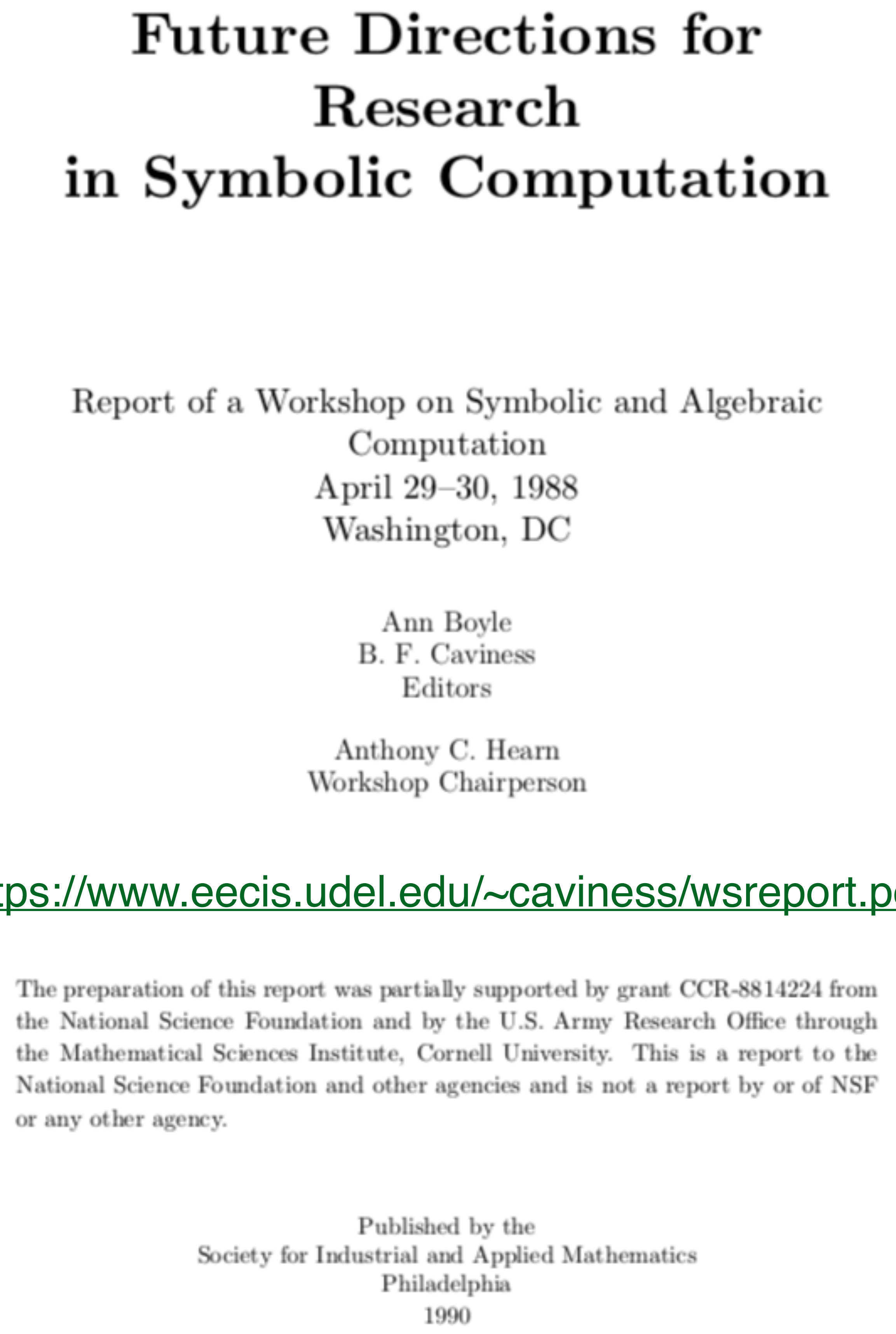
The past: 1988



FUTURE DIRECTIONS FOR RESEARCH IN SYMBOLIC COMPUTATION

Report of a Workshop on Symbolic and Algebraic Computation
Anthony C. Hearn, Workshop Chair

SIAM Reports on Issues in the Mathematical Sciences



Future Directions for Research in Symbolic Computation

Report of a Workshop on Symbolic and Algebraic Computation
April 29–30, 1988
Washington, DC

Ann Boyle
B. F. Caviness
Editors

Anthony C. Hearn
Workshop Chairperson

https://www.eecis.udel.edu/~caviness/wsreport.pdf

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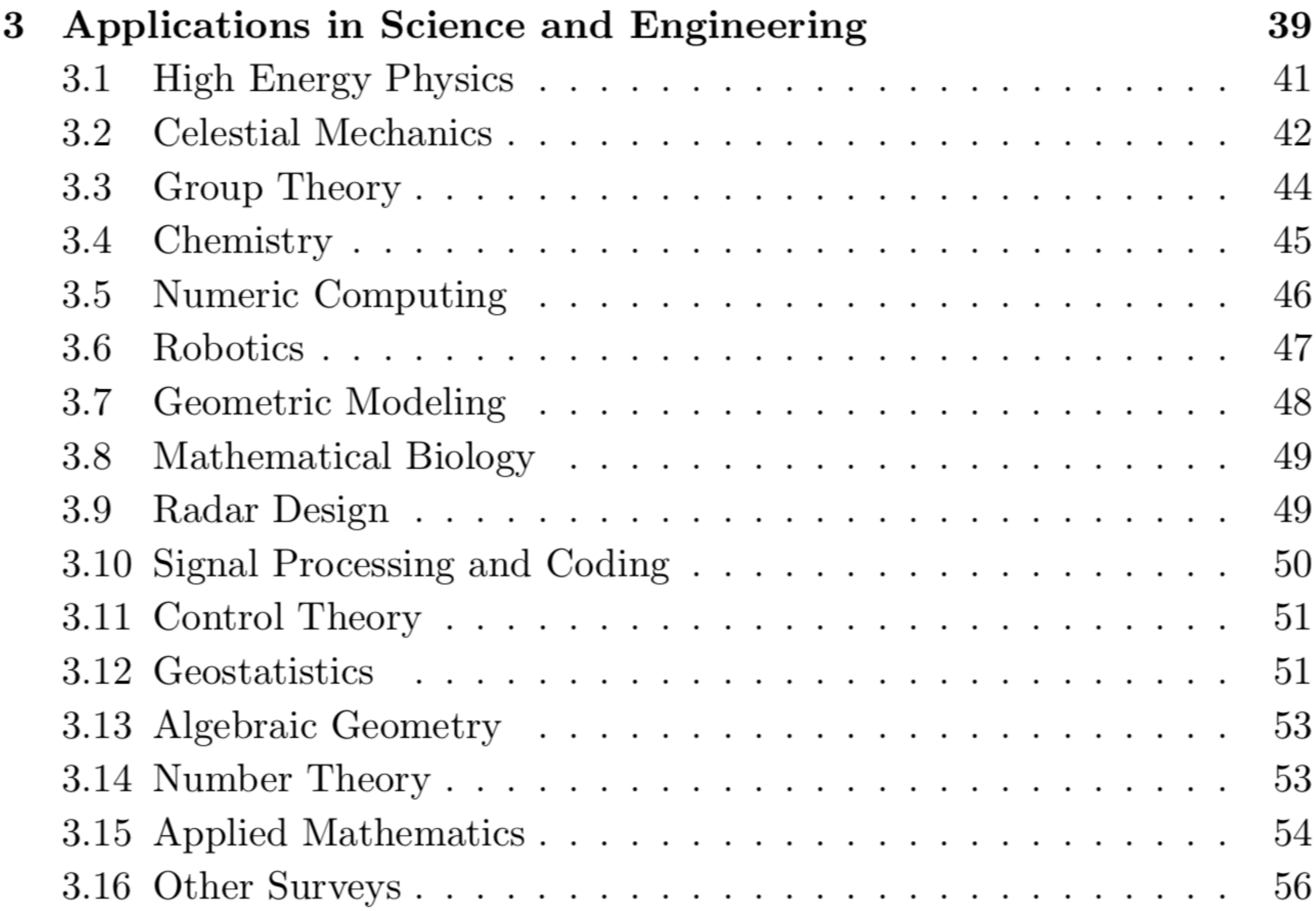
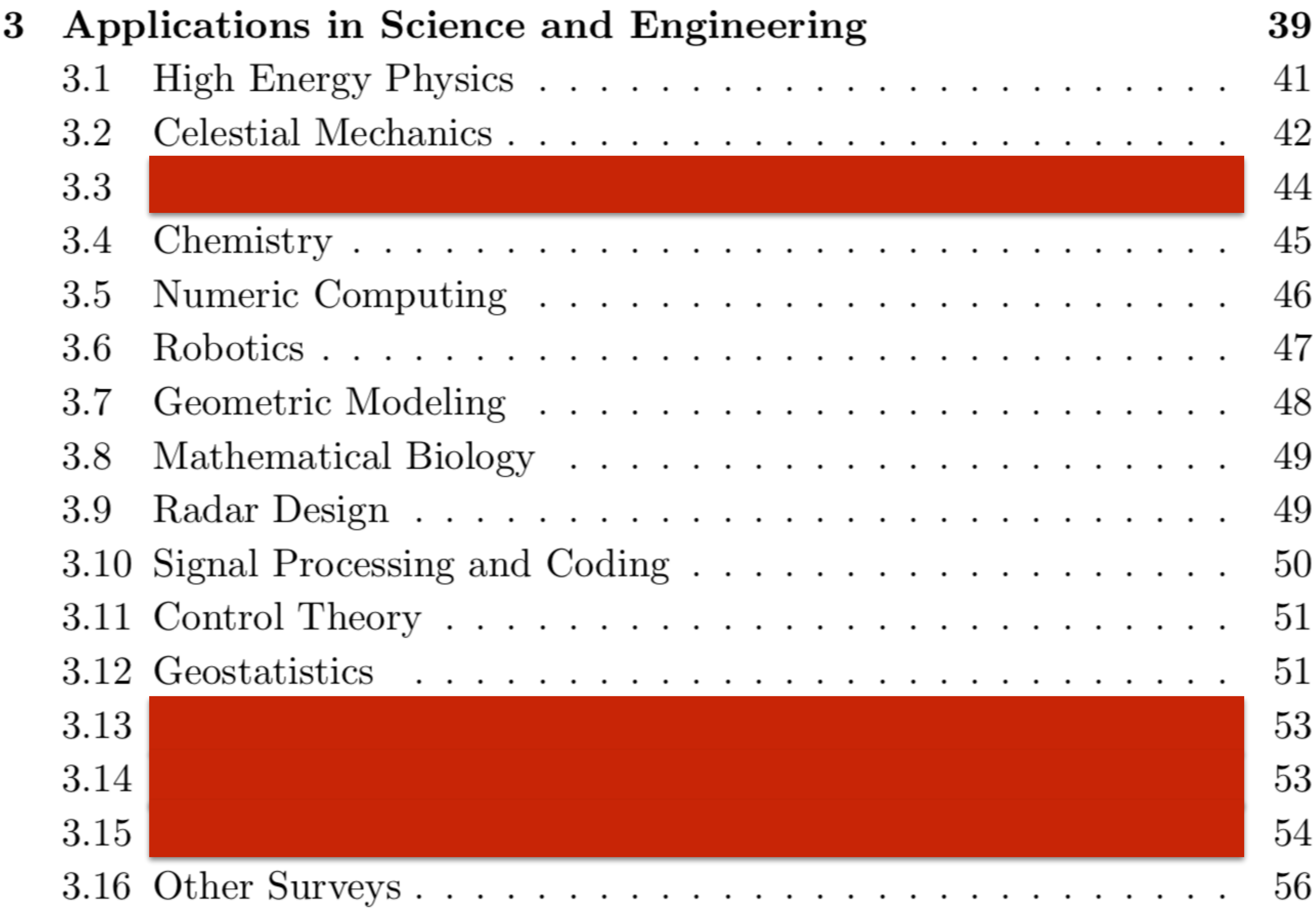
Published by the
Society for Industrial and Applied Mathematics
Philadelphia
1990

