Uses Made of Computer Algebra in Physics

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Computer algebra is a tool building activity. This paper is a review of acceptance of this tool by physicists and theoretical chemists during the period from the EUROSAM-79 survey to the Spring of 1988, as reflected by the literature which quotes computer algebra.

After considering the traditional areas of application; celestial mechanics, relativity and quantum mechanics, we extend our examination to other areas of physics which would appear, from the literature, to be using computer algebra efficiently: fluid mechanics, plasma physics, optics, perturbation technology, continuum mechanics, numerical analysis for physics, mechanics, non-linear evolution equations, theoretical chemistry and other applications.

1. Introduction

Computer algebra has from its earliest days been concerned with providing a tool with which researchers in other fields can determine new results. This paper is a survey of the literature produced in physics and some theoretical chemistry from the survey of EUROSAM-79, to Spring 1988. There have been a number of other general reviews during this period, such as that of Gerdt *et al.*(1980), but most of these are in particular application areas or environments. We looked at a wide range of areas, in order to get a feeling for the overall penetration of computer algebra into the physical sciences.

A significant feature of the past decade has been the attempt to popularise computer algebra, both by presentations to other communities, and by producing systems on the smaller and cheaper computers now available. Our aim in writing this survey is in part to investigate the extent to which this work has produced results; we would expect this to be reflected in a general increase in the volume of papers which acknowledge the significant use of computer algebra, and in a broadening of the range of applications. Another change we might hope to see would be a widening of the number of systems used, in contrast to 1979 when users, unless taking advantage of specialist systems, concentrated on one system, REDUCE.

First we consider the familiar areas of application which have been active for a number of years; celestial mechanics, relativity and quantum mechanics, and then we pass on to new areas where the efficient use of computer algebra is reported. At the end there is a statement of the methods by which these references were obtained.

2. Celestial Mechanics

Celestial mechanics was one of the earliest application areas of computer algebra, but as the typical calculations are in terms of Fourier series the major systems have not made the impact of the specialist systems. The number of publications citing computer algebra has fallen recently, but systems like TRIGMAN continue to be used, as can be seen from Ricklefs *et al.*(1983) and Jefferys & Ries(1979). What seems to have happened in celestial mechanics is that computer algebra has become an everyday tool for many workers, but as their requirements are so particular, each group has its own system; the

phrase of Deprit is that the systems are like a toothbrush, in that they are used every day, but are not lent to others.

3. Relativity

There are a number of reviews of applications of computer algebra in relativity which have appeared over the period of our survey, such as Cohen et al.(1984), MacCallum(1984), and MacCallum(1986). Here we restrict ourselves to drawing attention to the style of use.

Relativity is a subject in which some specialist algebra systems still survive and prosper. Principal among these is SHEEP which has been the main tool of a number of research groups, and in particular the Queen Mary College and Stockholm groups. They have produced several papers describing the progress made on classification of the Riemann tensor based on studies of the multiplicity of roots of a quartic equation, and MacCallum(1983) and MacCallum(1985) in which SHEEP is used as an essential tool in the investigation of Einstein-Maxwell equations of high symmetry. The work of this group on the equivalence problem is now at a high level, with results being produced rather than just the program; see for example MacCallum & Åman(1986).

The other system that is frequently used in general relativity is CAMAL, as for example in Wainwright(1981) who investigates exact spatially inhomogeneous solutions of Einstein's equation, Wainwright(1983) where it is used it to obtain a new solution with certain properties and Wainwright & Anderson(1984) on isotropic singularities.

Even in this area which has produced its own strong tradition the mainstream computer algebra systems are found. For instance REDUCE was used by Perjés (1984) in investigations of stationary vacuum fields with a conformally flat three-space. Here the algebra system was not calculating field equations or classifying metrics, but in a fashion found all over physics, rearranging equations, substituting for variables and collecting terms. The MAPLE system was the vehicle for a Newman-Penrose relativity package written by Czapor & McLenaghan(1987). REDUCE has also been used by Baekler & Hehl(1984,1985), McCrea(1982,1984), Carlson(1980), Dautcourt et al.(1981), and Dautcourt(1983).

The indicial tensor system STENSOR was presented at various conferences during the period, and recently the EXCALC system has been produced for REDUCE. This latter system is an exterior calculus system which has been applied to general relativity (Schrüfer et al.(1987)). Before the availability of this system REDUCE had certainly been used in relativity, but we expect EXCALC to make a significant change, and to bring REDUCE into the mainstream of relativity studies.

