swMATH
The Publication-based Approach to Software

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Zuse Institute Berlin (ZIB)

Open Science Days 2019
5./6. February 2019

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MODAL
Mathematical Optimization and Data Analysis Laboratories

zbMATH
the first resource for mathematics

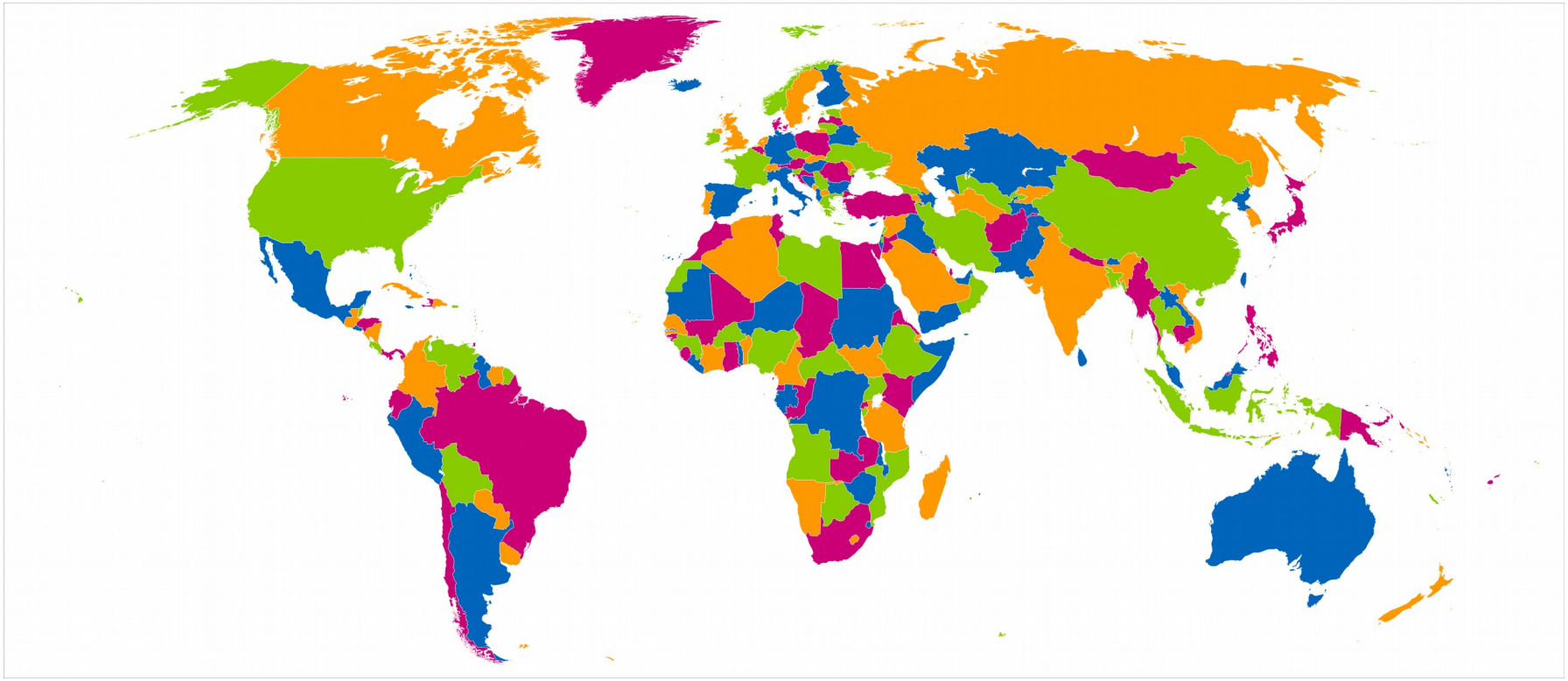
The Zuse Institute Berlin (ZIB)

is an interdisciplinary research institute for applied mathematics and data-intensive high-performance computing. Its research focuses on modeling, simulation and optimization with scientific cooperation partners from academia and industry.

Scientific Software in Mathematics

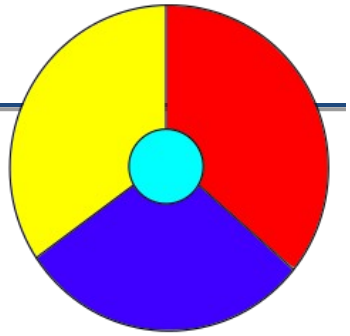
- Increasing role of scientific software
- Less credit for software developer
- An established infrastructure is missing
  - Standards
  - Information Services
  - „Reinvent the wheel“
  - Verification
  - Reproducibility

Famous Example: Four Color Theorem



„Every planar map can be colored with at most four colors“

Verifiability and Reproducibility



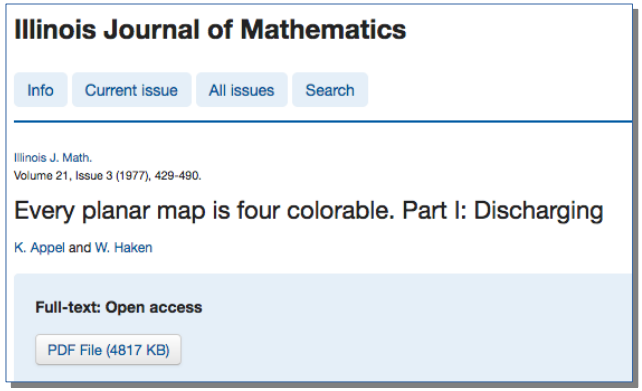
Have you ever tried to verify the four color theorem?

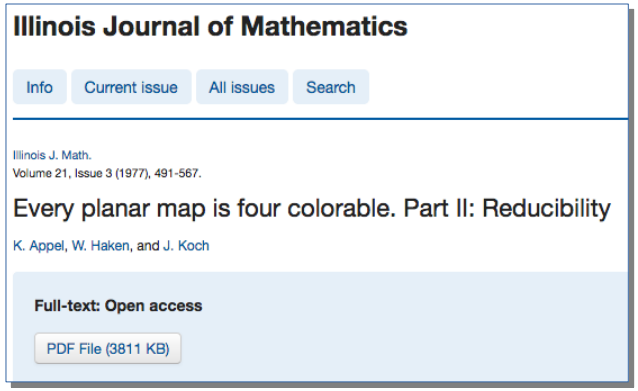
„Every planar map can be colored with at most four colors"

en.wikipedia.orgwiki/Four_color_theorem:

- proved in 1976 by K. Appel & W. Haken using a computer
- their proof were not accepted at all (infeasible for a human to check by hand)
- in 1997 was published a simpler proof by Robertson, Sanders, Seymour, and Thomas
- in 2005 the theorem was proved by Benjamin Werner and Georges Gonthier with Coq, a theorem-proving software

Four Color Theorem: The Article





2. The computer programs

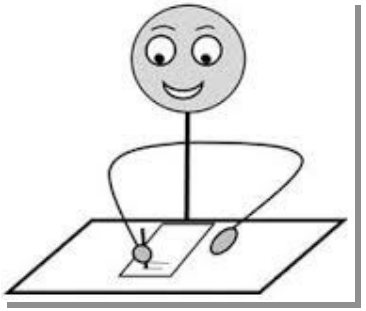
runs over 1,200 hours on IBM /370

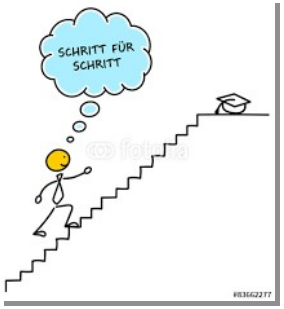
D-reduction was done dynamically (see [2]) in the sense that once a coloration was proved good, its goodness was immediately available for use in the testing of other colorations. The programs for D-reduction are extensions and modifications of those in [20].

The computer programs were greatly influenced by the facilities available. We had access to IBM computers (a 360-75 at Urbana-Champaign, a 370-158 at the University's Chicago Circle Campus, and later a 370-168 of the University of Illinois administrative data processing unit). For this reason the programs were written in IBM assembler language to attempt to maximize efficiency. When we inquired, the operations staff suggested that we use less computer time at the expense of larger amounts of core storage. Therefore, to save steps we chose to use large tables. The core storage requirements were as follows: for twelve-rings, 220,000 bytes; for thirteen-rings, 600,000 bytes; for fourteen-rings, 1,700,000 bytes.