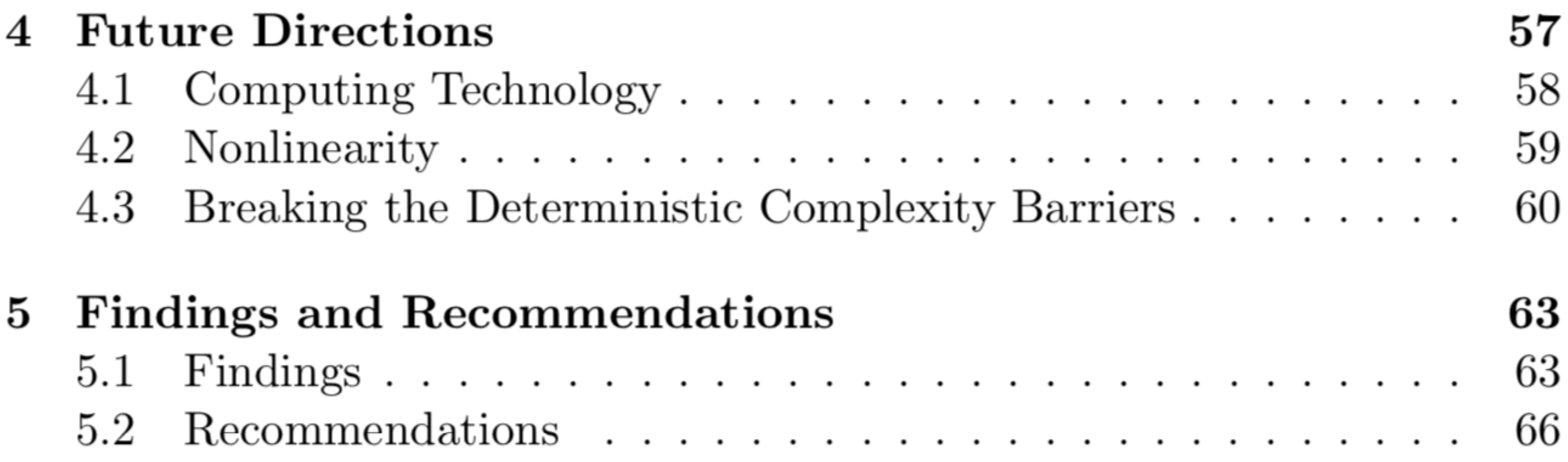
The past: 1988

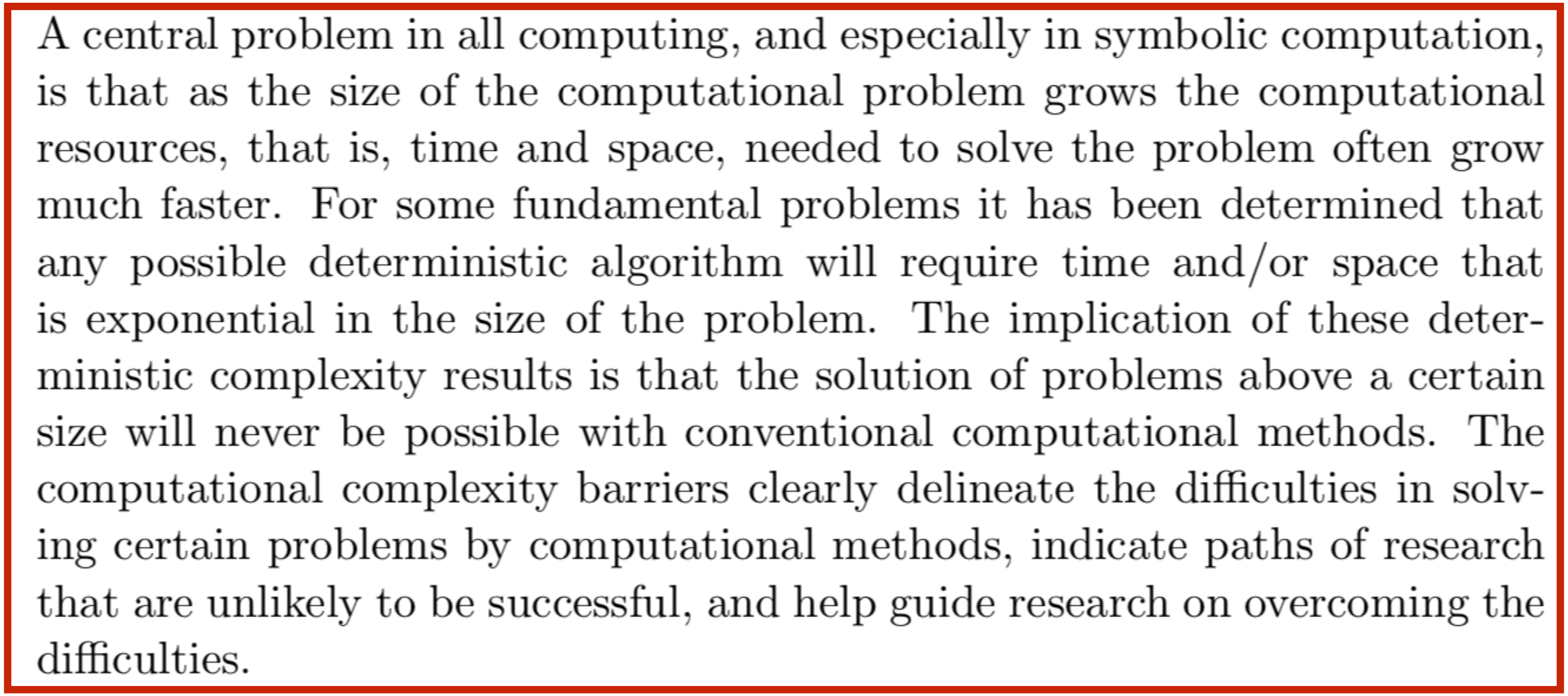


The past: 1988



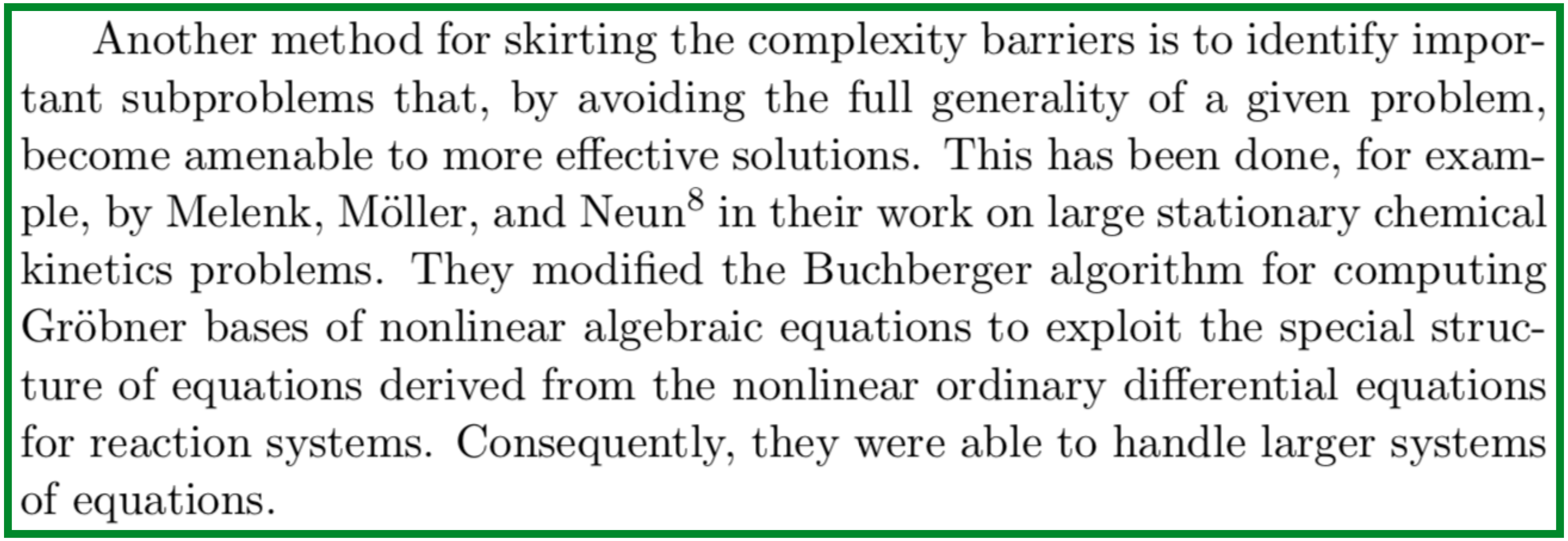
The past: 1988



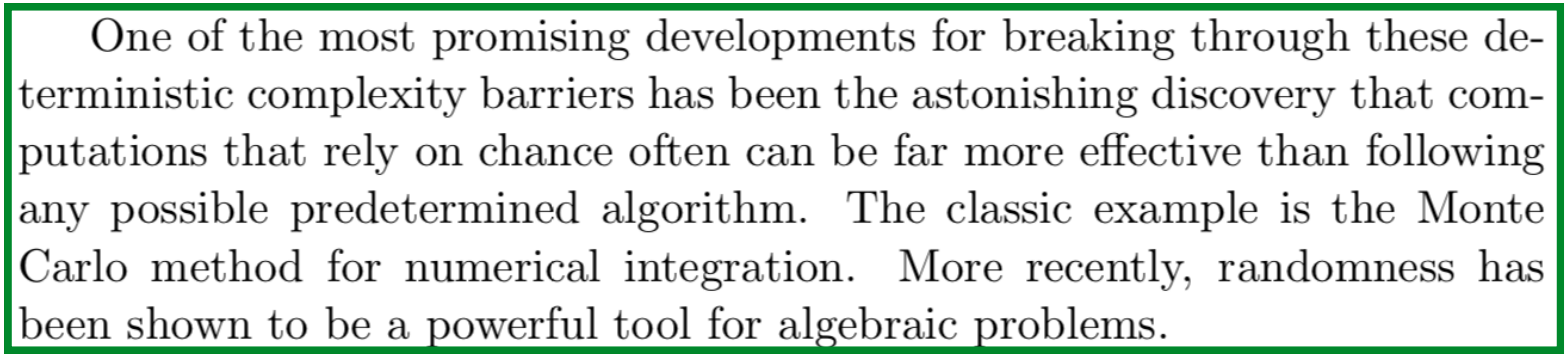


A central problem in all computing, and especially in symbolic computation, is that as the size of the computational problem grows the computational resources, that is, time and space, needed to solve the problem often grow much faster. For some fundamental problems it has been determined that any possible deterministic algorithm will require time and/or space that is exponential in the size of the problem. The implication of these deterministic complexity results is that the solution of problems above a certain size will never be possible with conventional computational methods. The computational complexity barriers clearly delineate the difficulties in solving certain problems by computational methods, indicate paths of research that are unlikely to be successful, and help guide research on overcoming the difficulties.

The past: 1988

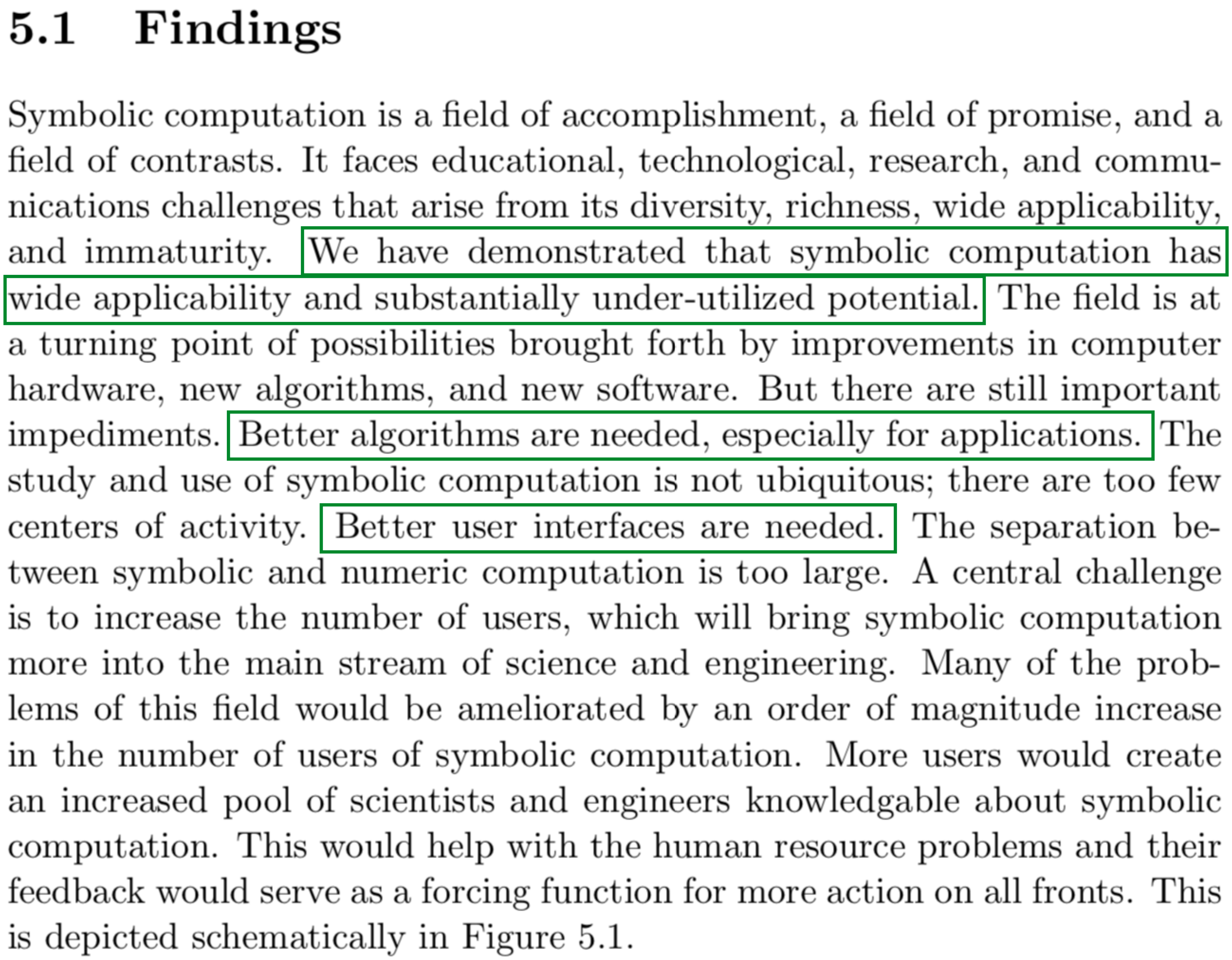


Another method for skirting the complexity barriers is to identify important subproblems that, by avoiding the full generality of a given problem, become amenable to more effective solutions. This has been done, for example, by Melenk, Möller, and Neun[8] in their work on large stationary chemical kinetics problems. They modified the Buchberger algorithm for computing Gröbner bases of nonlinear algebraic equations to exploit the special structure of equations derived from the nonlinear ordinary differential equations for reaction systems. Consequently, they were able to handle larger systems of equations.



One of the most promising developments for breaking through these deterministic complexity barriers has been the astonishing discovery that computations that rely on chance often can be far more effective than following any possible predetermined algorithm. The classic example is the Monte Carlo method for numerical integration. More recently, randomness has been shown to be a powerful tool for algebraic problems.