A new trend among the relativists is numerical relativity, and here algebraic computing is playing a part, for example in generating the starting equations for numerical calculation (Stewart(1984), MacCallum(1986)). MacCallum also describes the use to which the newer systems for generating FORTRAN (such as GENTRAN) can be put. The importance of computer algebra in this growing field can be judged from the statement of Nakamura in MacCallum(1987), "it seems that the use of the algebraic computing software is indispensible in constructing codes as well as checking and analyzing numerical results".

Returning to the sheep derivative STENSOR, this has been used used by Amerighi et al.(1986) in investigating the superfield action for degenerate central-charge multiplets for both supersymmetric Yang-Mills and supergravity theories. This is not strictly speaking general relativity, but grows out of the same school.

For other examples of the uses of computer algebra in relativity we would refer to Kersten & Martini(1984), Prince(1986) and Joly(1987). A different emphasis is found in Beig & Simon(1980) who produce an algorithm for calculating multipole moments of a static space-time, noting this algorithm as suitable for symbolic manipulation.

4. Quantum Field Theory

High energy physics has been a very active area for applications of computer algebra. The systems REDUCE and SCHOONSCHIP have been used for many years, and this continues. Computer algebra is frequently used in QED, and as experiments become more accurate the need for higher orders of theoretical calculation will ensure that the demand for the systems persists.

As examples of the kind of calculation for which this area has regularly called on computer algebra we give only a few; Mzhaviya *et al.*(1986) studied rare four fermion *K*-meson decay, and used SCHOONSCHIP, while Akundov *et al.*(1986) used the same system for studying electromagnetic corrections in inelastic lepton-nuclean scattering.

REDUCE's high-energy physics package has been modified to work with quantum gravity by Gastmans *et al.*(1979), the modifications being to work in the higher dimensional space.

The original REDUCE system for quantum electro-dynamics is still being used, for example in Adkins(1985) and two papers presenting identical results, Adkins & Brown(1983) and Lepage *et al.*(1983). Broadhurst(1985) used REDUCE to calculate explicitly the 1-loop member of a class of massless, dimensionally regularized Feynman diagrams, in order to verify an explicit formula, while Berends *et al.*(1981) used it in a traditional way for 25 Feynman diagrams to produce experimental results which could be checked against experiment. This last work was the starting point of what is called the CALCUL collaboration, and this approach has led to further work which uses REDUCE (Gunion & Kunszt(1985), Łukaszuk *et al.*(1987)).

Another feature of quantum field theory which is rarely found elsewhere is the use of two independent algebra systems to check the accuracy of the answer, for example Aurenche *et al.*(1984) used REDUCE and SCHOONSCHIP in the extension of calculations to a higher order to keep pace with experimental results.

5. Other Quantum Physics

There are many other areas of physics related to quantum theory, and here computer algebra is becoming a much used tool.

For example Müller & Müller-Kirsten(1981), investigating single-channel and two-channel Schrödinger equations state "...we describe an iteration procedure which has already been applied to a large number of other problems. With the help of REDUCE it is now possible to do these algebraic computations on the computer, so that the necessary expressions are obtained within a reasonable time". It is this liberation of the physicist from the restrictions of his ability to perform the manipulations which has produced the largest growth area.

The very knowledge that automation of algebra is possible affects physics. Bessis *et al.*(1985), in their derivation of a closed form expression for the Dirac-Coulomb radial r^i integrals, remark that their formula is well suited to evaluation by REDUCE or MACSYMA, and this is one of the advantages of the formulation. Similarly Aguilera-Navarro *et al.*(1987) use computer algebra to rearrange ideal-gas-based low-density expansions; to them REDUCE or MACSYMA provide just the expertise they require to substitute forms into equations, and so make their formulation possible.

Rodionov & Taranov(1987) used REDUCE to calculate the geodetic interval of the Riemannian manifold by calculating the multiple covariant derivatives of orders 7 and 8. Direct use of REDUCE was not sufficient, but some investigations of the structure of the problem produced some recurrence relations.

Sometimes one finds algebra systems being used for reasons other than the usual algebraic ones. Laursen & Samuel(1981), as part of their work on an exact integration for mass independent n-bubble diagrams in leptonic g-2, used the rational capabilities of REDUCE to get values explicitly for the 13th order, much higher than was possible by hand. And there is still evidence of distrust or unavailability of computer algebra. Koh *et al.*(1982) for example did their lengthly calculations by hand before checking them with REDUCE.