Scientific Workflow

Scientist





Software Developer

Scientific Software in Mathematics

Scientific Software

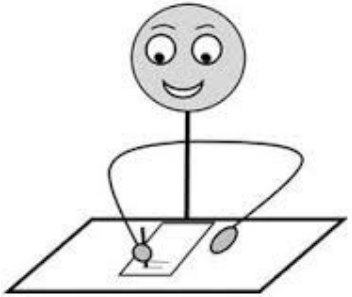
- plays an important role within the scientific workflow
- produces new scientific results
- is (sometimes/often) the base of a proof
  - e.g. four color problem/Vierfarbenproblem

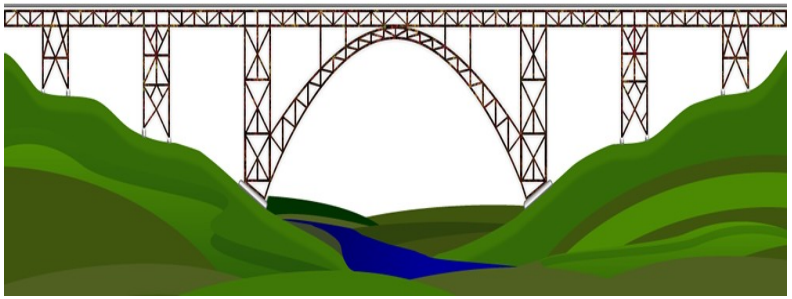
Scientific Software Developer

- receives little or no scientific recognition
- gets no or less academic reputation
- gets no credit points in his academic career

Bridging the Gap: www.swmath.org

- makes important software visible
- findable (unique and persistent identifier)
- accessible





- main idea: publication-based approach
- general: machine-based analysis of the content of publications
- cooperation with Zentralblatt MATH (zbMATH)

What is zbMATH (zbMATH.org)?

zbMATH is an abstracting and reviewing service in pure and applied mathematics

Jahrbuch

über die

Fortschritte der Mathematik

im Verein mit anderen Mathematikern

herausgegeben

von

Carl Ohrtmann, Felix Müller, Albert Wangerin.

Fünfter Band.

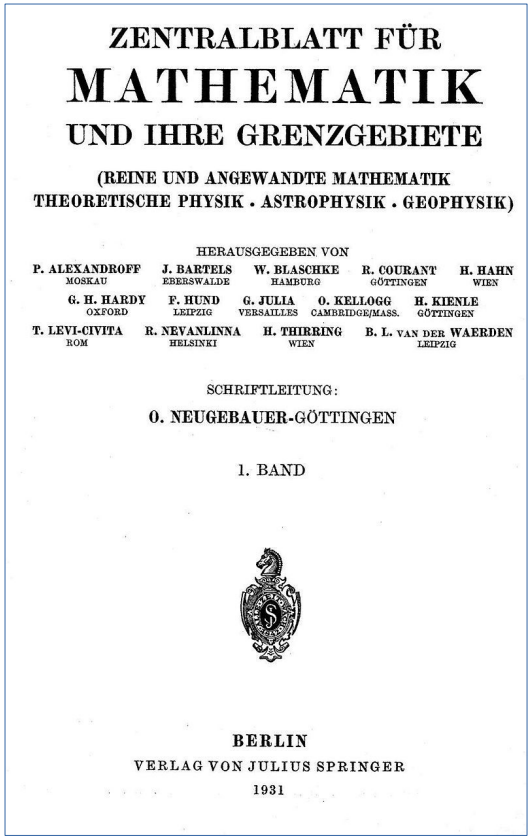
Jahrgang 1873.

Berlin.

Druck und Verlag von Georg Reimer.

1875.

1868-1942



ZENTRALBLATT FÜR

MATHEMATIK

UND IHRE GRENZGEBIETE

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zbMATH in Numbers

- zbMATH covers all available published and peer-reviewed articles, books, conference proceedings as well as other publication formats
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Achterberg, Tobias

SCIP: solving constraint integer programs. (English) Zbl 1171.90476

Math. Program. Comput. 1, No. 1, 1-41 (2009).

Summary: Constraint integer programming (CIP) is a novel paradigm which integrates constraint programming (CP), mixed integer programming (MIP), and satisfiability (SAT) modeling and solving techniques. In this paper we discuss the software framework and solver SCIP (Solving Constraint Integer Programs), which is free for academic and non-commercial use and can be downloaded in source code. This paper gives an overview of the main design concepts of SCIP and how it can be used to solve constraint integer programs. To illustrate the performance and flexibility of SCIP, we apply it to two different problem classes. First, we consider mixed integer programming and show by computational experiments that SCIP is almost competitive to specialized commercial MIP solvers, even though SCIP supports the more general constraint integer programming paradigm. We develop new ingredients that improve current MIP solving technology. As a second application, we employ SCIP to solve chip design verification problems as they arise in the logic design of integrated circuits. This application goes far beyond traditional MIP solving, as it includes several highly non-linear constraints, which can be handled nicely within the constraint integer programming framework. We show anecdotally how the different solving techniques from MIP, CP, and SAT work together inside SCIP to deal with such constraint classes. Finally, experimental results show that our approach outperforms current state-of-the-art techniques for proving the validity of properties on circuits containing arithmetic.

Cited in **144** Documents

MSC:

90C11	Mixed integer programming
68T20	AI problem solving (heuristics, search strategies, etc.)
90C27	Combinatorial optimization
90-04	Machine computation, programs (optimization)
90-08	Computational methods (optimization)

Keywords:
constraint programming; integer programming; SAT

Software:
Decision tree for optimization software; MIPLIB; Chaff; Valse-XT; SoPlex; Mosek; SCIL; SIMPL; CPLEX; MiniSat; Siege; ABACUS; MIPLIB2003; CLP; Zimpl; FEASPUMP; SCIP; Benchmarks for Optimization Software; COIN-OR; Tabu search; XPRESS

PDF | BibTeX | XML | Cite | Full Text: DOI

zbMATH Entry (cont.)

Software:
Decision tree for optimization software; MIPLIB; Chaff; Valse-XT; SoPlex; Mosek; SCIL; SIMPL; CPLEX; MiniSat; Siege; ABACUS; MIPLIB2003; CLP; Zimpl; FEASPUMP; SCIP; Benchmarks for Optimization Software; COIN-OR; Tabu search; XPRESS

PDF | BibTeX | XML | Cite Full Text: DOI

References:

[1] Achterberg T.: Conflict analysis in mixed integer programming. Discret. Optim. 4(1), 4--20 (2007) (special issue: Mixed Integer Programming) · Zbl 1169.90414 · doi:10.1016/j.disopt.2006.10.006

[2] Achterberg, T.: Constraint Integer Programming. Ph.D. Thesis, Technische Universität Berlin (2007). http://opus.kobv.de/tuberlin/volltexte/2007/1611/

[3] Achterberg T., Berthold T.: Improving the feasibility pump. Discret. Optim. 4(1), 77--86 (2007) (special issue: Mixed Integer Programming) · Zbl 1170.90443 · doi:10.1016/j.disopt.2006.10.004

[4] Achterberg, T., Berthold, T., Koch, T., Wolter, K.: Constraint integer programming: a new approach to integrate CP and MIP. In: Perron, L., Trick, M.A. (eds.) Integration of AI and OR techniques in constraint programming for combinatorial optimization problems, 5th international conference, CPAIOR 2008. Lecture Notes in Computer Science, vol. 5015, pp. 6--20. Springer, Heidelberg (2008) · Zbl 1142.68504

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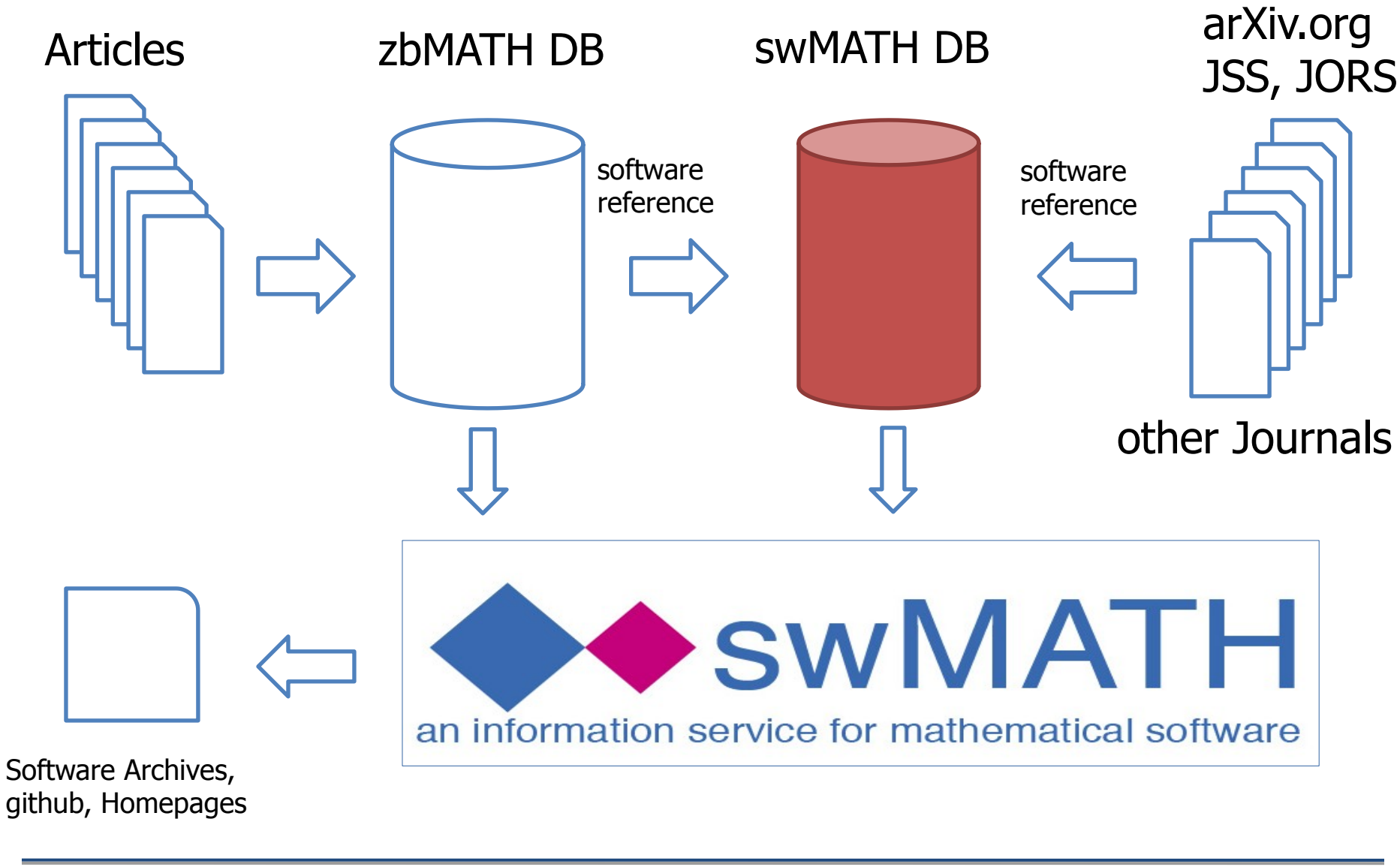
Main Idea: Publication-based Approach