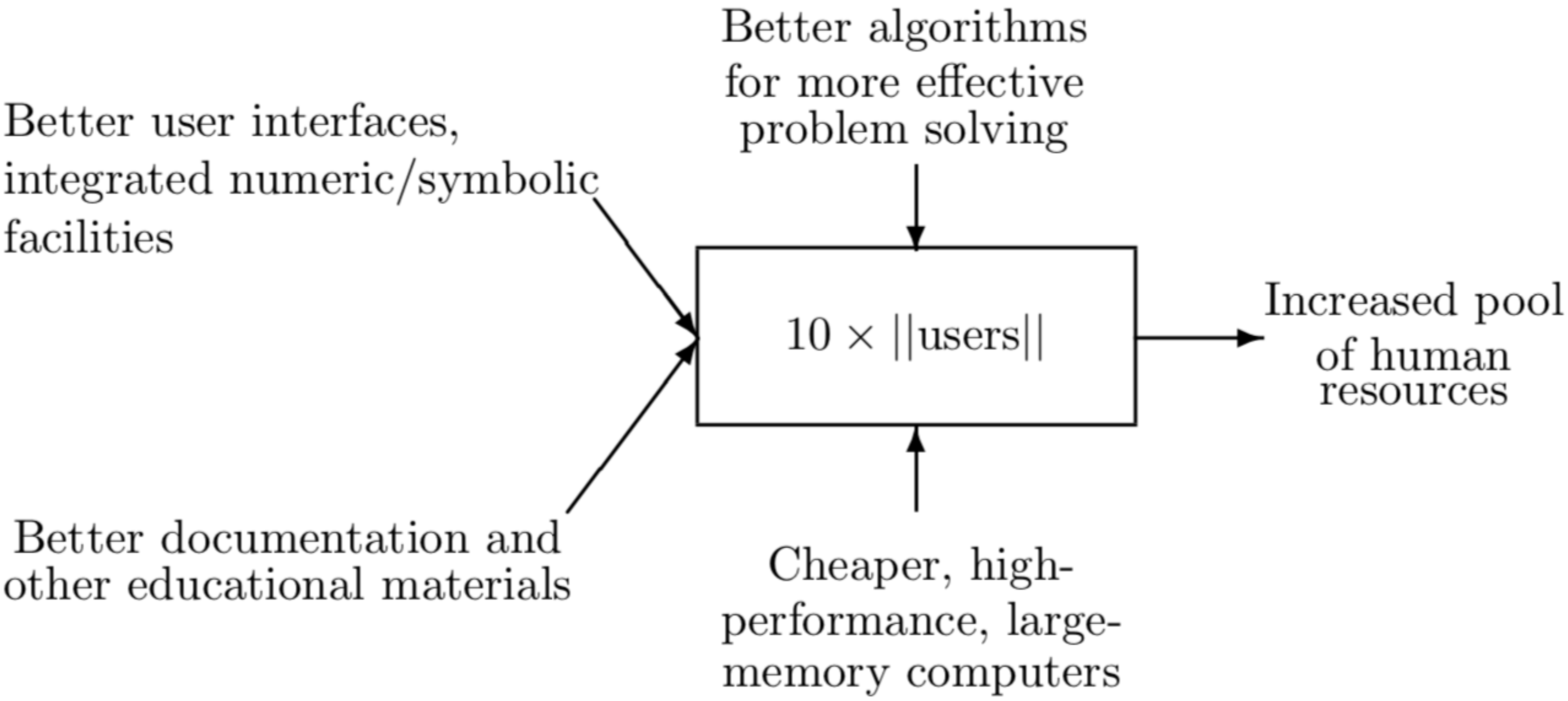
The past: 1988



5.1 Findings

Symbolic computation is a field of accomplishment, a field of promise, and a field of contrasts. It faces educational, technological, research, and communications challenges that arise from its diversity, richness, wide applicability, and immaturity. We have demonstrated that symbolic computation has wide applicability and substantially under-utilized potential. The field is at a turning point of possibilities brought forth by improvements in computer hardware, new algorithms, and new software. But there are still important impediments. Better algorithms are needed, especially for applications. The study and use of symbolic computation is not ubiquitous; there are too few centers of activity. Better user interfaces are needed. The separation between symbolic and numeric computation is too large. A central challenge is to increase the number of users, which will bring symbolic computation more into the main stream of science and engineering. Many of the problems of this field would be ameliorated by an order of magnitude increase in the number of users of symbolic computation. More users would create an increased pool of scientists and engineers knowledgable about symbolic computation. This would help with the human resource problems and their feedback would serve as a forcing function for more action on all fronts. This is depicted schematically in Figure 5.1.

The past: 1988



Better user interfaces, integrated numeric/symbolic facilities

Better algorithms for more effective problem solving

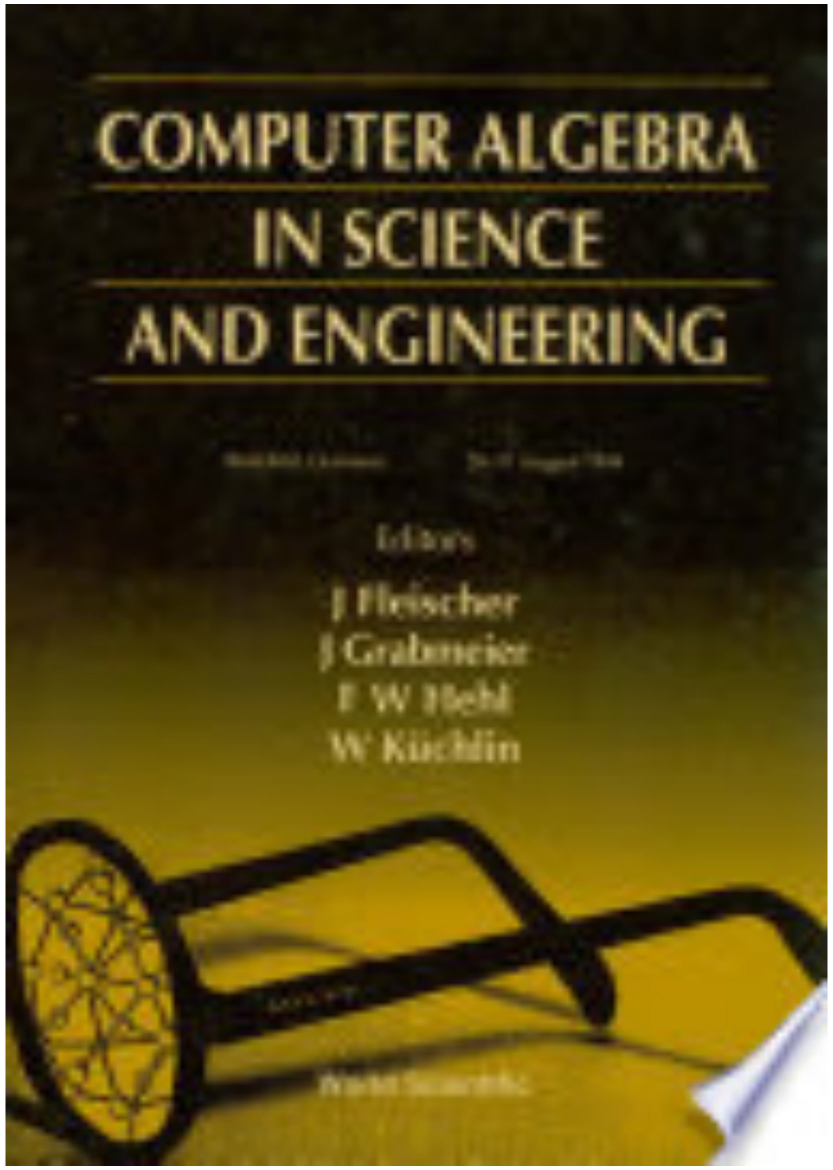
$10 \times ||\text{users}||$

Increased pool of human resources

Better documentation and other educational materials

Cheaper, high-performance, large-memory computers

The past: the nineties

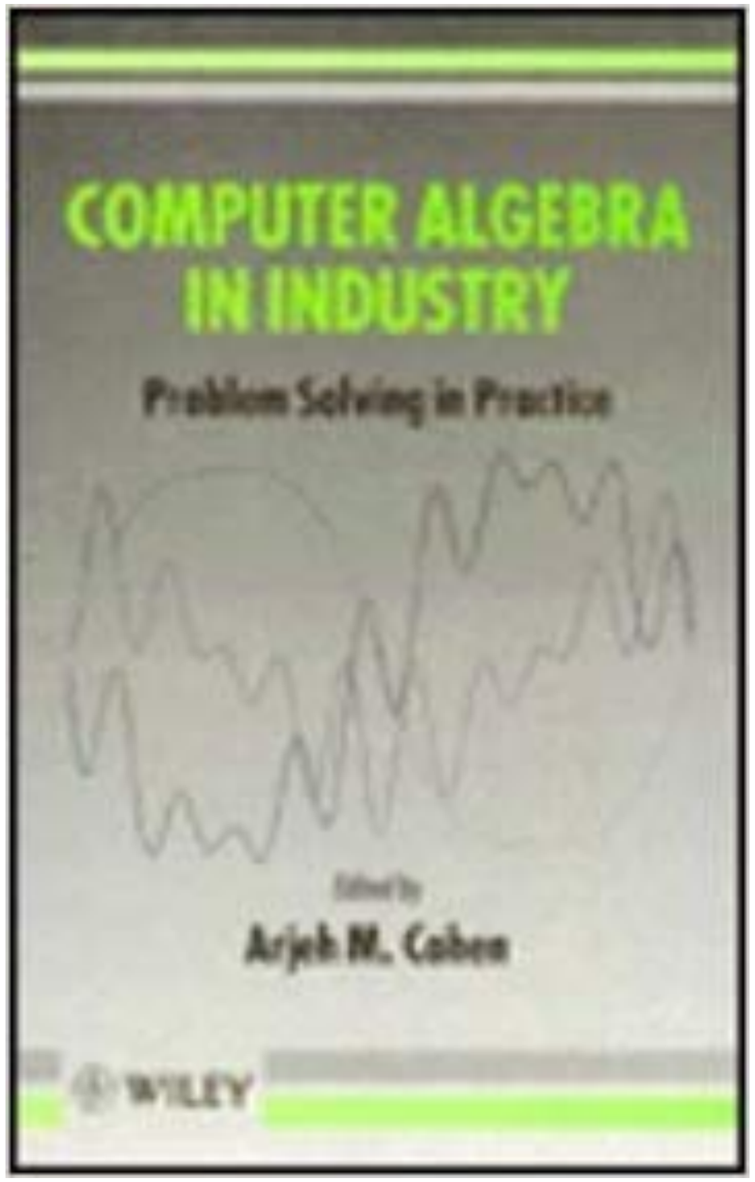


COMPUTER ALGEBRA
IN SCIENCE
AND ENGINEERING

Editors
J Fleischer
J Grabmeier
F W Hehl
W Küchlin

World Scientific

1995



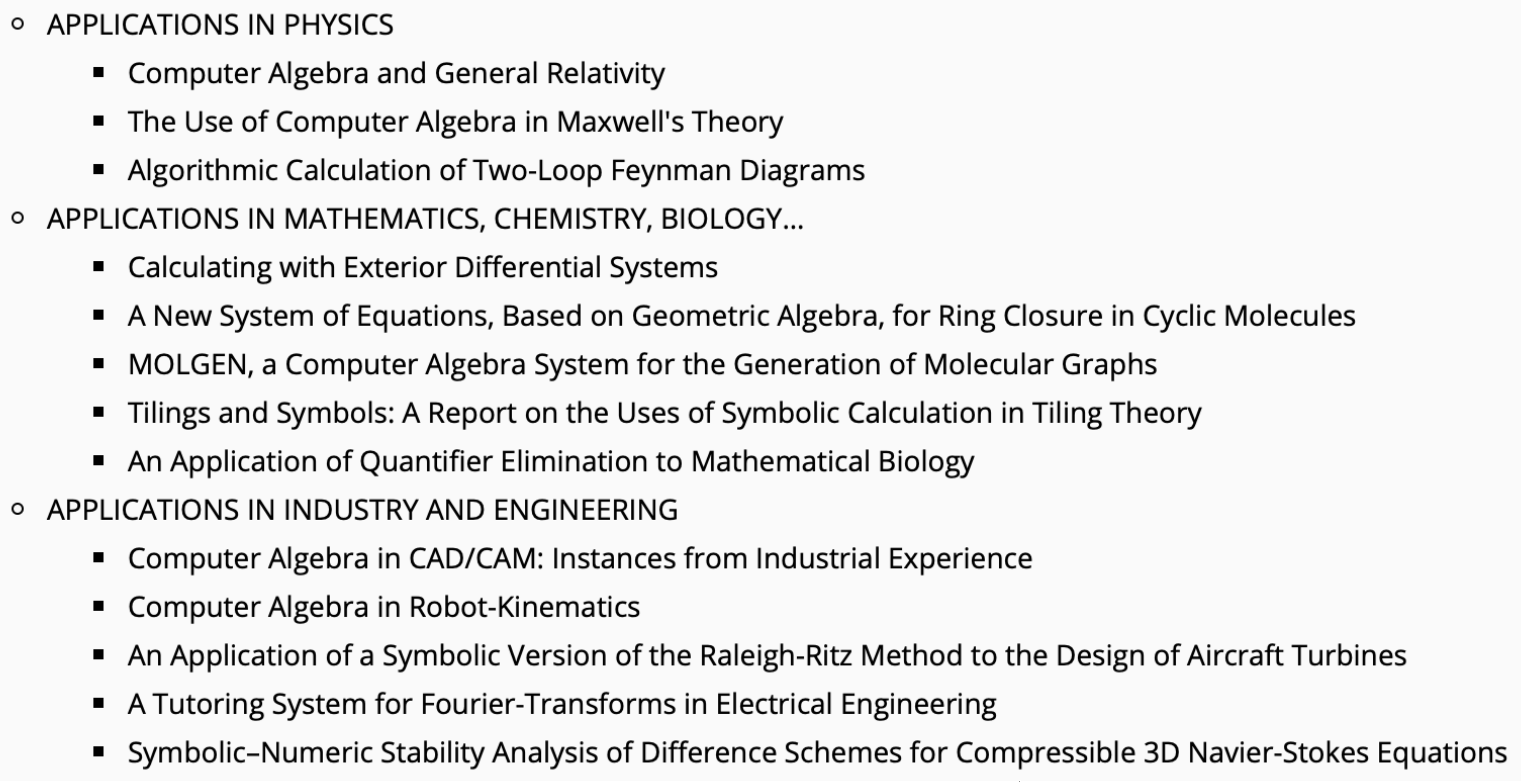
COMPUTER ALGEBRA
IN INDUSTRY
Problem Solving in Practice