The mixed use of FORTRAN and REDUCE is found in Baker *et al.*(1982), where various derivatives were calculated algebraically, but the double series was evaluated numerically, and Pattnaik *et al.*(1983) realised that inverting a matrix algebraically would be more accurate than a numerical inverse, and used REDUCE for this part of their work.

6. Fluid Mechanics and Plasma Physics

In the EUROSAM-79 review it was predicted that fluid mechanics would be the next major physical area in which computer algebra would be applied. In this section we look at the publications in fluids in general to see if this prediction was accurate.

MACSYMA has been used as a general tool by Roache & Steinberg in generating the FORTRAN equations for solving three dimensional boundary fitting problems, as described in Roache & Steinberg(1984) and in Steinberg & Roache(1985). In essence they are using symbolic procedures to generate recurrence relationships for finite difference solutions. MACSYMA has also been used by Berger(1987) to produce asymptotic approximations to the Onsager equation for a gas centrifuge. In considering steady flows with free surfaces Hui & Tenti(1982) used MACSYMA for evaluating their recursion formulae, but lamented the limiting speed, and looked forward to a generation of smaller and faster algebra systems.

Perturbation expansions are also the subject of the work of Kotorynski(1986), who used REDUCE to perform the calculations for steady flow through twisted pipes, but who also remarked that the techniques he developed for this problem are applicable to a variety of other pipe flow tasks. REDUCE was also the basis for the work of Zahalak et al.(1987) in considering the deformations of cylindrical liquid-filled membranes by viscous shear. They draw attention to the use of classical perturbation techniques combined with computer algebra as an alternative to numerical calculation. Indeed, this has been a feature of many application papers for a number of years, starting with celestial mechanics in the 1960s. It is such an important technique that we devote a section below to perturbation theory and computer algebra.

That computer algebra is becoming a factor in fluid mechanics can be seen by the work concerning the forces and couples acting on two nearly touching spheres in low-Reynolds-number flows, done by Jeffrey & Onishi(1984). They extend a linear approximation up to the terms in ε ln ε; to quote their introduction, "Otherwise the only new principle in the calculation is the handling of long algebraic expressions, which was accomplished by using the computer algebra systems CAMAL and REDUCE". It is in a fluids paper that we find evidence that some of the more recent parts of REDUCE are actually used. Feuillebois(1984), in investigating sedimentation with vertical inhomogeneities, remarked that the availability of REDUCE and its integrator made the formulation of the problem much simpler. We also find throw-away remarks, as in Miric & Su(1984), who in their perturbation and integration work "acknowledge the use of Reduce2".

Astrophysical fluid mechanics was one of the fields which Fitch thought would spearhead computer algebra use in fluids. This prediction can now be seen to be premature. The paper of Lebovitz(1979) on ellipsoidal potentials of polynomial distributions of matter is the kind of work which was expected. The calculations here are very large, and we are aware of other, but even larger, calculations in the same spirit, but as yet there is no publication.

In plasmas it was previously noted that there were applications using MACSYMA. This seems to be continuing, for example in the work of Gladd(1984), where this system is used for many of the steps. Mynick(1987) goes further in using MACSYMA as one of the two cornerstones of PAP, a Plasma Apprentice Program. REDUCE has also been used, as in De Menna et al.(1987), working with perturbation techniques.

7. Optics

In 1979 we noticed a small community of computer algebra users in optics, using CAMAL and REDUCE. There has been growth in the field, but not to the extent that was suggested.

Hawkes wrote two review articles; Hawkes(1981a) concentrates on the use of computer algebra in aberration studies, drawing attention to the great potential there, while Hawkes(1981b) takes a more general view of computers in optics, and includes computer algebra within this wider scope. In Hawkes(1983) the aberration coefficients of microwave cavity lenses of second order are calculated with CAMAL.

A different view of aberration calculations is shown in Dragt(1982), where use of Lie algebraic theory gives a method of calculating the higher order aberrations more easily than classical methods. While he does not use computer algebra, he suggests that his techniques are well suited for it, and predicts ninth or higher order terms could be generated.