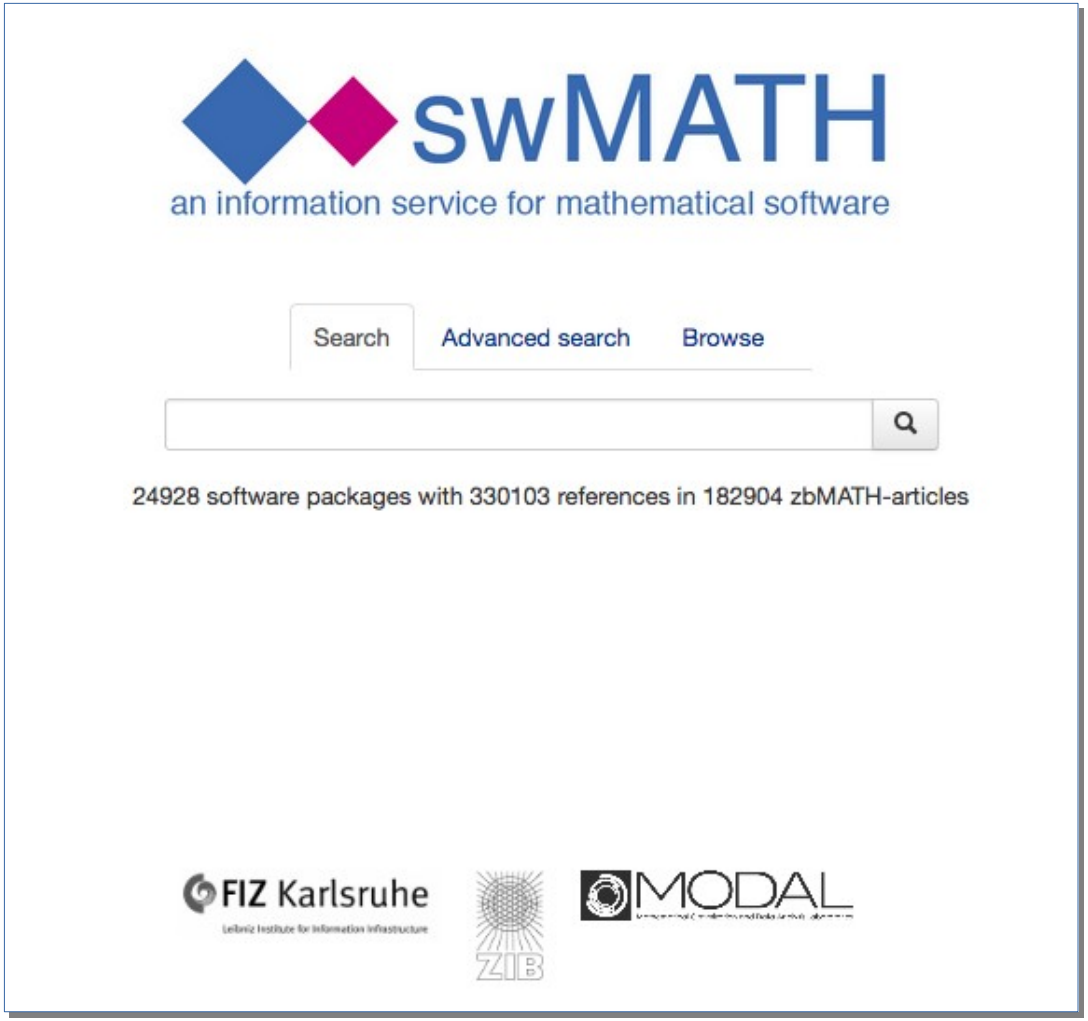
- identification and analysis of software references in publications
  - → which articles refer/review software in zbMATH?
  - → store the result (publication/software) into a database

- swMATH offers a list of all publications and articles listed in Zentralblatt MATH (zbMATH) that refer to software
- swMATH includes also articles which describe the background and technical details of a program, as well as those publications in which a piece of software is applied or used for research

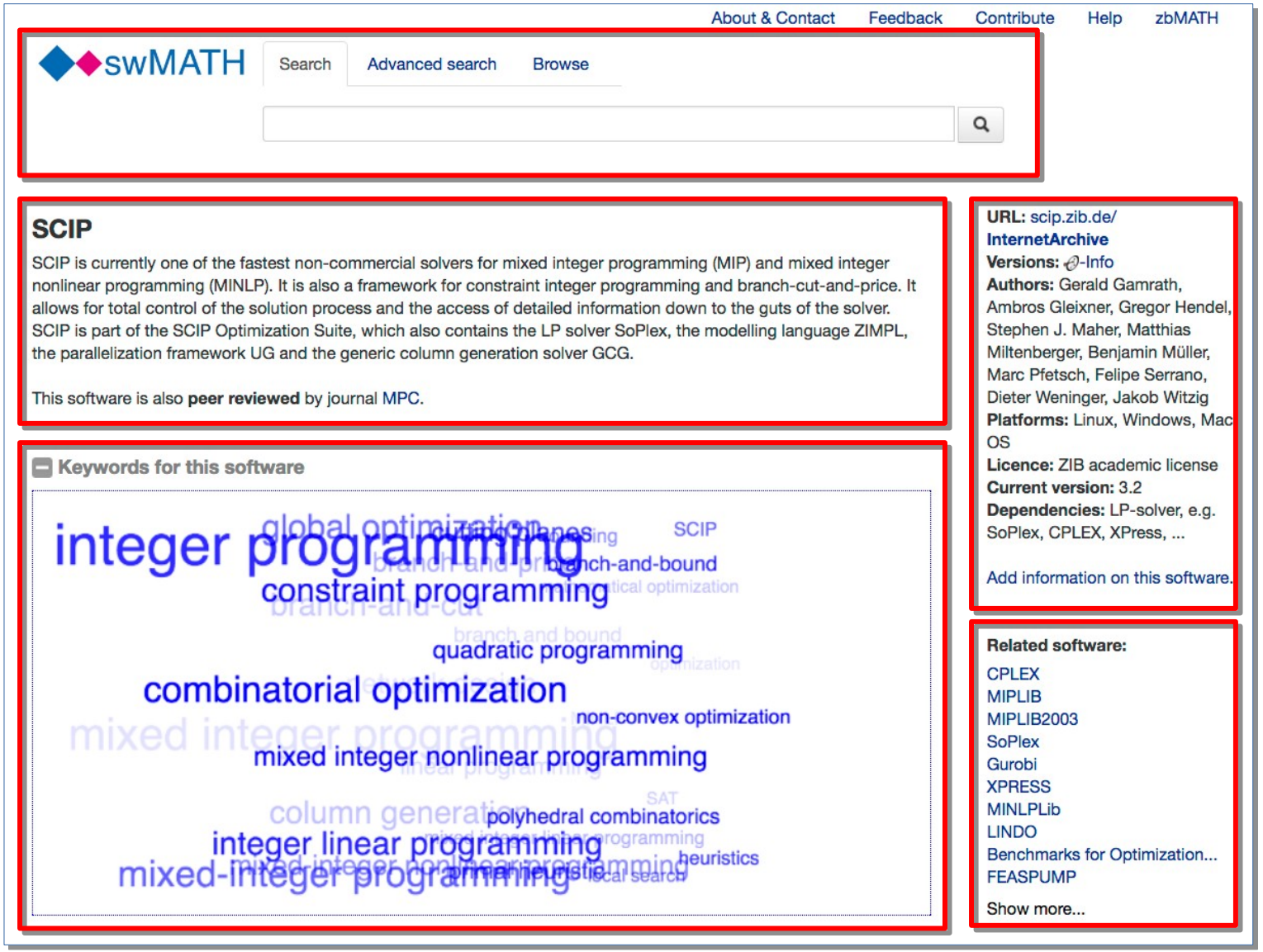
Building swMATH



Quick Overview: www.swmath.org



Example: Searching for SCIP



Example cont.