Edited by
Arjeh M. Cohen

WILEY

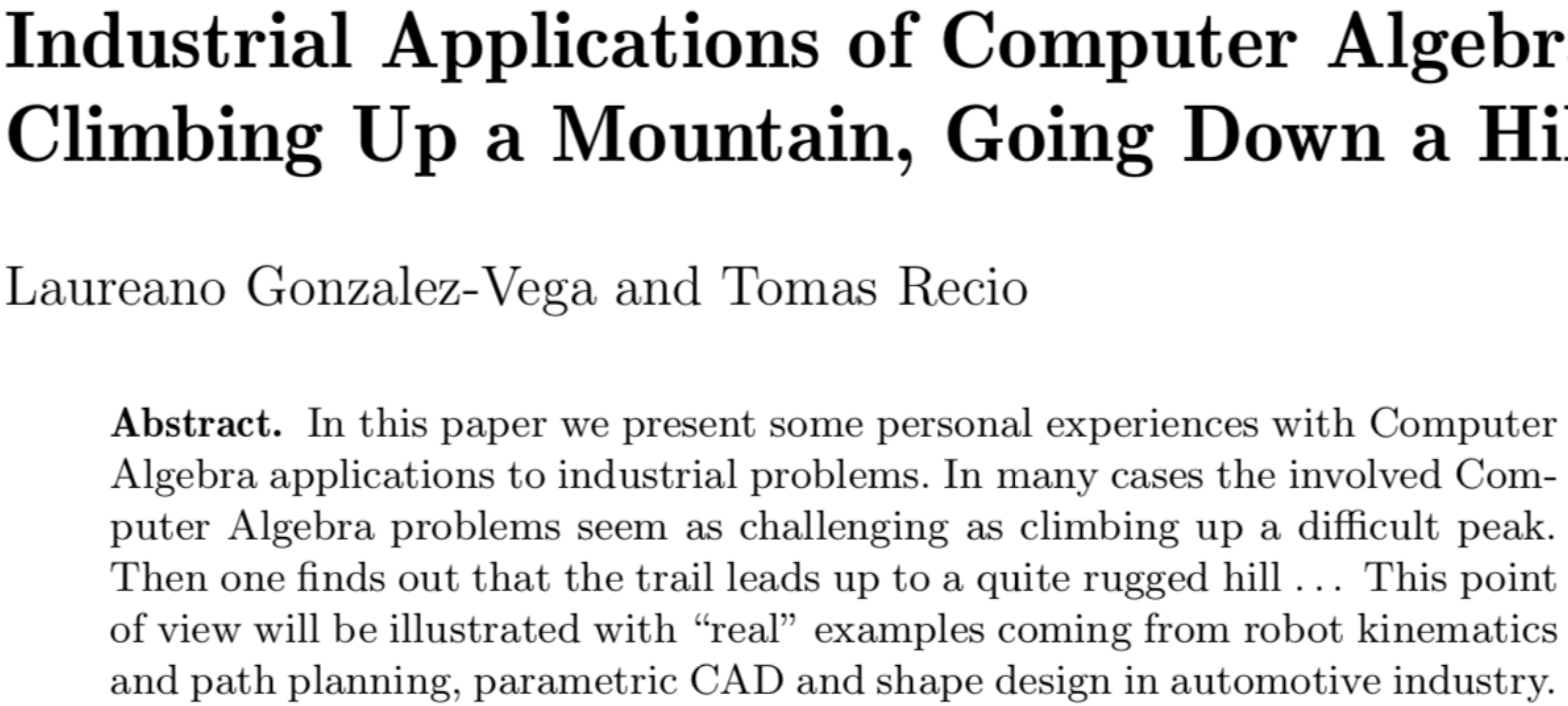
1993, 1995

The past: the nineties



- APPLICATIONS IN PHYSICS
  - Computer Algebra and General Relativity
  - The Use of Computer Algebra in Maxwell's Theory
  - Algorithmic Calculation of Two-Loop Feynman Diagrams
- APPLICATIONS IN MATHEMATICS, CHEMISTRY, BIOLOGY…
  - Calculating with Exterior Differential Systems
  - A New System of Equations, Based on Geometric Algebra, for Ring Closure in Cyclic Molecules
  - MOLGEN, a Computer Algebra System for the Generation of Molecular Graphs
  - Tilings and Symbols: A Report on the Uses of Symbolic Calculation in Tiling Theory
  - An Application of Quantifier Elimination to Mathematical Biology
- APPLICATIONS IN INDUSTRY AND ENGINEERING
  - Computer Algebra in CAD/CAM: Instances from Industrial Experience
  - Computer Algebra in Robot-Kinematics
  - An Application of a Symbolic Version of the Raleigh-Ritz Method to the Design of Aircraft Turbines
  - A Tutoring System for Fourier-Transforms in Electrical Engineering
  - Symbolic–Numeric Stability Analysis of Difference Schemes for Compressible 3D Navier-Stokes Equations

The past: 2001



Industrial Applications of Computer Algebra: Climbing Up a Mountain, Going Down a Hill

Laureano Gonzalez-Vega and Tomas Recio

Abstract. In this paper we present some personal experiences with Computer Algebra applications to industrial problems. In many cases the involved Computer Algebra problems seem as challenging as climbing up a difficult peak. Then one finds out that the trail leads up to a quite rugged hill . . . This point of view will be illustrated with "real" examples coming from robot kinematics and path planning, parametric CAD and shape design in automotive industry.

In: Casacuberta C., Miró-Roig R.M., Verdera J., Xambó-Descamps S. (eds). **European Congress of Mathematics**. Progress in Mathematics 202. Birkhäuser **(2001)**.

The past: 2001

In the earlier times, a handful of successful Computer Algebra stories made their way to the communication media. We can recall articles published in the Scientific News (1981), New York Times (1988), Nature (1981), Scientific American (1981), etc. One could argue that it was, perhaps, just because of the scientific novelty of symbolic computation —performing in a few minutes or seconds some computations that required, previously, a titanic effort for humans— and that some of these were news on non-industrial aspects of Computer Algebra.

In section 3, we will summarily describe the more intrinsic cooperation problems posed in the promising field of Computer Algebra applications in Robotics: certainly, we were trying to climb up a high mountain ... Section 4 is devoted to present the more modest aims of an ongoing cooperation project which is effectively changing the practice of a concrete enterprise: we can say that we are now exploring the challenging top of a rugged hill.

In: Casacuberta C., Miró-Roig R.M., Verdera J., Xambó-Descamps S. (eds). **European Congress of Mathematics**. Progress in Mathematics 202. Birkhäuser **(2001)**.

The past: 2001

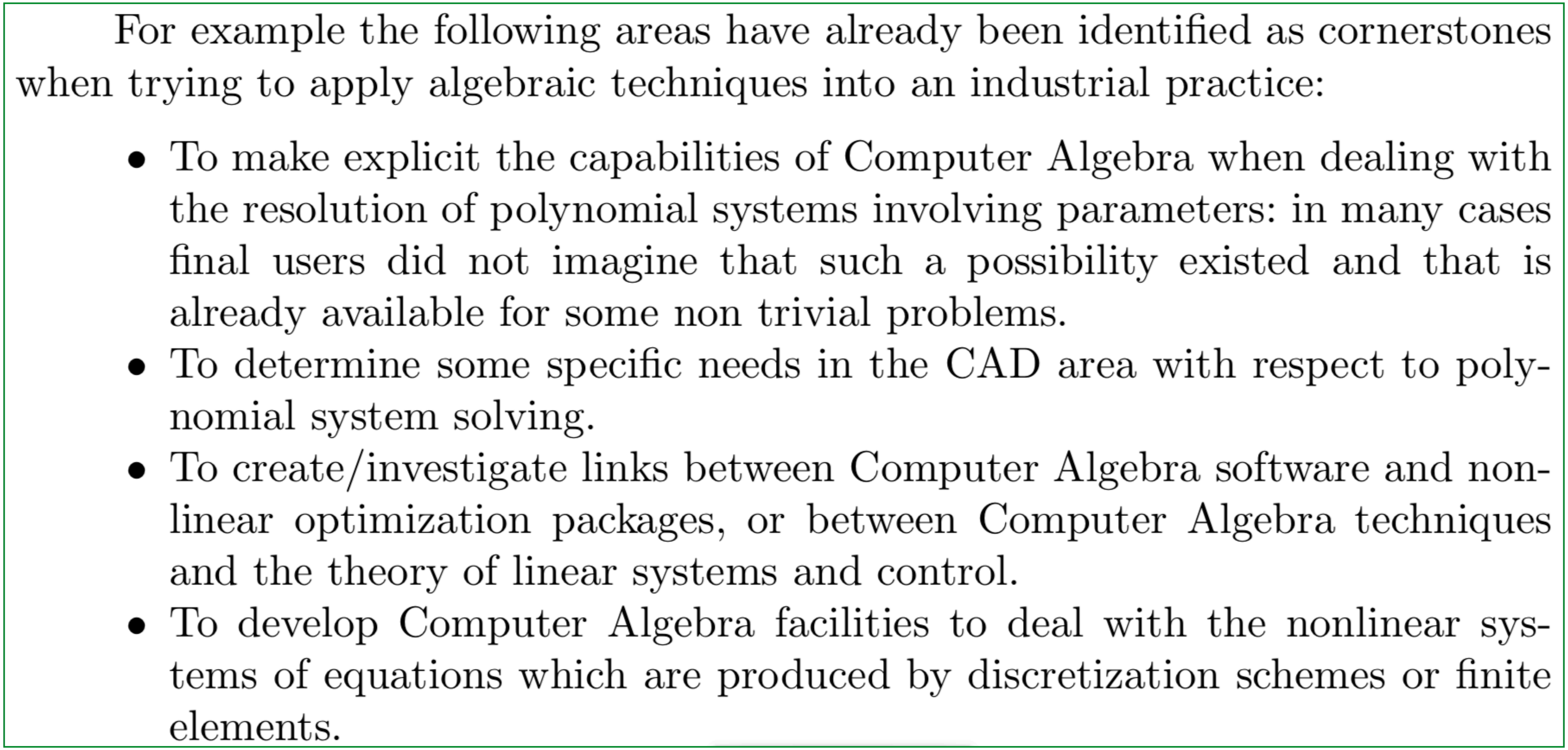
Working with industrial partners is quite uncomfortable for us, academics.

They obstinately care about solving a problem, but just in most cases, or at least in some cases, or even in “this” particular case, instead of caring about solving it in general. Sometimes the solution they search for is conceptually rather simple, but tiresome to execute in practice. Other times they do not care about the problem they just have posed, if they see that you do not progress fast enough to solve it; and then they merely switch their mathematical model to a different and simpler one, asking you to forget about the interesting question you have just started to think about …

It is difficult to get a paper properly done under these changing conditions, it seems impossible to bind in a Ph.D. thesis based on such “rush hour” solutions … . As a result, only very few and very obstinate scholars persist working in this near-zero atmosphere (i.e. extremely poor in academic oxygen: publications and dissertations).

In: Casacuberta C., Miró-Roig R.M., Verdera J., Xambó-Descamps S. (eds). **European Congress of Mathematics**. Progress in Mathematics 202. Birkhäuser (**2001**).

The past: 2001

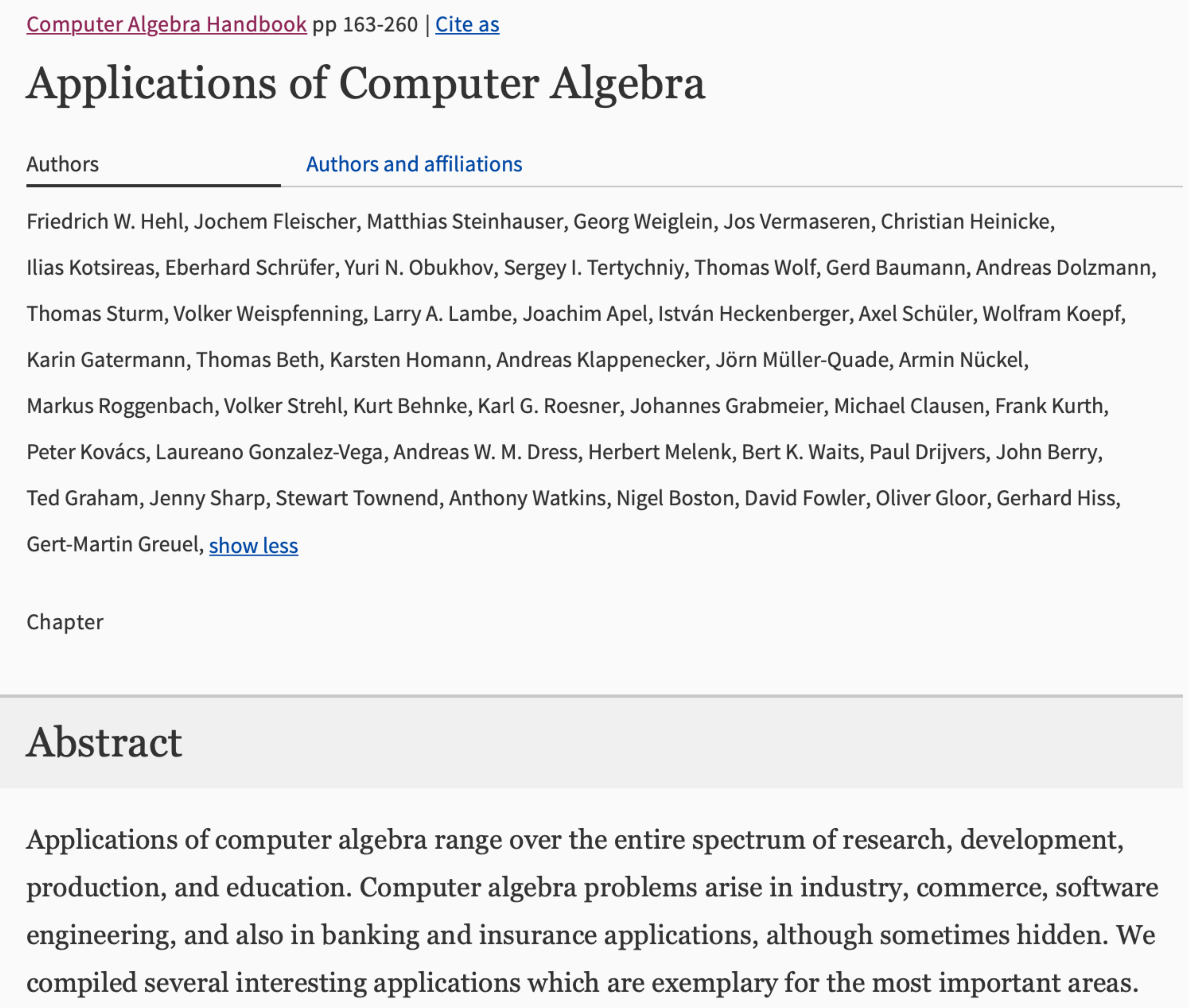


For example the following areas have already been identified as cornerstones when trying to apply algebraic techniques into an industrial practice:

- To make explicit the capabilities of Computer Algebra when dealing with the resolution of polynomial systems involving parameters: in many cases final users did not imagine that such a possibility existed and that is already available for some non trivial problems.
- To determine some specific needs in the CAD area with respect to polynomial system solving.
- To create/investigate links between Computer Algebra software and nonlinear optimization packages, or between Computer Algebra techniques and the theory of linear systems and control.
- To develop Computer Algebra facilities to deal with the nonlinear systems of equations which are produced by discretization schemes or finite elements.

