Computer Algebra

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(LIFIA / INPG)

As soon as computers became available the wish to manipulate symbols rather than numbers was considered. This resulted in what is called symbolic computing. The sub-field of symbolic computing which deals with the symbolic solution of mathematical problems is known today as Computer Algebra. The discipline was rapidly organized, in 1962, by a special interest group on symbolic and algebraic manipulation, SIGSAM, of the Association for Computing Machinery. Soon after, the first major Computer Algebra Systems (CAS) were designed and available. Simultaneously, several specialized packages were successful and greatly contributed to the fame of the field. For instance, SCHOONSHIP was used at CERN to solve problems in high energy physics from the early 1970s.

A main characteristic of the computer algebra community was its diversity. Indeed, it gathered mathematicians mostly interested in designing algebraic algorithms, computer scientists motivated by the will to manipulate symbols and, surprisingly enough, many users who designed their own CAS. Despite the fact that the discipline is now well established in computer science departments, these three classes of practitioners still remain active. The field is still lacking good textbooks. The only exception [1] was planned as a collection of the basic material needed to set up courses at all levels of the curriculum. Also illustrative are the proceedings of the annual conferences usually published in *Lecture Notes in Computer Science* of Springer-Verlag and the *SIGSAM Bulletin*. Since 1985, the *Journal of Symbolic Computing* covers the research activities of the field and is eagerly looking for contributions to its "Letters on Applications" section.

Before outlining the tools of Computer Algebra, what it can bring to physicists and what the new frontiers of the field are, it is relevant to point out that a CAS is presently a very powerful technical assistant to perform algebraic computations. Its benefits are the accuracy, speed and reliability of calculations, the handling of very large pieces of algebra which would be hopeless without computer aid, the possibility to get insight into a calculation, to experiment ideas interactively and to save time for less technical problems. When compared to numerical computing, it is also much closer to human reasoning.

Computer Algebra Systems

Computer Algebra systems may be classified into two different categories: general purpose systems and specialized packages. The latter are generally very efficient at solving some well defined classes of problem. Most often, their architecture reflects their goal and it is seldom possible to transport them to different makes of computer. General purpose systems are expected to be less efficient for very specialized applications, but easily portable and they offer a large library of algorithms. Their architectures share many common features:

(i) a programming language which is Pascal or Algol-like with a strong flavour of Lisp,

(ii) a kernel constituted by the basic functions performing the generic operations on mathematical expressions such as input, output, representations, simplification, substitutions, term generation, flow control, storage and special commands,

(iii) one or several modules of algebraic algorithms embedding the mathematical knowledge of the system.

Specialized CAS have always originated from research needs and stick to them. Although general purpose CAS have sometimes a similar origin, they have evolved to become "consumers" oriented products and, in fact, some have become commercial products which is a common trend in computer science. Nevertheless, it must be noted that most of the very important applications have been worked out using general CAS.

Over the years, more than 70 CAS have been designed [1]. A major reason for such a diversity of systems lies with the technology of computers. Twenty years ago, a general purpose CAS was already a large piece of software at a time when computer resources were short and expensive. Consequently, computer centre managers were not easily persuaded to install such systems. This is another reason why many specialized CAS have been developed in many different institutions. From the very beginning it was felt that the breakthrough of Computer Algebra is linked to the availability of adequate computers: several megabytes of main memory and very large capacity disks. Since the advent of the VAX's and the personal workstations, this era is opened and indeed the use of CAS is spreading very quickly.

What are the main CAS of possible interest to physicists? A fairly balanced answer is to quote MACSYMA, REDUCE, SMP, MAPLE among the general purpose ones and SCHOONSHIP, SHEEP and CAYLEY among the specialized ones. MACSYMA is the largest of all CAS. This means that its library of procedures, methods and techniques is the most complete. This originates in the fact that for many years it was only accessible at MIT through networking and all relevant programs written by users were added to its library. Today it is distributed by Symbolics Inc., except for the US Department of Energy version which is subject to possible restrictions. It is Lisp-based and available on many different computers starting from the SUN's and VAX's. REDUCE, also Lisp-based, is less powerful but very clean, well debugged and well documented. Over 1000 copies are distribued worldwide as of today and it is probably the most used of all CAS. SMP and MAPLE are written in C. SMP is announced to be as powerful as MACSYMA but this remains to be fully proved and the debugging completed. Eventually, it ought to be very well suited to the physicist's needs. MAPLE is listed here since it is the system to select for a classroom environment. Indeed, it enables many jobs to be run efficiently simultaneously. Both REDUCE and MAPLE are available on machines ranging from the MacPlus (MAPLE) and IBM PC's (REDUCE) to the Cray's. According to the opinion of Computer Algebra specialists, SCHOONSHIP is a rather crude system but it is perfectly tailored to the needs of high energy physicists and still in use. It is written in machine code for the CDC's and now for the Atari micro-computer. CAYLEY is specialized to group theory and SHEEP to tensors and thus to general relativity.