References in zbMATH (referenced in 237 articles , 4 standard articles)

Showing results 1 to 20 of 237. Sorted by year (citations) 20

1 2 3 ... 10 11 12 next

Andrea Callia D'Iddio, Michael Huth: Manyopt: An Extensible Tool for Mixed, Non-Linear Optimization Through SMT. Solving (2017) arXiv

2. Assarf, Benjamin; Gawrilow, Ewgenij; Herr, Katrin; Joswig, Michael; Lorenz, Benjamin; Paffenholz, Andreas; Rehn, Thomas: Computing convex hulls and counting integer points with polymake (2017)
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4. Brinkmann, Philip; Ziegler, Günter M.: A flag vector of a 3-sphere that is not the flag vector of a 4-polytope (2017)
5. Cussens, James; Järvisalo, Matti; Korhonen, Janne H.; Bartlett, Mark: Bayesian network structure learning with integer programming: polytopes, facets and complexity (2017)
6. Gleixner, Ambros M.; Berthold, Timo; Müller, Benjamin; Weltge, Stefan: Three enhancements for optimization-based bound tightening (2017)
7. Göttlich, Simone; Potschka, Andreas; Ziegler, Ute: Partial outer convexification for traffic light optimization in road networks (2017)
8. Haws, David; Cussens, James; Studený, Milan: Polyhedral approaches to learning Bayesian networks (2017)
9. Humpola, Jesco; Serrano, Felipe: Sufficient pruning conditions for MINLP in gas network design (2017)
10. Ichim, Bogdan; Katthän, Lukas; Moyano-Fernández, Julio José: How to compute the Stanley depth of a module (2017)
11. Khan, Kamil A.; Watson, Harry A.J.; Barton, Paul I.: Differentiable McCormick relaxations (2017)
12. Lima, Ricardo M.; Grossmann, Ignacio E.: On the solution of nonconvex cardinality Boolean quadratic programming problems: a computational study (2017)
13. Modaresi, Sina; Vielma, Juan Pablo: Convex hull of two quadratic or a conic quadratic and a quadratic inequality (2017)
14. Newby, Eric; Ali, M.M.: Linear transformation based solution methods for non-convex mixed integer quadratic programs (2017)
15. Pecin, Diego; Pessoa, Artur; Poggi, Marcus; Uchoa, Eduardo: Improved branch-cut-and-price for capacitated vehicle routing (2017)
16. Pferschy, Ulrich; Staněk, Rostislav: Generating subtour elimination constraints for the TSP from pure integer solutions (2017)
17. Puranik, Yash; Sahinidis, Nikolaos V.: Bounds tightening based on optimality conditions for nonconvex box-constrained optimization (2017)
18. Witzig, Jakob; Berthold, Timo; Heinz, Stefan: Experiments with conflict analysis in mixed integer programming (2017)
19. Andreatta, G.; Casula, M.; De Francesco, C.; De Giovanni, L.: A branch-and-price based heuristic for the stochastic vehicle routing problem with hard time windows (2016)
20. Berthold, Timo; Farmer, James; Heinz, Stefan; Perregaard, Michael: Parallelization of the FICO Xpress-Optimizer (2016)

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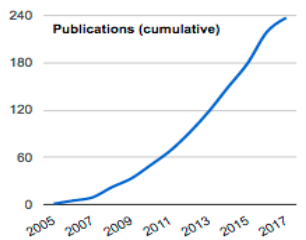
MSC classification / top

- Top MSC classes
  - **05** Combinatorics
  - **52** Convex and discrete...
  - **65** Numerical analysis
  - **68** Computer science
  - **90** Optimization
- Other MSC classes

Publication year

- 2010 - today
- 2005 - 2009
- 2000 - 2004
- before 2000

Chart: cumulative / absolute



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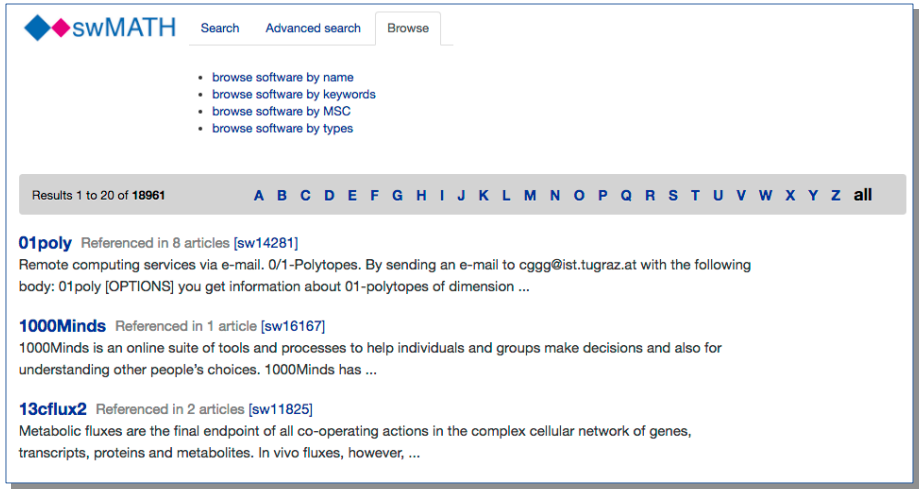