In: Casacuberta C., Miró-Roig R.M., Verdera J., Xambó-Descamps S. (eds). **European Congress of Mathematics**. Progress in Mathematics 202. Birkhäuser (**2001**).

The past: 2003



Computer Algebra Handbook pp 163-260 | Cite as

Applications of Computer Algebra

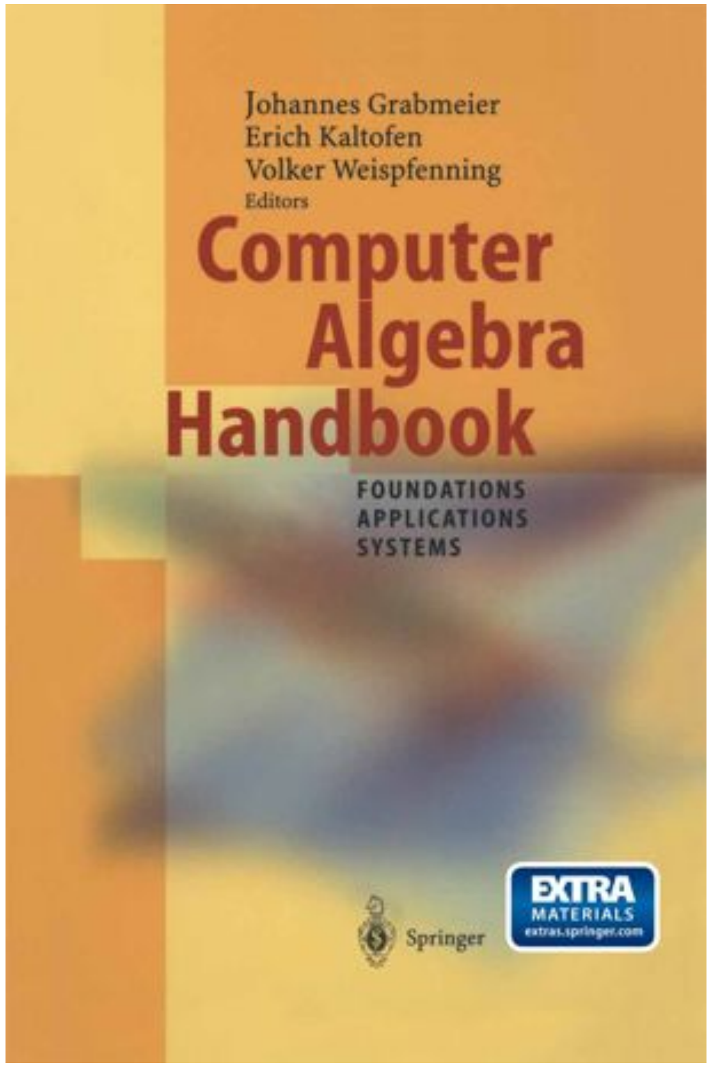
Authors   Authors and affiliations

Friedrich W. Hehl, Jochem Fleischer, Matthias Steinhauser, Georg Weiglein, Jos Vermaseren, Christian Heinicke, Ilias Kotsireas, Eberhard Schrüfer, Yuri N. Obukhov, Sergey I. Tertychniy, Thomas Wolf, Gerd Baumann, Andreas Dolzmann, Thomas Sturm, Volker Weispfenning, Larry A. Lambe, Joachim Apel, István Heckenberger, Axel Schüler, Wolfram Koepf, Karin Gatermann, Thomas Beth, Karsten Homann, Andreas Klappenecker, Jörn Müller-Quade, Armin Nückel, Markus Roggenbach, Volker Strehl, Kurt Behnke, Karl G. Roesner, Johannes Grabmeier, Michael Clausen, Frank Kurth, Peter Kovács, Laureano Gonzalez-Vega, Andreas W. M. Dress, Herbert Melenk, Bert K. Waits, Paul Drijvers, John Berry, Ted Graham, Jenny Sharp, Stewart Townend, Anthony Watkins, Nigel Boston, David Fowler, Oliver Gloor, Gerhard Hiss, Gert-Martin Greuel, show less

Chapter

Abstract

Applications of computer algebra range over the entire spectrum of research, development, production, and education. Computer algebra problems arise in industry, commerce, software engineering, and also in banking and insurance applications, although sometimes hidden. We compiled several interesting applications which are exemplary for the most important areas.



Johannes Grabmeier
Erich Kaltofen
Volker Weispfenning
Editors

Computer Algebra Handbook

FOUNDATIONS
APPLICATIONS
SYSTEMS

Springer

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2003

From the past to the present

Maplesoft

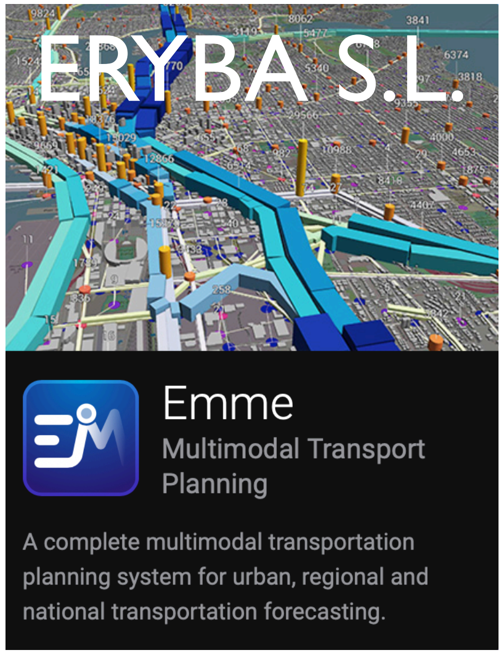
Addlink
Software Científico

nag

TopSolid

CDM
CANDEMAT

DPT



ERYBA S.L.

Emme
Multimodal Transport Planning

A complete multimodal transportation planning system for urban, regional and national transportation forecasting.

CENTRO TECNOLÓGICO CTC

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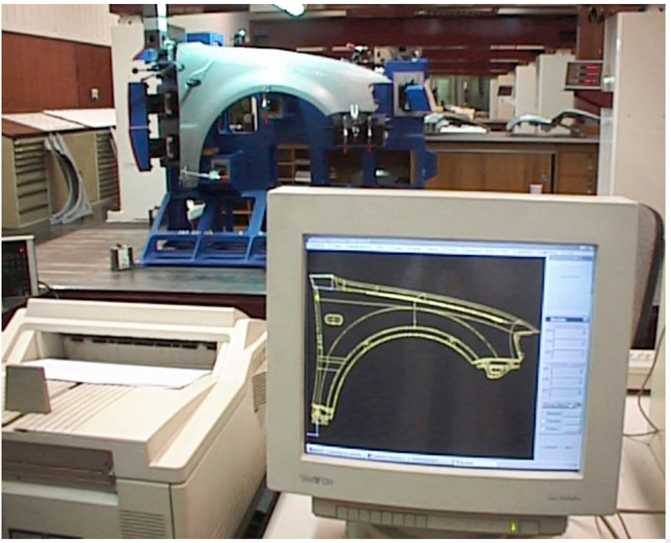
Equations & Formulae

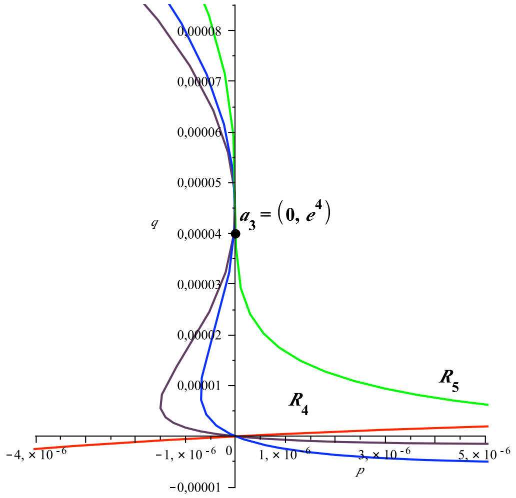
Polynomials

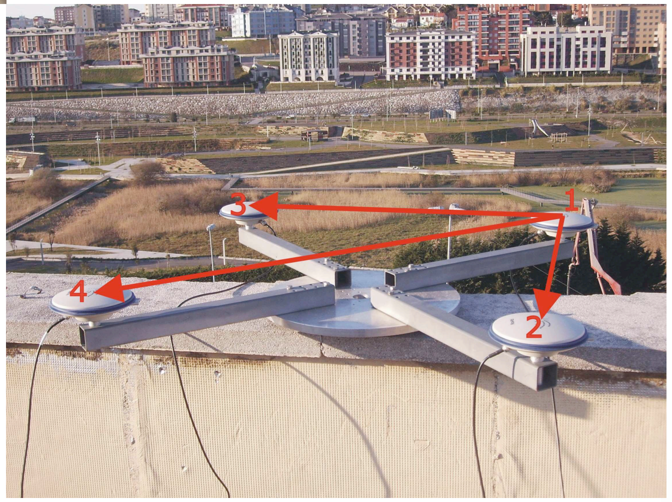


$$
\begin{aligned}
X &= (h+n)\cos\varphi\cos\lambda \\
Y &= (h+n)\cos\varphi\sin\lambda \\
Z &= (h+n(1-e^2))\sin\varphi
\end{aligned}
$$

[Gema, …]

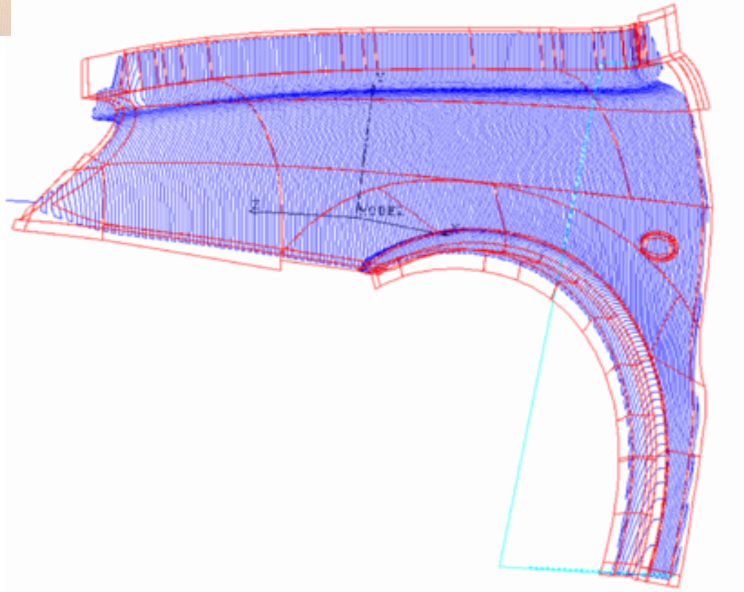
Algorithms





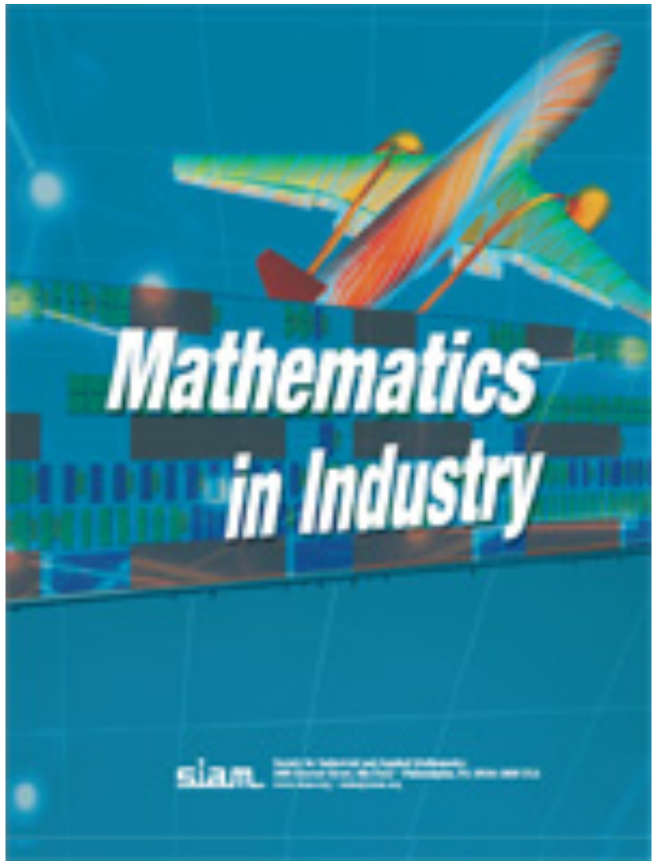
Software

[JC, LFT, JS, MF, …]



Curves & Surfaces

The future

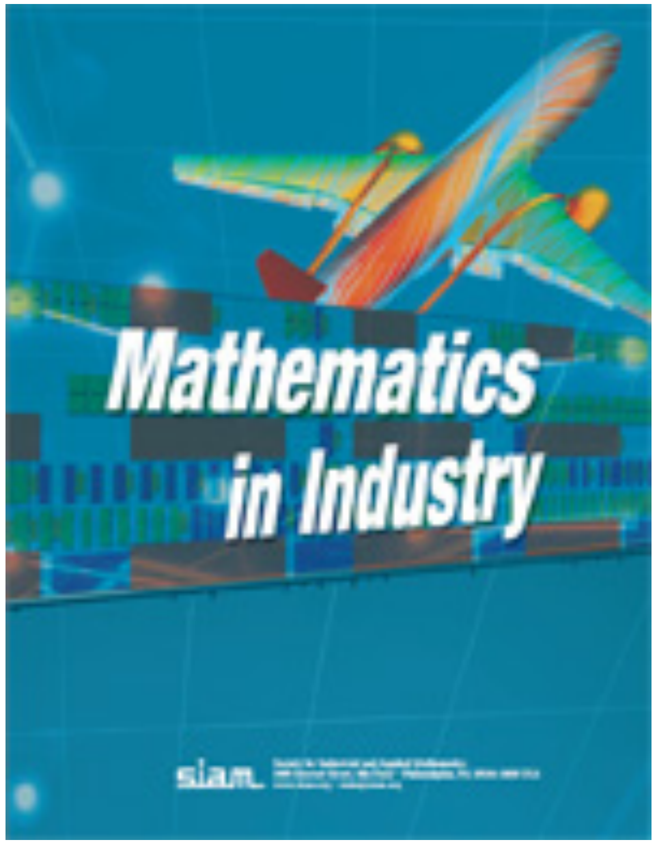


Mathematics in Industry

siam

Many of the recommendations and insights in the 1996 report remain valid today. However, the landscape of mathematical and computer sciences in industry has changed. Organisations now collect orders of magnitude more data than they used to, and face the challenge of extracting useful information from it. Computing technology has continued to advance rapidly, and companies are making more and more aggressive use of high-performance parallel computing.