A frequent question from potential users is which CAS is best suited to their problem and if it appears that the required methods are not immediately available they may be tempted to design

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Simple Example of the Use of a Computer Algebra System (Reduce) in a Combined Algebraic-numerical Problem.

Problem: Find the minimum value of

$$\int_0^{\pi} (x+y)^5 \cos(x)\,dx$$

The following REDUCE session solves the algebraic part:

```
(x+y)↑5*cos(x);                 enter function into ws (work space)
int(ws,x);                      integrate with respect to x
sub(x=pi,ws)-sub(x=0,ws);       definite integral from 0 to π
on fort;                        turn on Fortran generation
ws;                             generate Fortran for the definite integral
df(ws,y);                       and for its derivative with respect to y
```

REDUCE generates the following ouput:

```
      FC=5.*(2.*Y**4+4.*Y**3*PI+6.*Y**2*PI**2-24.*Y**2+
     . 4.*Y*PI**3-24.*Y*PI+PI**4-12.*PI**2+48.)

      GC=20.*(2.*Y**3+3.*Y**2*PI+3.*Y*PI**2-12.*Y+PI**3-
     . 6.*PI)
```

The above statements can then be used with a numerical minimization package which requires the function and its first derivative.

their own system. It is necessary to point out that this means implementing all the general features which are required in symbolic manipulation. Consequently it is much better to select a CAS and to add their own techniques. Indeed, a CAS is also a programming language so that this approach is always more efficient than starting from scratch. Examples of running 10 of the most important CAS are reproduced in [2] which thus gives a flavour of what programming with CAS is.

Algebraic Algorithms

The heart and power of CAS are their library of algebraic algorithms. In such a short survey it is not possible to specify each system. It is enough to know that the following capabilities are available within one or another CAS and are very general: Arithmetics on integers including arbitrarily long ones, on rational and (partially) algebraic numbers, p-adic and modular ones as well. Manipulation of rational fractions and of polynomials defined over diverse fields, including their arithmetics, factorization, gcd, zeros determination... Linear algebra including matrix with symbolic elements operations such as inverse, determinant, product... Solutions of equations and of systems of equations, both linear and algebraic, are now well mastered. To handle power series is easy. Non commutative algebra is sometimes possible. To differentiate is trivial. To evaluate indefinite integrals is a much more difficult task but, nowadays symbolic integrators are very performant and more reliable than tables. The Rish's theory of integration in finite terms [1] is a highlight of the research activity in the field.

Among the capabilities which are only partially implemented are the evaluation of definite integrals for which the computation of limits is still a difficult problem, the solution of ordinary and partial differential equations, which are difficult mathematical problems anyhow, and the handling of special functions. The capabilities available in present systems do not always reflect the state of knowledge in algebraic algorithm design. For instance new powerful methods to solve differential equations in closed forms have been found but are not yet fully implemented.

Prototypical Applications

CAS have been applied to many different fields of physics [1]. In high energy physics, a breakthrough application has been to perform the tedious algebra arising from the calculation of Feynman diagrams in quantum electrodynamics and to determine the theoretical values of the anomalous magnetic moments of the electron and muon and of the Lamb-shift effect at high orders of the perturbative expansion. Also noticeable are several diagram calculations in quantum chromodynamics and the two loops computation in the standard SU(2) × U(1) model.

In celestial mechanics an outstanding result is the duplication in 1970 by Deprit and co-workers, of the 1867 work of Delaunay on the calculation of the orbit of the moon with corrections up to order 9. To get an error free result took them only 20 hours on a mini-computer instead of 20 years of Delaunay's life. In this example, the capability to implement a Poisson series representation in a CAS was the key to their success. The same type of computation is applicable to the orbit of satellites for instance.

In general relativity specialized (CLAM, SHEEP,...) as well as general purpose systems such as MACSYMA are used to solve the basic equations starting with the definition of the covariant metric tensor which determines the length of a line element in space. Then, the Christoffel's symbol and Rieman's, Ricci's and Einstein's tensors are obtained and the 10 Einstein's field equations solved. CAS are useful to point out the possible equivalence of some metrics. Many other applications have been reported on.