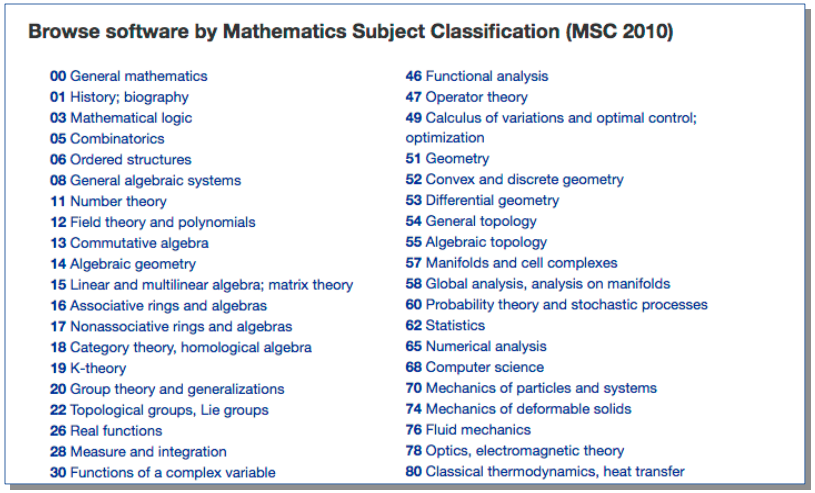

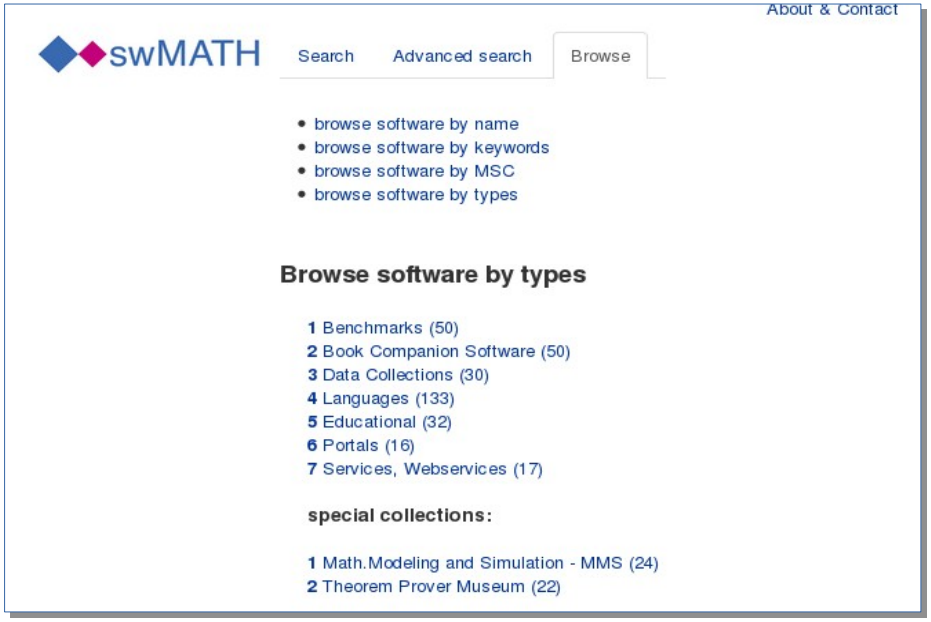

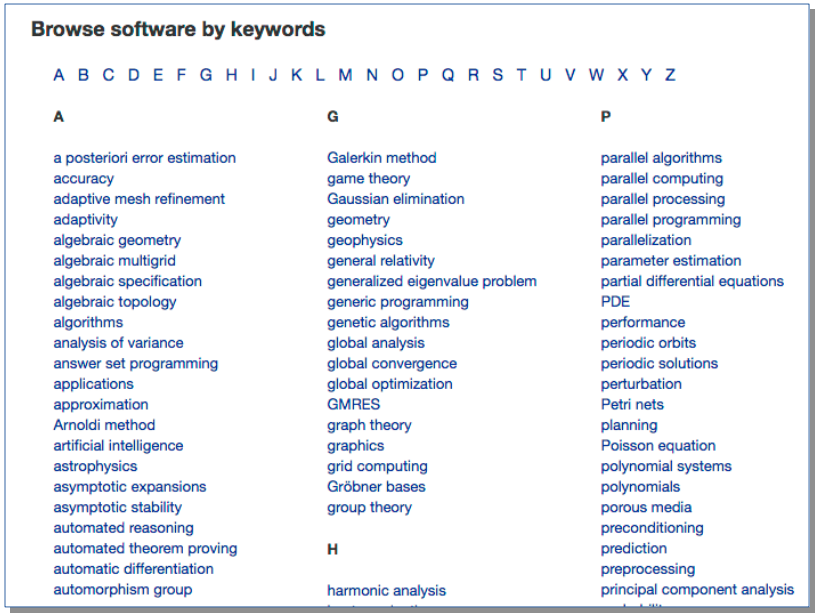

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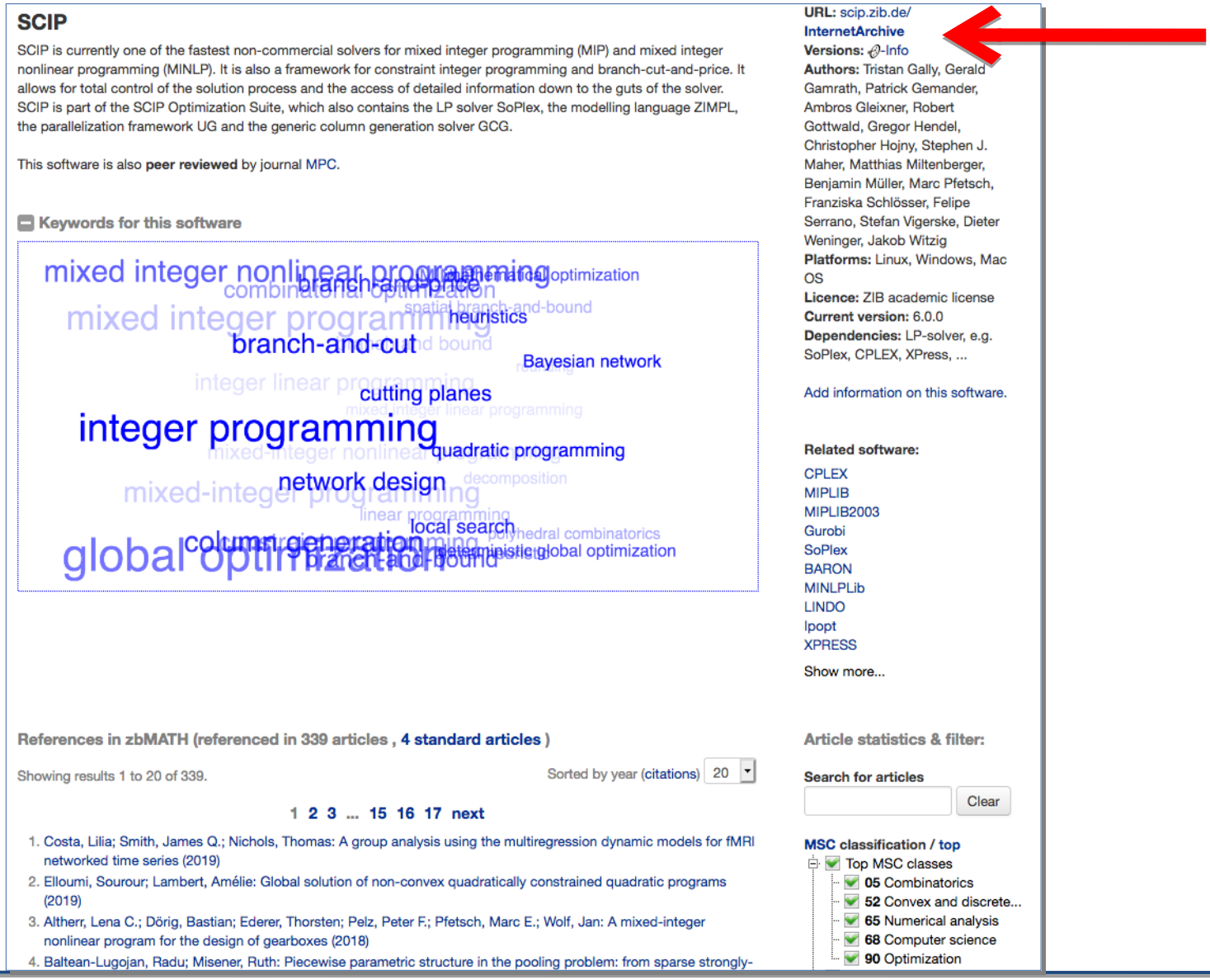

SCIP

SCIP is currently one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming (MINLP). It is also a framework for constraint integer programming and branch-cut-and-price. It allows for total control of the solution process and the access of detailed information down to the guts of the solver. SCIP is part of the SCIP Optimization Suite, which also contains the LP solver SoPlex, the modelling language ZIMPL, the parallelization framework UG and the generic column generation solver GCG.

This software is also **peer reviewed** by journal MPC.

Keywords for this software

mixed integer nonlinear programming
branch-and-price
combinatorial optimization
mixed integer programming
heuristics
branch-and-cut
Bayesian network
integer linear programming
cutting planes
integer programming
quadratic programming
network design
mixed-integer programming
decomposition
linear programming
local search
column generation
polyhedral combinatorics
deterministic global optimization
global optimization
branch and bound

URL: scip.zib.de/
InternetArchive
Versions: Info
Authors: Tristan Gally, Gerald Gamrath, Patrick Gemander, Ambros Gleixner, Robert Gottwald, Gregor Hendel, Christopher Hojny, Stephen J. Maher, Matthias Miltenberger, Benjamin Müller, Marc Pfetsch, Franziska Schlösser, Felipe Serrano, Stefan Vigerske, Dieter Weninger, Jakob Witzig
Platforms: Linux, Windows, Mac OS
Licence: ZIB academic license
Current version: 6.0.0
Dependencies: LP-solver, e.g. SoPlex, CPLEX, XPress, ...

Add information on this software.

Related software:

CPLEX
MIPLIB
MIPLIB2003
Gurobi
SoPlex
BARON
MINLPLib
LINDO
Ipopt
XPRESS

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References in zbMATH (referenced in 339 articles , 4 standard articles)

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1. Costa, Lilia; Smith, James Q.; Nichols, Thomas: A group analysis using the multiregression dynamic models for fMRI networked time series (2019)
2. Elloumi, Sourour; Lambert, Amélie: Global solution of non-convex quadratically constrained quadratic programs (2019)
3. Altherr, Lena C.; Dörig, Bastian; Ederer, Thorsten; Pelz, Peter F.; Pfetsch, Marc E.; Wolf, Jan: A mixed-integer nonlinear program for the design of gearboxes (2018)
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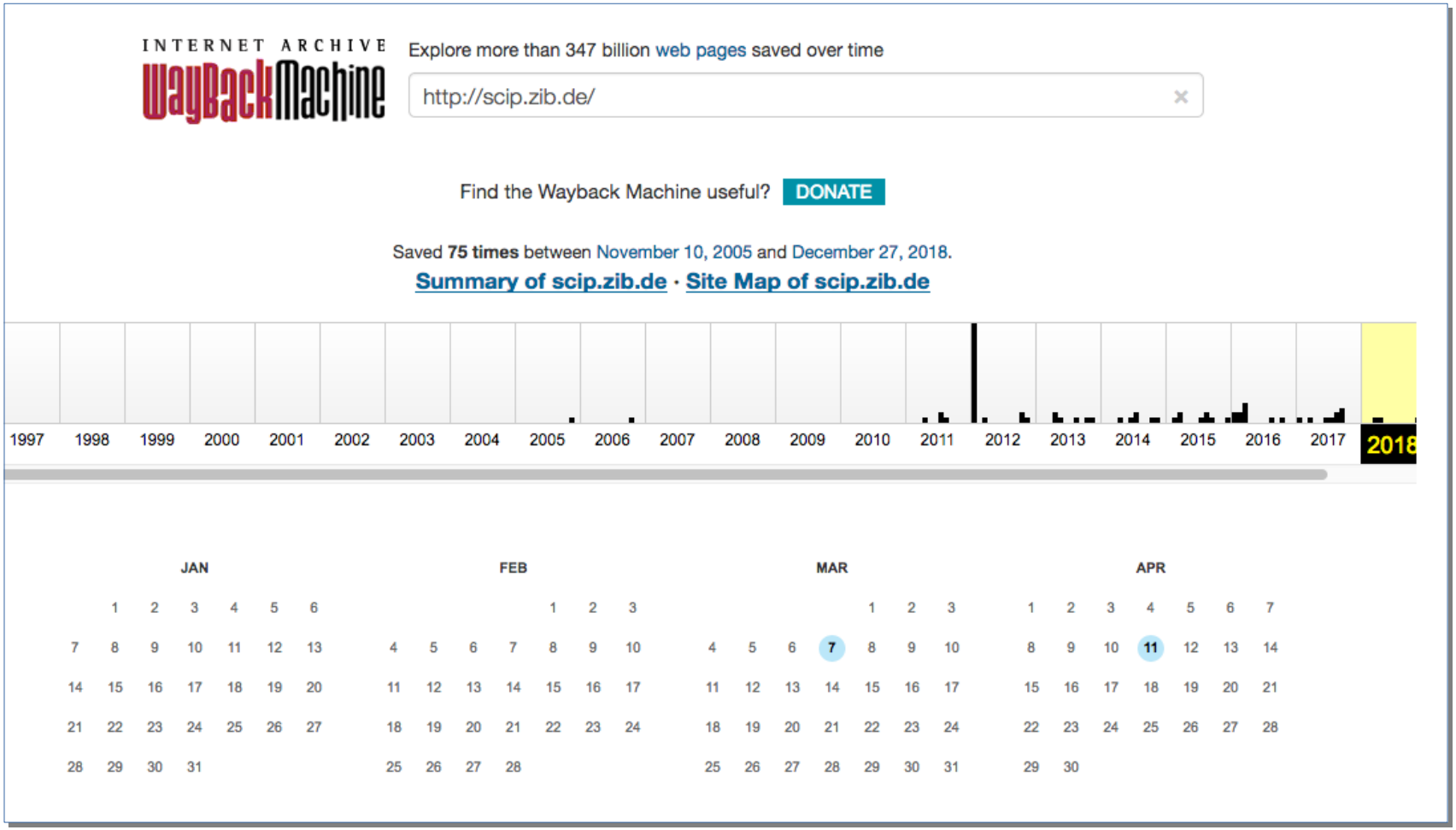
- Top MSC classes
  - **05** Combinatorics
  - **52** Convex and discrete...
  - **65** Numerical analysis
  - **68** Computer science
  - **90** Optimization