The future



Mathematics in Industry

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Our most important conclusion is that the mathematical and computational sciences continue to find many applications, both traditional and novel, in industry. Some of these applications have very dramatic effects on the bottom line of their companies, often in the **tens of millions of dollars**. Other applications may not have an easily measured impact on the bottom line but simply allow the company to conduct business in a 21st-century data-rich marketplace. Finally, some applications have great value as contributions to science. We want to emphasize that technology transfer, including the transfer of mathematical ideas, is not a one-way street; a technology designed for or by one company often ends up enriching science as a whole.

The future

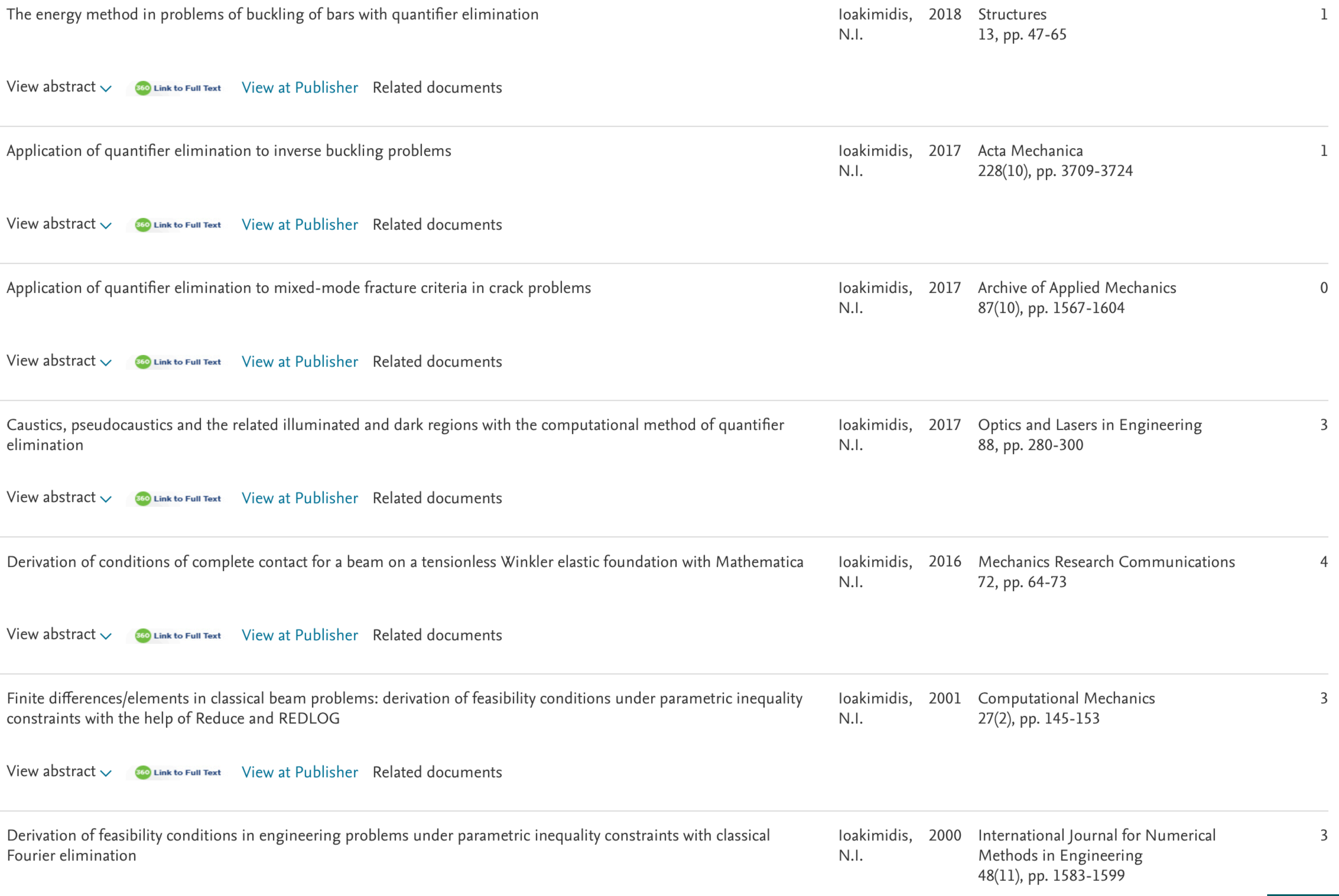
Conclusions (very personal):

- Difficult to argue that Symbolic Computation (**alone**) has direct applications in industry (may be).
- Easy to argue that Symbolic Computation can be very useful and helpful in applications in industry (and it is !).

What to do in the near-future?

- Get closer to the (**potential**) applications.
- Get closer to the (**engineering**) academia outside Mathematics.

Getting closer: N. Ioakimidis



The energy method in problems of buckling of bars with quantifier elimination	Ioakimidis, N.I.	2018	Structures 13, pp. 47-65	1
Application of quantifier elimination to inverse buckling problems	Ioakimidis, N.I.	2017	Acta Mechanica 228(10), pp. 3709-3724	1
Application of quantifier elimination to mixed-mode fracture criteria in crack problems	Ioakimidis, N.I.	2017	Archive of Applied Mechanics 87(10), pp. 1567-1604	0
Caustics, pseudocaustics and the related illuminated and dark regions with the computational method of quantifier elimination	Ioakimidis, N.I.	2017	Optics and Lasers in Engineering 88, pp. 280-300	3
Derivation of conditions of complete contact for a beam on a tensionless Winkler elastic foundation with Mathematica	Ioakimidis, N.I.	2016	Mechanics Research Communications 72, pp. 64-73	4
Finite differences/elements in classical beam problems: derivation of feasibility conditions under parametric inequality constraints with the help of Reduce and REDLOG	Ioakimidis, N.I.	2001	Computational Mechanics 27(2), pp. 145-153	3
Derivation of feasibility conditions in engineering problems under parametric inequality constraints with classical Fourier elimination	Ioakimidis, N.I.	2000	International Journal for Numerical Methods in Engineering 48(11), pp. 1583-1599	3

Getting closer: N. Ioakimidis

The energy method in problems of buckling of bars with quantifier elimination	Ioakimidis, N.I.	2018	Structures 13, pp. 47-65	1

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Derivation of feasibility conditions in engineering problems under parametric inequality constraints with classical Fourier elimination	Ioakimidis, N.I.	2000	International Journal for Numerical Methods in Engineering 48(11), pp. 1583-1599	3

From 1995: 22 papers

Getting closer: Alicia Dickenstein

PHOSHO-DEPHOSPHORYLATION: "FUTILE" CYCLE

$$S_0 + E \underset{k_{\mathrm{off}}}{\overset{k_{\mathrm{on}}}{\rightleftarrows}} ES_0 \overset{k_{\mathrm{cat}}}{\to} S_1 + E$$

$$S_1 + F \underset{\ell_{\mathrm{off}}}{\overset{\ell_{\mathrm{on}}}{\rightleftarrows}} FS_1 \overset{\ell_{\mathrm{cat}}}{\to} S_0 + F$$

E and F *enzymes*, S_0 and S_1 *substrates*, S_0E and S_1F *intermediates*

and we represent it with:

$$\begin{tikzcd} S_0 \arrow[r, bend left, "E"] & S_1 . \arrow[l, bend left, "F"] \end{tikzcd}$$

Getting closer: Michael Barton

We have 2nd order matching constraints

$$\begin{aligned} \nabla_{\mathbf{v}} d &= r'(s) \\ \nabla_{\mathbf{v}}(\nabla_{\mathbf{v}} d) = \nabla^2_{\mathbf{v}} d &= r''(s) \end{aligned}$$

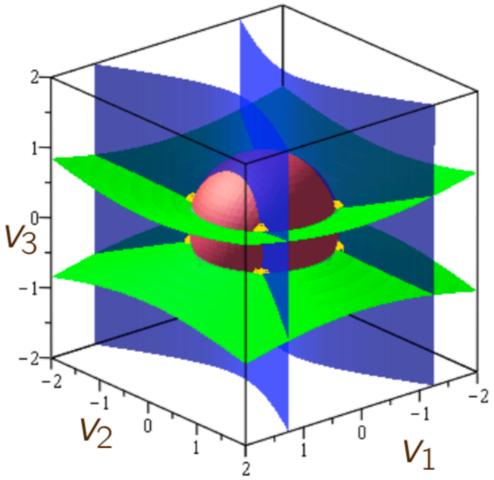
and surface distance approximation

$$\widetilde{d}(\mathbf{x}, \Gamma) = x_3 + \frac{1}{2(h-\rho_1)} x_1^2 + \frac{1}{2(h-\rho_2)} x_2^2$$

and seek a unit vector $\mathbf{v} = (v_1, v_2, v_3)$.

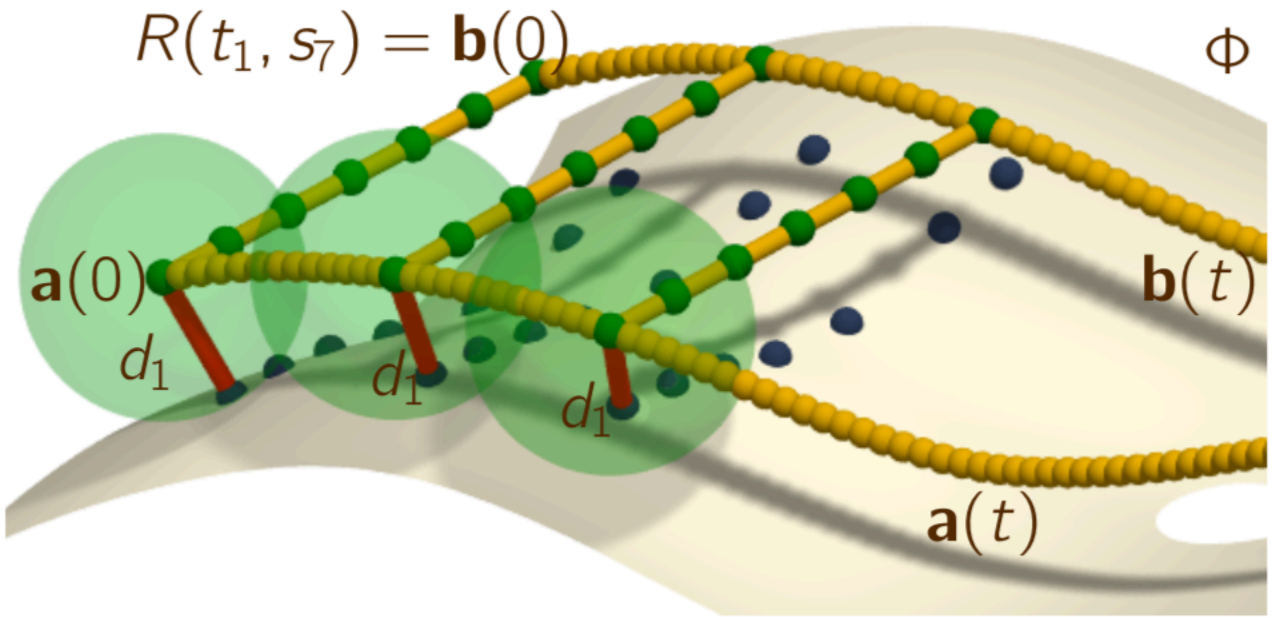
We obtain

$$\begin{aligned} v_1^2 + v_2^2 &= 1 - r'(s)^2 \\ \frac{v_1^2}{r(s)-\rho_1} + \frac{v_2^2}{r(s)-\rho_2} &= r''(s). \end{aligned}$$



4 solutions
(in general)

optimize both surface of revolution and its motion



Getting closer: C. Bajaj, B. Juttler,

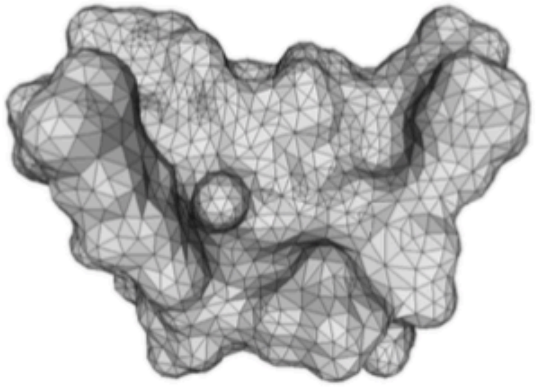
ISOGEOMETRIC ANALYSIS

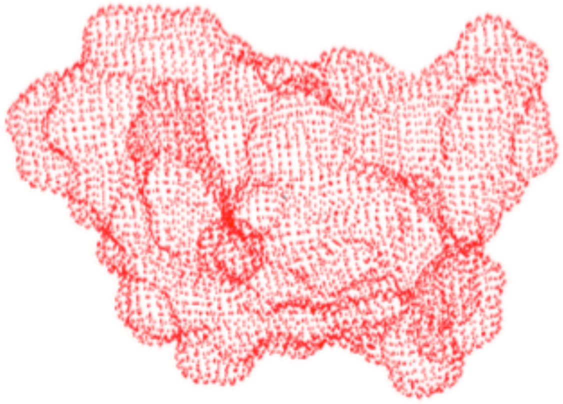
Fast Computation of Born Radii

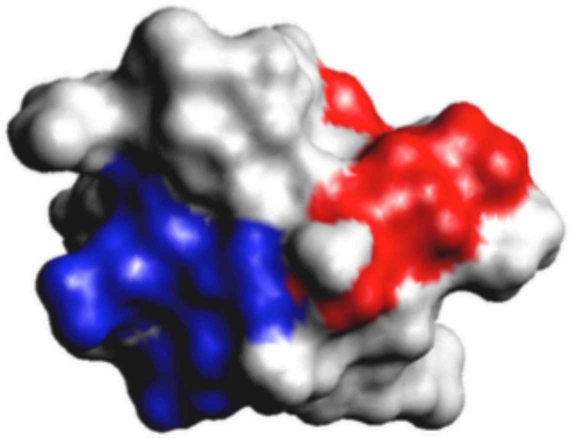
$$R_i^{-1} = \frac{1}{4\pi}\int_{\Gamma} \frac{(\mathbf{r}-\mathbf{x}_i).\mathbf{n}(\mathbf{r})}{|\,\mathbf{r}-\mathbf{x}_i\,|^4}\, dS \approx \frac{1}{4\pi}\sum_{k=1}^{N} w_k \frac{(\mathbf{r}_k-\mathbf{x}_i).\mathbf{n}(\mathbf{r}_k)}{|\,\mathbf{r}_k-\mathbf{x}_i\,|^4} \qquad \mathbf{r}_k \in \Gamma$$

Algorithm:

1. Generate a *smooth* algebraic spline boundary element model for the molecular surface Γ .
2. Cubature: choose w_k and $\mathbf{r}_k$ properly so that *higher order* accuracy can be obtained for *small* N. [Parameterization]
3. *Fast summation* using non-uniform FFT to evaluate R_i , $i = 1,\ldots,M$.