Since CAS are devoted to symbolic mathematics, they are obviously used by mathematicians as well. It is worthwhile to notice that although they encompass only a little part of the whole knowledge of mathematicians, they can be used to solve, from scratch, some of the "open problems" in the relevant section of the *American Mathematical Monthly*.

A general feature of applications is that most of them involve simple and straightforward but long and tedious algebra. While many years ago the use of a CAS was always acknowledged in published papers (several hundreds of them) nowadays, they are often regarded as casual tools and no longer referenced.

New Frontiers

Despite the many successful applications of CAS in many fields of science, they have obviously some drawbacks. Apart from technical ones which are irrelevant for this brief survey, the major weakness is probably that, surprisingly enough, they know very little mathematics. To bypass this limitation, two different research directions are possible and investigated. The first is to concentrate on enlarging the library of available algebraic algorithms and procedures. As outlined previously, several breakthroughs have been achieved in the design of algebraic algorithms and there is no reason to believe that this trend will stop. This ensures that existing CAS will remain alive and expand in the foreseeable future. An alternative approach is to consider that CAS are not only suitable to manipulate formulae as they exclusively do today, but that they must also accommodate the concept of mathematical objects and their associated properties. The IBM project SCRATCHPAD, which is well under way, is the first CAS of this generation. But, it is possible further to enlarge the concepts upon which computer algebra is based by stating that its ultimate goal is to represent and manipulate mathematical knowledge. Then, artificial intelligence techniques become compulsory. Unfortunately, mathematics is a very complex domain and the techniques developed for the usual domains of artificial intelligence such as expert systems or robotics are not elaborated enough for its needs. This latter trend [3] is thus a longer term research track which aims to design completely new types of mathematical systems but not to replace present CAS.

Further information and references are available from the author.

REFERENCES

[1] *Computer Algebra: Symbolic and Algebraic Computation* 2nd ed., Eds. B. Buchberger *et al.* (Springer-Verlag) 1983.

[2] Yun D.Y.Y. and Stoutmyer D.R., 'Symbolic Mathematical Computation', *Encyclopedia of Computer Science and Technology*, Eds. Belzer, Holzman & Kent, **15** (1980) 235-310.

[3] Calmet J., "Intelligent Computer Algebra Systems: Myth, Fancy or Reality?' To appear in *Proc. of the Trends in Computer Algebra,* Conference. Bad Neuenahr, FRG. May 1987, LNCS (Springer-Verlag) 1988.

A Delegate Enquires

Dear Sir

May I use your columns to write to the Individual Ordinary Members of the EPS? I am a recently-elected delegate of the IOM's to the Council of the EPS. I believe I could do this job more effectively (and this goes for other Council members too) if any IOM with strong views about any aspect of how the EPS runs its affairs — conferences, journals, general structure (including financial matters), or indeed anything else — would write to me about it. I can then form a better idea of what EPS members' attitudes are on the issues they find important. The next Council meeting is on 24-25 March 1988, so it would be especially helpful to have any comments before then.

Such comments need not, of course, be restricted to remarks (favourable or unfavourable) about current practices; ideas for the future development of the EPS and views on broader issues would also be valuable. I should mention further that I am not intending in the least to suggest that adequate channels of communication do not exist already in the EPS; it is simply that I personally feel I could play a more useful role as a delegate if I were better informed.

Yours sincerely,

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Optics Elections

Elections will be held shortly of the 12 members of the Board of the **Optics Division**. Candidates proposed by the Provisional Board are listed below, but additional nominations are invited.

These should be supported by three members of the Division coming from at least two countries and the candidates agreement to stand should be appended.

J. Bescos, Optics Institute, Madrid
K. Biedermann, Royal Inst. of Technology, Stockholm
J.J.M. Braat, Philips Research Lab., Eindhoven
J. Bulabois, Franche-Comté Univ., Besançon
R. Dändliker, Inst. of Microtechniques, Neuchâtel
J.C. Dainty, Imperial College, London
H.A. Ferwerda, University, Groningen
J.-P. Huignard, Thomson-CSF, Orsay
O.J. Løkberg, Norway
E.R. Pike, Kings College, London
A. Podmaniczky, Technical University, Budapest
V. Russo, IROE, Florence
O.D.D. Soares, University, Porto

Nominations should be sent to the EPS Secretariat by the end of March, 1988.