… leads to the WayBackMachine



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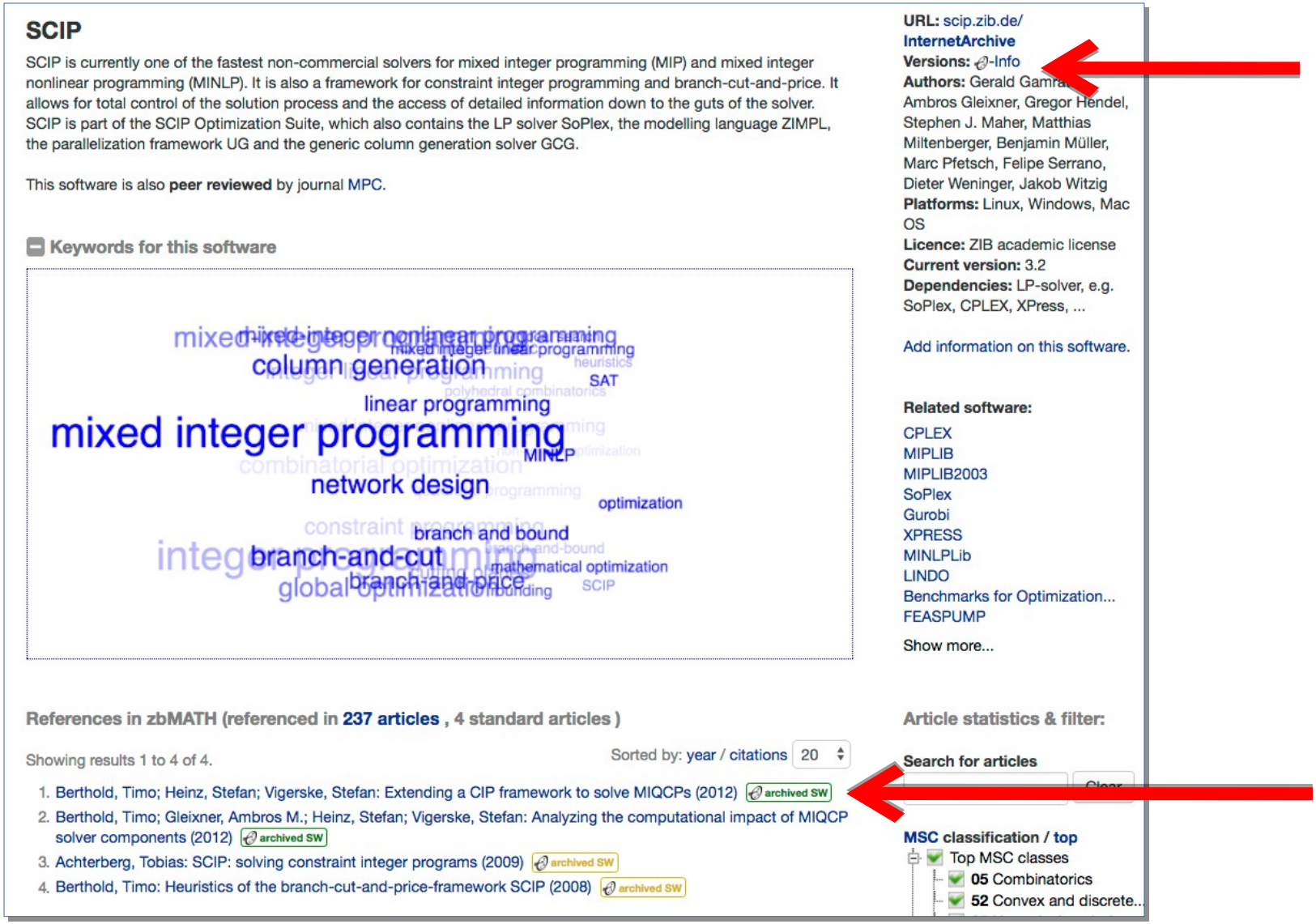
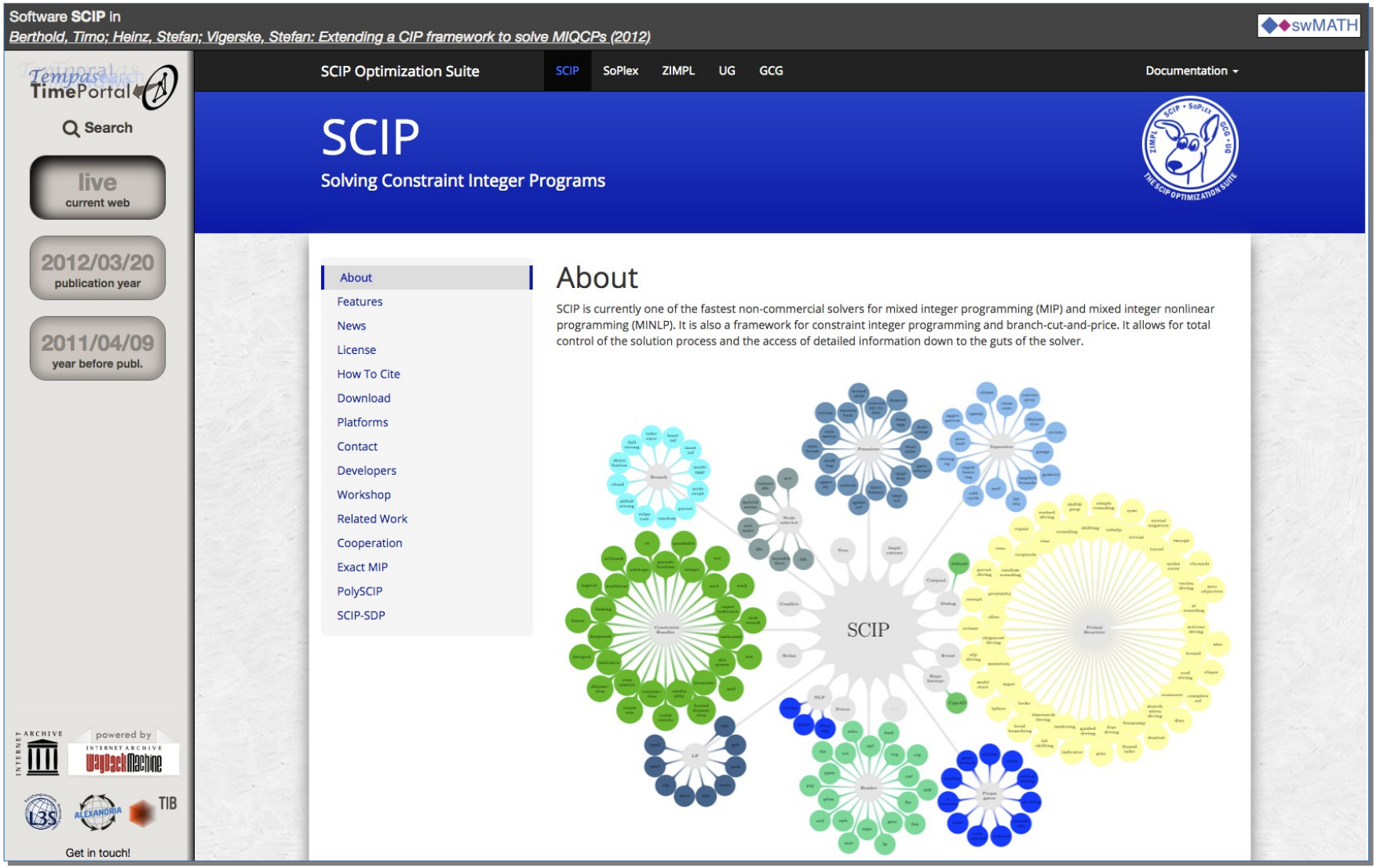
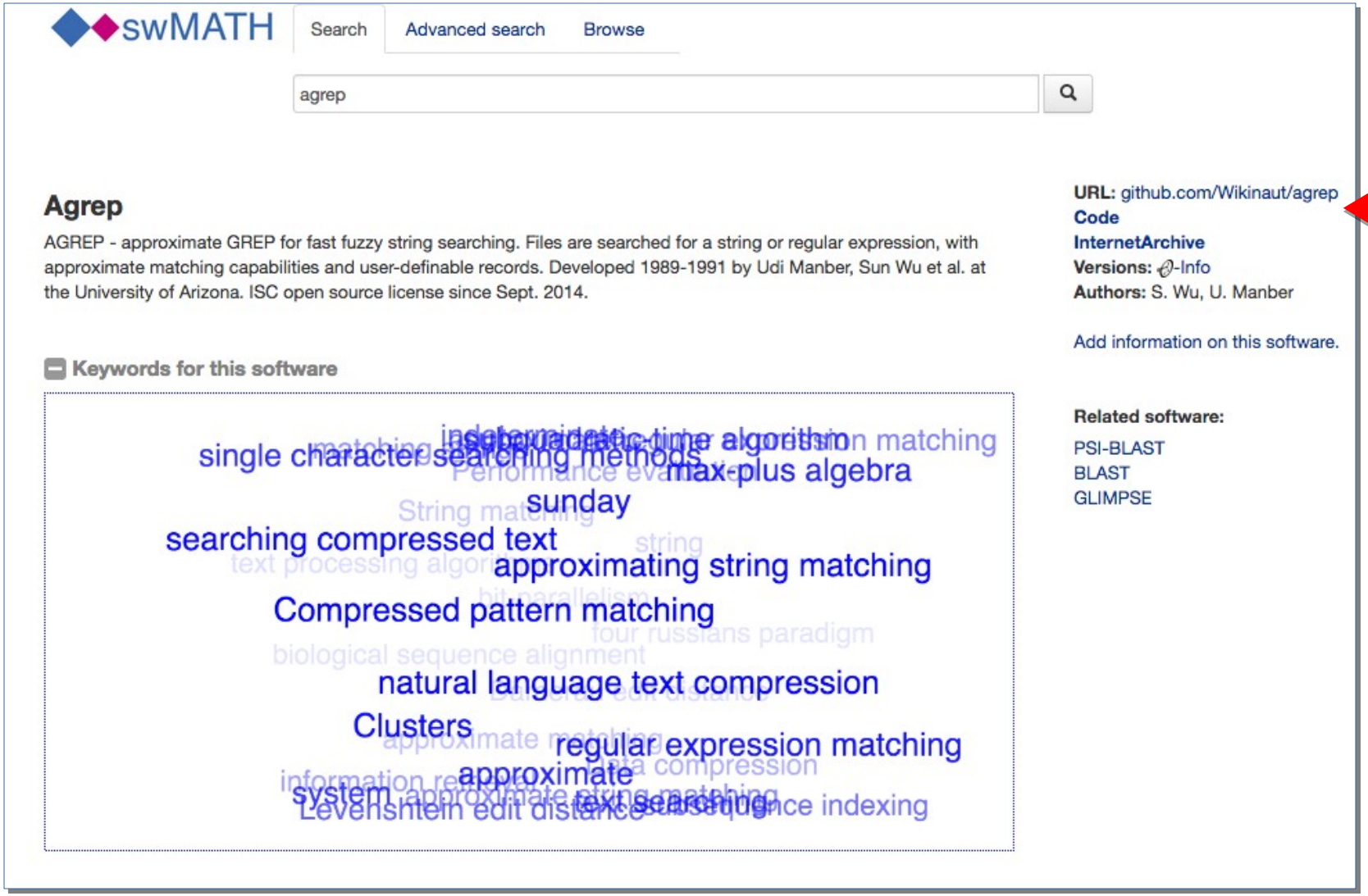