The future: opportunities

F. Chazal, B. Michel. An introduction to Topological Data Analysis: fundamental and practical aspects for data scientists. 2017. arXiv:1710.04019.

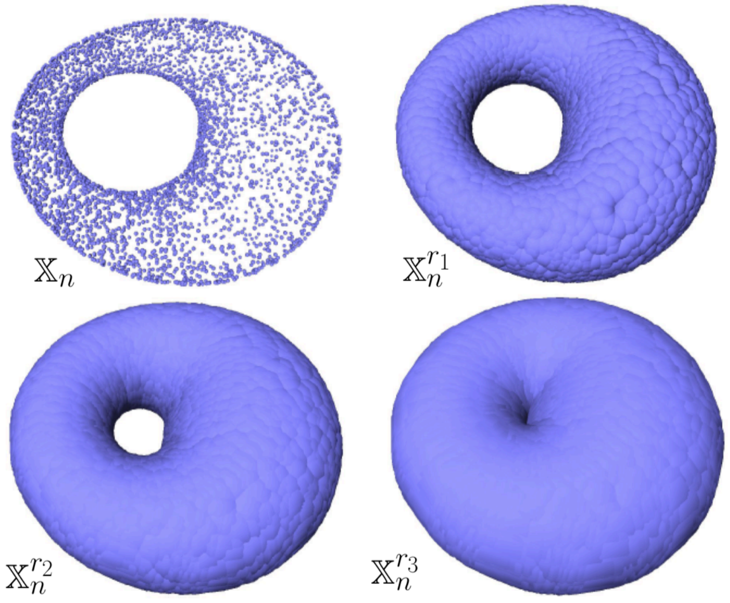


Figure 7: The example of a point cloud $\mathbb{X}_n$ sampled on the surface of a torus in $\mathbb{R}^3$ (top left) and its offsets for different values of radii $r_1 < r_2 < r_3$. For well chosen values of the radius (e.g. r_1 and r_2), the offsets are clearly homotopy equivalent to a torus.

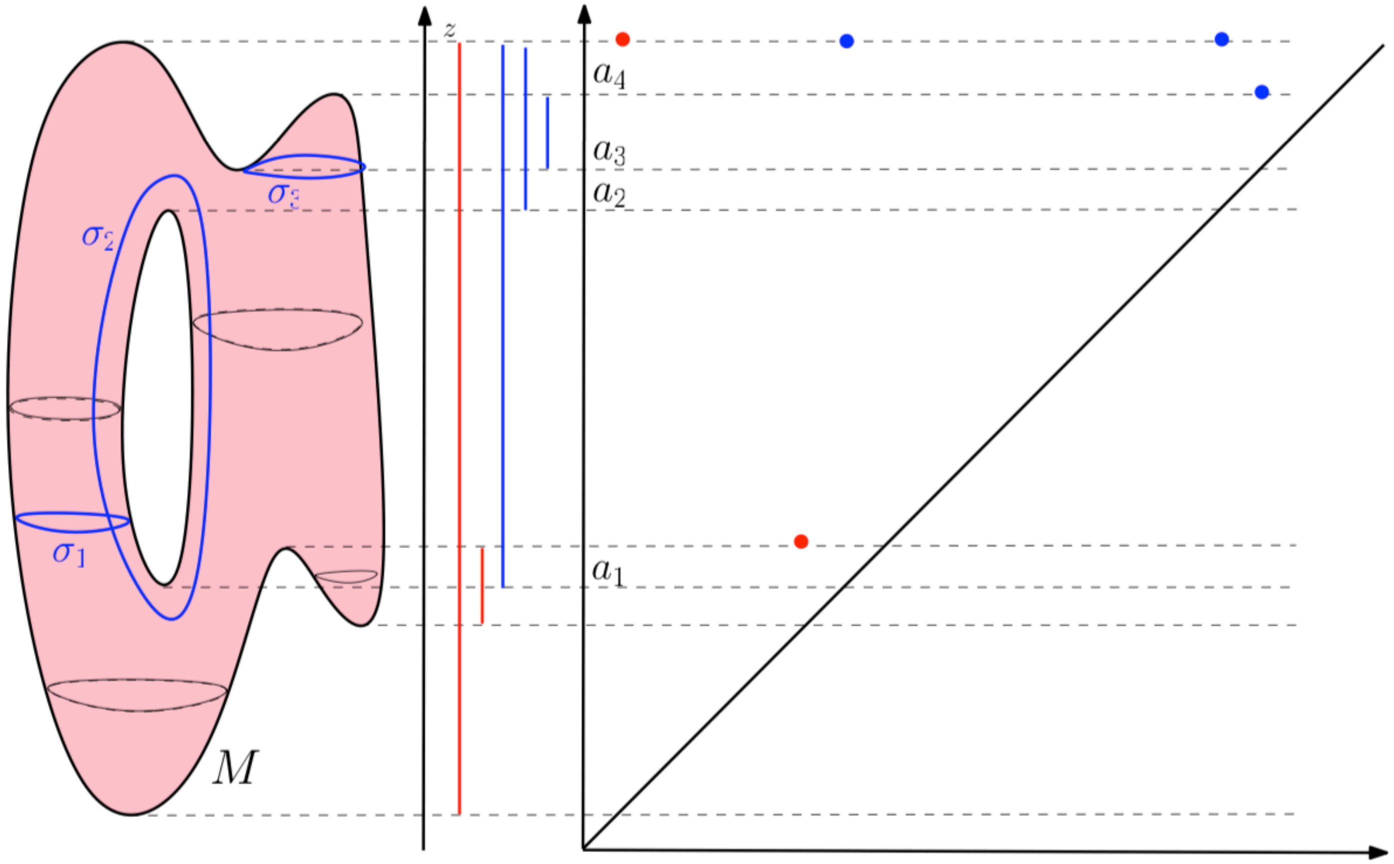
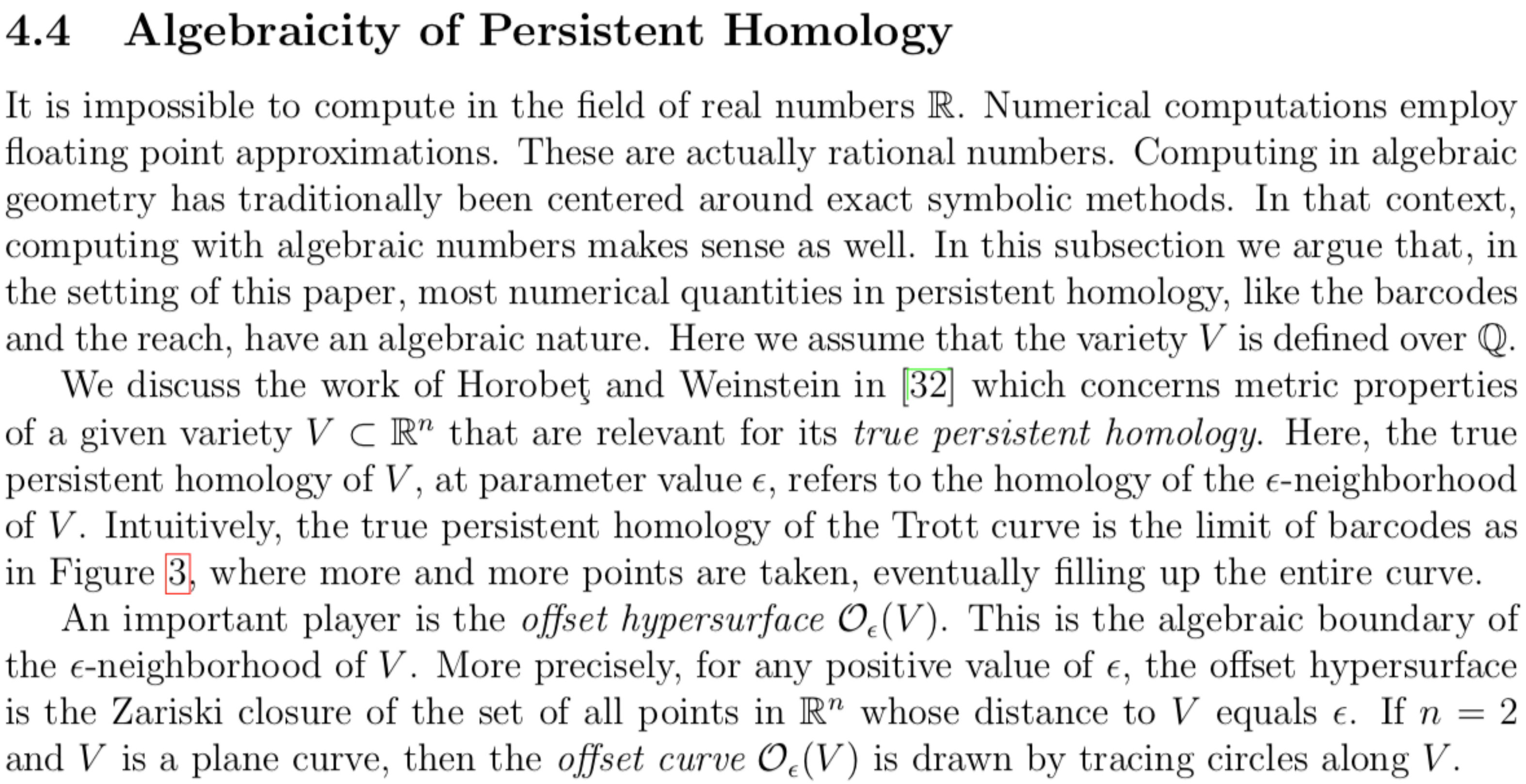


Figure 12: The persistence barcode and the persistence diagram of the height function (projection on the z-axis) defined on a surface in $\mathbb{R}^3$.

Topological Data Analysis

[Ana, Luis Felipe, Andratx, …]

The future: opportunities



4.4 Algebraicity of Persistent Homology

It is impossible to compute in the field of real numbers $\mathbb{R}$. Numerical computations employ floating point approximations. These are actually rational numbers. Computing in algebraic geometry has traditionally been centered around exact symbolic methods. In that context, computing with algebraic numbers makes sense as well. In this subsection we argue that, in the setting of this paper, most numerical quantities in persistent homology, like the barcodes and the reach, have an algebraic nature. Here we assume that the variety V is defined over $\mathbb{Q}$.

We discuss the work of Horobeţ and Weinstein in [32] which concerns metric properties of a given variety $V \subset \mathbb{R}^n$ that are relevant for its *true persistent homology*. Here, the true persistent homology of V, at parameter value ϵ, refers to the homology of the ϵ-neighborhood of V. Intuitively, the true persistent homology of the Trott curve is the limit of barcodes as in Figure 3, where more and more points are taken, eventually filling up the entire curve.

An important player is the *offset hypersurface* $\mathcal{O}_\epsilon(V)$. This is the algebraic boundary of the ϵ-neighborhood of V. More precisely, for any positive value of ϵ, the offset hypersurface is the Zariski closure of the set of all points in $\mathbb{R}^n$ whose distance to V equals ϵ. If $n = 2$ and V is a plane curve, then the *offset curve* $\mathcal{O}_\epsilon(V)$ is drawn by tracing circles along V.