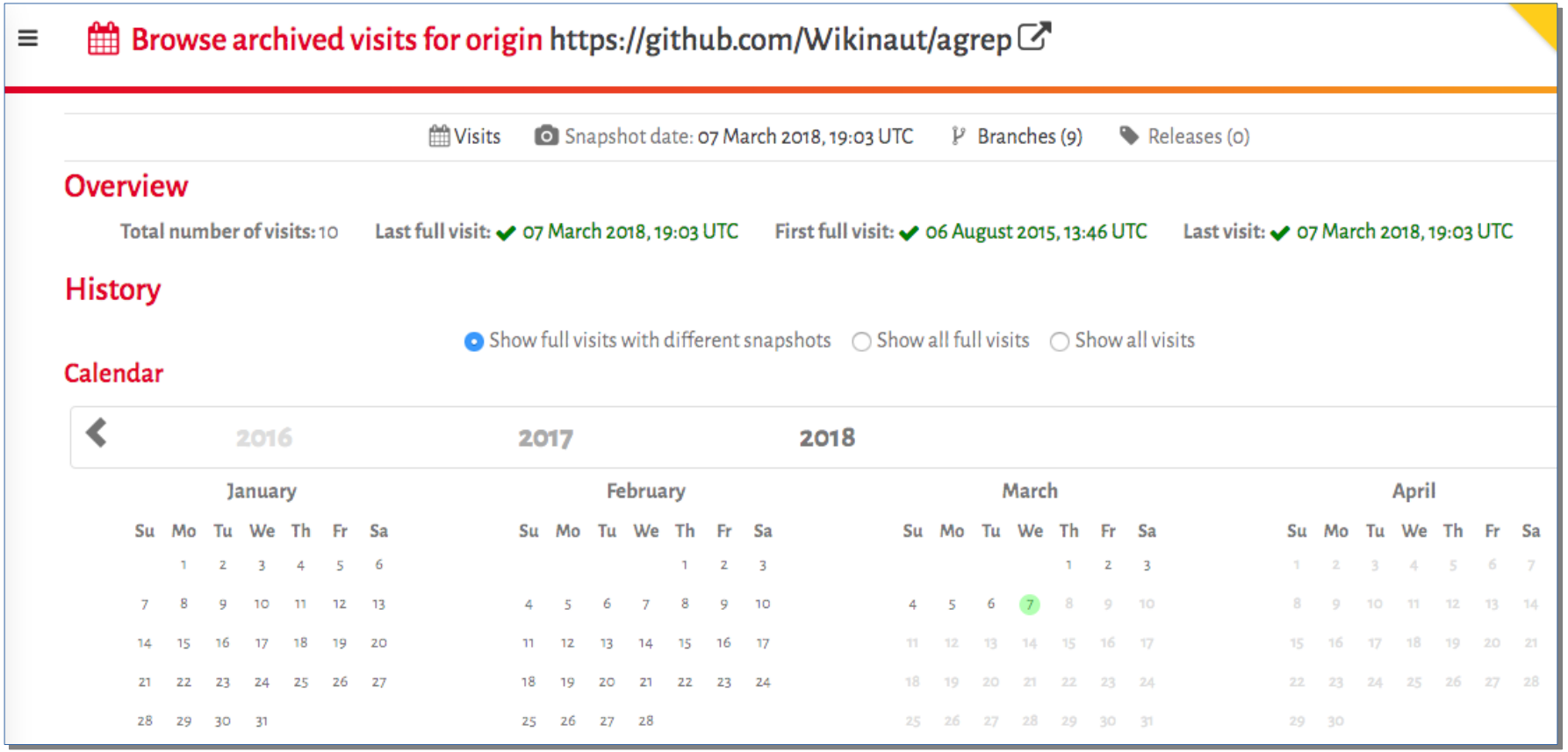
… leads to Tempas TimePortal (L3S)



Link to Github and to Software Heritage Archive



Software Heritage

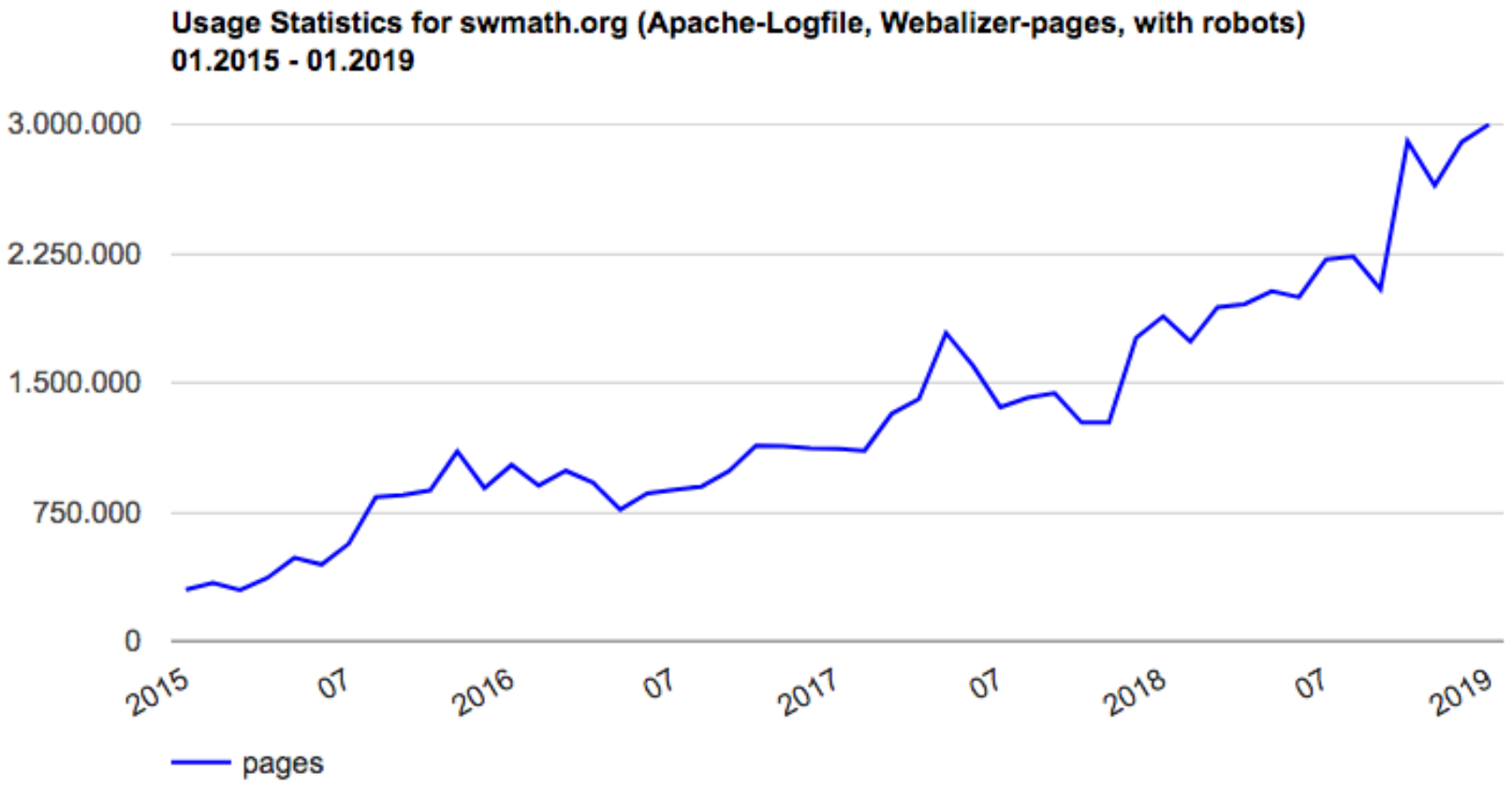


Some Statistics

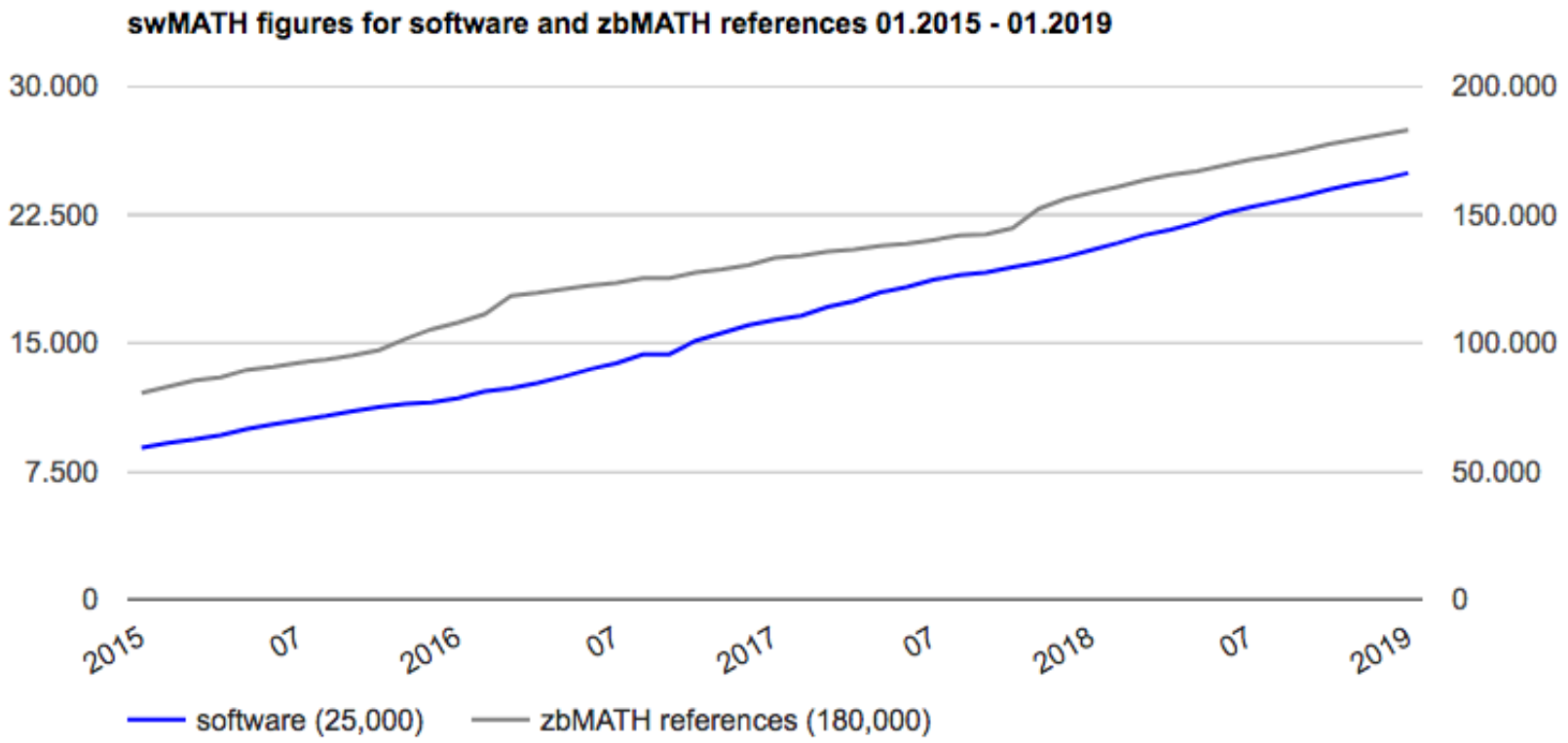
- swMATH has been started in 2011, a joined project of Research Institute Oberwolfach (MFO) and FIZ Karlsruhe
- currently a project of the BMBF research campus MODAL with FIZ Karlsruhe/zbMATH and Zuse Institute Berlin (ZIB)

- ~ 25.000 Software Packages
- ~ 330.000 Software References in
- ~ 182.000 zbMATH and other Scientific Articles

Usage of swMATH



Software and zbMATH References



Some Results (I)

- swMATH provides general information about software, especially about software products (or containers): information about all software artifacts which are under a common name
- we have extended the swMATH pages by linking to further Internet information resources if existing:
  - Websites of the software - problem: not permanent
  - Internet Archive - problem: archive not complete
  - Software Heritage - problem: SWH provides artifacts (revisions/commits, releases), but not direct versions
- verification of scientific results needs more information about the version of the software used

Some Results (II)

swMATH makes the software container citable*:*

- each swMATH page gets a unique and persistent identifier
- swMATH page are so-called „landing pages“ in the terminology of the Software Citation Principles

Some Results (III)

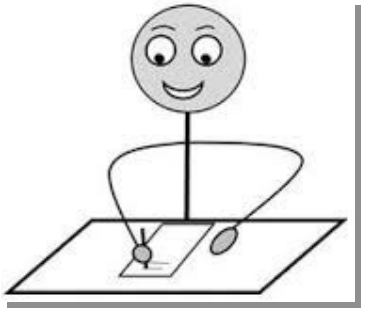
- the numbers of citations listed in swMATH is an indicator of acceptance, spread and quality of the software

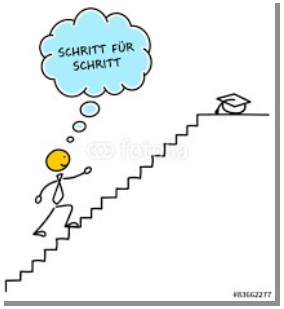
- software developer
  - → receives more scientific recognition
  - → gets more academic reputation
  - → gets more credit points in his academic career

New Scientific Recognition

Scientist



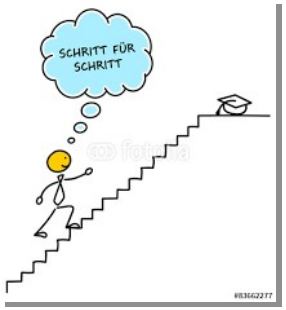





Software Developer





To-do

- The overall aim: developing an efficient infrastructure for (scientific) software based on the FAIR principles
  - → Findable, Accessible, Interoperable, Reusable
- Definition and dissemination of a software citation standard: under work, especially discussed in Software Citation Implementation working group of the FORCE11 initiative
  - → The definition of a software citation standard is not trivial: Software is a complex and structured object and cannot be reduced to software code
- Developing of efficient machine-based methods for analysis of software information
- Compatibility, interoperability, and interaction of different software information services and archives

Thanks for your attention