Topological Data Analysis

[Ana, Luis Felipe, Andratx, …]

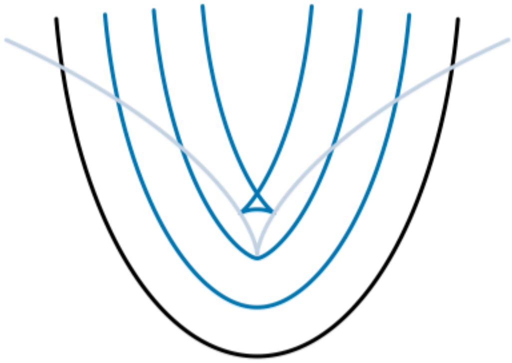
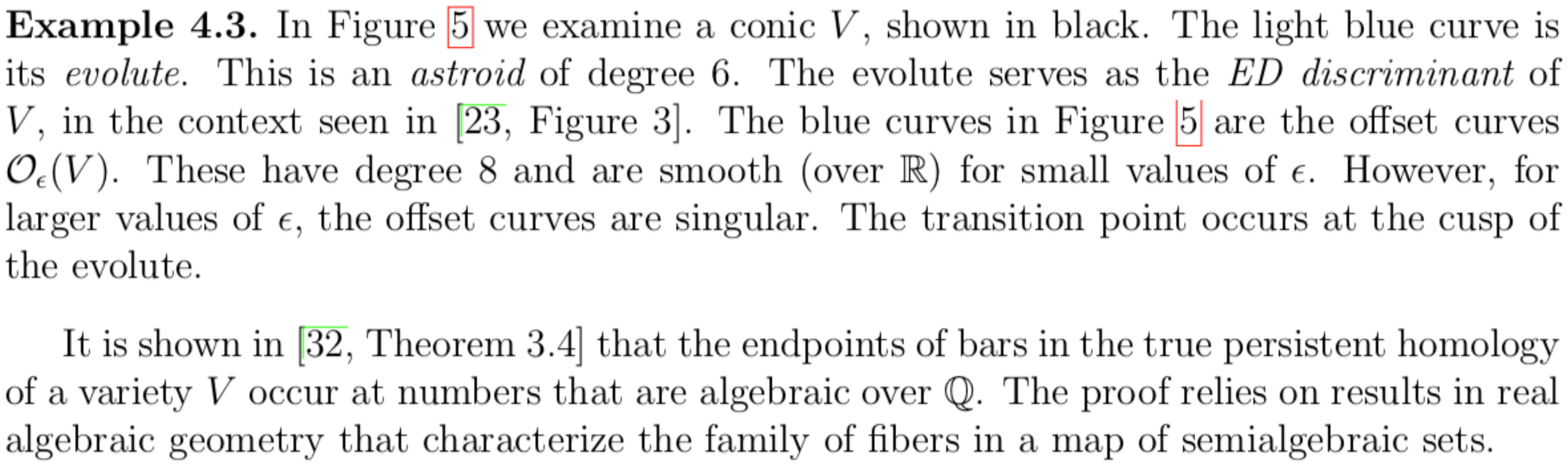


Figure 5: Offset curves (blue) and the evolute (light blue) of a conic (black).

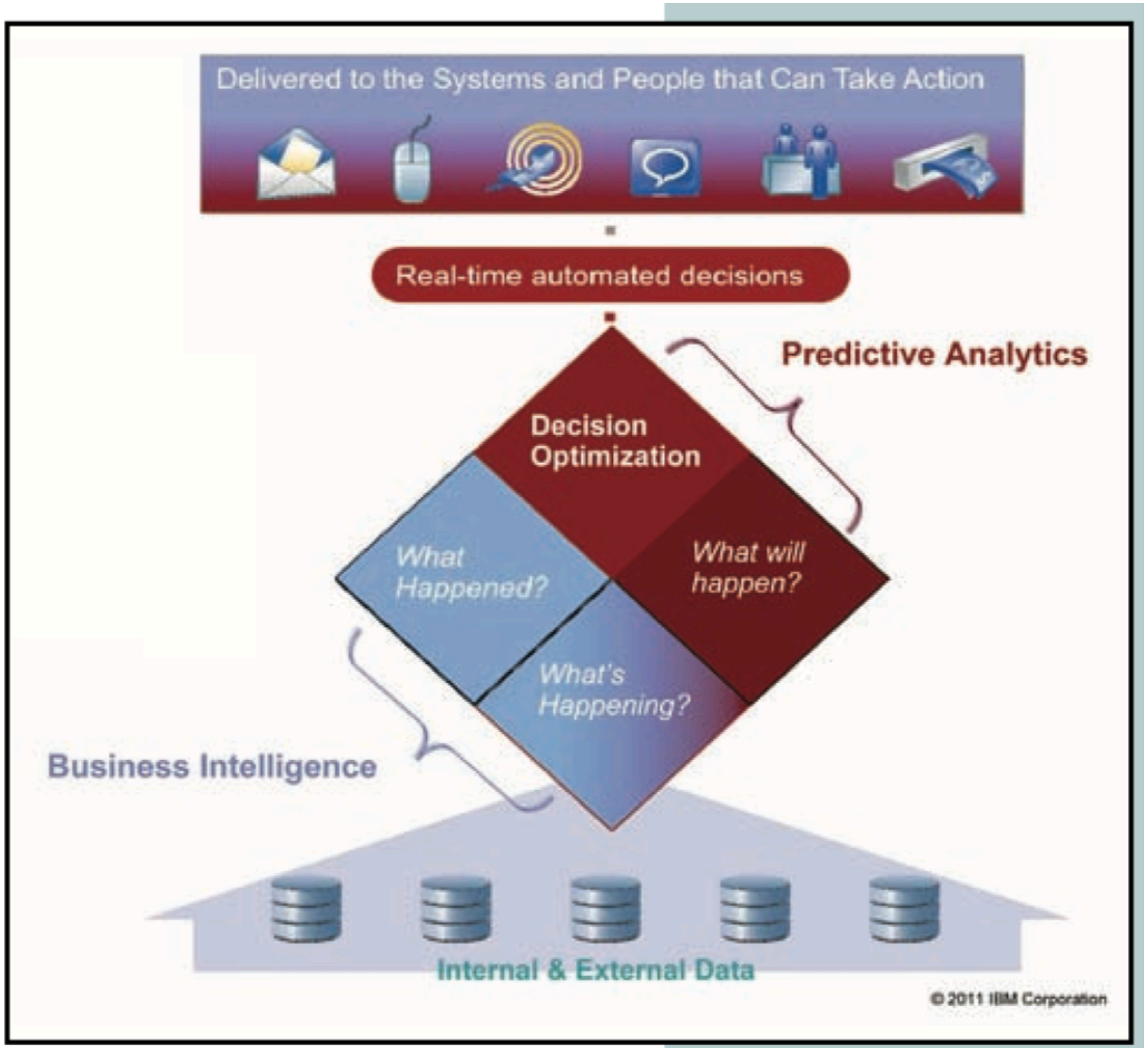
P. Breiding, S. K. Verovsek, B. Sturmfels, M. Weinstein: Learning Algebraic Varieties from Samples. 2018. arXiv:1802.09436



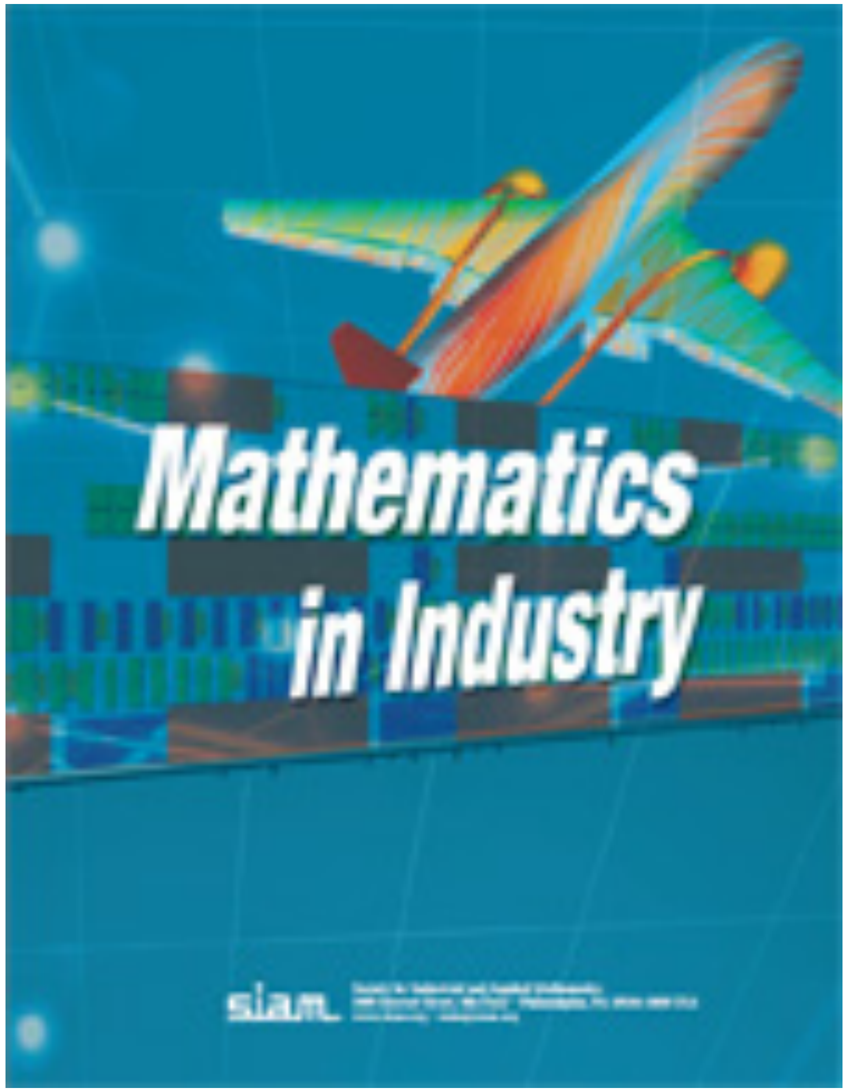
Example 4.3. In Figure 5 we examine a conic V, shown in black. The light blue curve is its *evolute*. This is an *astroid* of degree 6. The evolute serves as the *ED discriminant* of V, in the context seen in [23, Figure 3]. The blue curves in Figure 5 are the offset curves $\mathcal{O}_\epsilon(V)$. These have degree 8 and are smooth (over $\mathbb{R}$) for small values of ϵ. However, for larger values of ϵ, the offset curves are singular. The transition point occurs at the cusp of the evolute.

It is shown in [32, Theorem 3.4] that the endpoints of bars in the true persistent homology of a variety V occur at numbers that are algebraic over $\mathbb{Q}$. The proof relies on results in real algebraic geometry that characterize the family of fibers in a map of semialgebraic sets.

The future: opportunities



Automating decisions in business processes, IBM Corporation



The long and winding road

But “real” cooperation with industry is much more complex than dealing with the Mathematics behind the applied problems they are dealing with.

The long and winding road

Software interfaces

The language problem [JC]

The time constraints

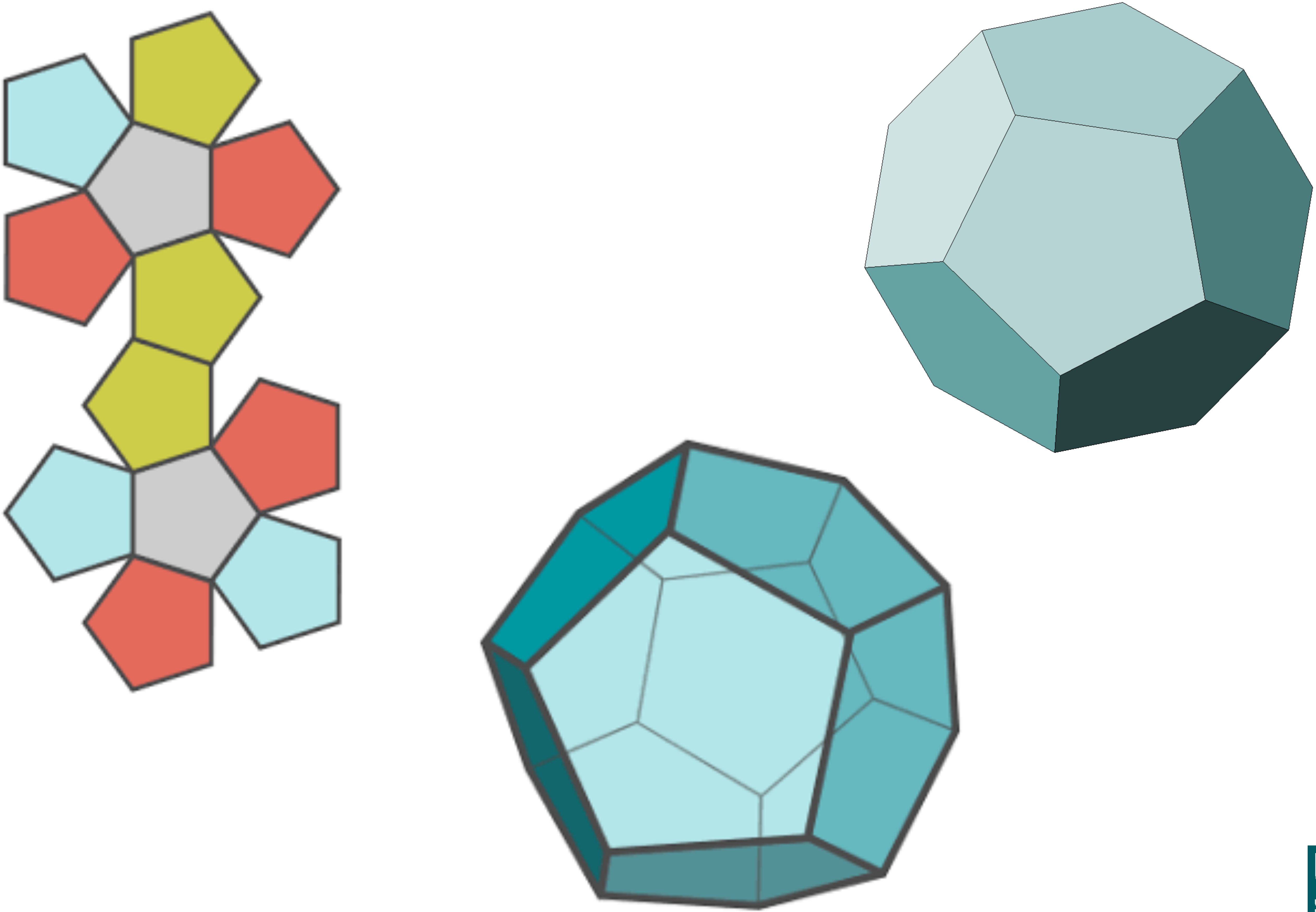
The constraints (any kind)

Entornos VUCA:

Volatility, Uncertainty,

Complexity & Ambiguity

The long and winding road



The long and winding road

The long and winding road
That leads to your door
Will never disappear
I've seen that road before
It always leads me her
Lead me to you door

The wild and windy night
That the rain washed away
Has left a pool of tears
Crying for the day
Why leave me standing here
Let me know the way

Many times I've been alone
And many times I've cried
Any way you'll never know
The many ways I've tried

But still they lead me back
To the long winding road
You left me standing here
A long long time ago
Don't leave me waiting here
Lead me to your door

But still they lead me back
To the long winding road
You left me standing here
A long long time ago
Don't leave me waiting here
Lead me to your door

John Lennon / Paul Mccartney
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