Computer algebra can be just a small part of a confidence building exercise before undertaking other work. Conwell et al.(1984) formulated the resonant spectra of a dielectric sphere in terms of Bessel functions. They used REDUCE to confirm independently that their numerical form of the particular function converged and was accurate, by expanding the function in series, and then using the bigfloat

package. While they describe it as slow and expensive, they were able to verify the accuracy of the routines used in zero-finding calculations.

Much work in optics, as elsewhere in physics, amounts to expansion in series of one kind or another. For Francescheti & Pinto(1985) it is Volterra series, for which they used REDUCE, but the mathematics would be familiar to many other specialists who use perturbation techniques.

Not all applications in optics require large scale computations. A tutorial style paper by Wyant(1981) shows how the matrix and trigonometric facilities of μMATH can be used in the Jones calculus for polarized light problems. This was using a Z80 processor and less than 48Kbytes.

8. Perturbation Technology

One technique which recurs in computer algebra is perturbation expansions. We have commented elsewhere in this paper on some of these, but there are also general papers which investigate the technique itself, for example with respect to the van der Pol equation, or to a class of equations. Dadfar *et al.*(1984) construct and analyse the power series of the limit cycle for the van der Pol equation with the aid of MACSYMA, a problem which has long been studied. Other authors have studied this equation, and have been reported in SIGSAM Bulletin and algebra conferences.

The problems of working with multiple time scales in nearly harmonic oscillators was considered by Weissman(1979) who used FORMAC to perform the calculations. While he remarks on the necessity for dealing with coupled oscillators, as yet there is no solution.

Perturbation theory has also produced its own algebra system; Fried & Ezra(1987) have created the PERTURB system, a C-based special algebra system which largely recreates the structures of Barton's CAMAL, and other celestial mechanics systems, apparently because MACSYMA is so large.

The existence of algebra systems influenced the thinking of Rosengaus & Dewar(1982) who argue that with their assistance it is not necessary to develop superconvergent techniques in perturbations of Hamiltonian systems, since the expansions can be made to high order.

9. Continuum Mechanics

An application field we had not seen in previous surveys is continuum mechanics. Frequently this involves perturbation expansions and other familiar techniques. MACSYMA was used by Frakes & Simmonds(1985) to help produce asymptotic solutions describing a circular plate under a concentrated load. The resulting forms from the algebra system were subsequently used in numerical evaluation. REDUCE was the system used by Pignataro *et al.*(1985) for postbuckling of uniformly compressed channels, where again algebraic manipulation generated the FORTRAN program for their model, but was also used to investigate the form of the solutions. Similar work by Rizzi & Tatone(1985) gives more details, publishing both the program in REDUCE and the output.

10. Numerical Analysis

Computer algebra is increasingly used in finite element construction, and in particular in continuum mechanics and engineering. Papers range from the very general and missionary such as Korncoff & Fenves(1979) who used MACSYMA to generate stiffness matrices symbolically, to specific crack analysis by Hussain *et al.*(1981). Saleeb & Chang(1987) developed a quadratic element for plate bending analysis with the aid of MACSYMA.

Other uses in numerical methods include the calculation of Padé approximants, as for example in Németh & Zimányi(1982) who used REDUCE and FORMAC. Connor *et al.*(1984) investigated numerically the uniform swallowtail in catastrophe theory, using REDUCE and SCHOONSCHIP for some algebraic manipulations, and then checking the results with MACSYMA; this is the most mistrustful attitude to computer algebra that we have seen reported.

11. Mechanics

As well as in those specialised areas which have become familiar to the computer algebra community, there have also been applications in mainstream mechanics. MACSYMA was applied to various problems in vibration by Rehak *et al.*(1987). They remark at various stages "...which we would not have attempted to evaluate without MACSYMA" and "..had it not been for MACSYMA....".

Handy(1987) used REDUCE to produce a straightforward method for the derivation of kinetic energy operators for the vibrations and rotations of molecules. He notes in the introduction "The purpose of this paper is to derive a simple and straightforward procedure for which it is possible to make the computer do all the hard work. After many years of investigating this problem, this author believes that this must be the reliable way to proceed". Surely many others would agree with this sentiment.

12. Non-linear Evolution Equations

In recent years there has been a new interest in non-linear systems. This has been reflected in computer algebra in several ways. Perhaps one of the earliest of cases is that of Edelen(1982) who wrote a REDUCE package for isovector methods, and applied it to mechanics of solids and fluids. Two main centres have emerged amongst the REDUCE users in this area, in Germany (Schwarz(1984) for example) and Holland (Kersten(1986) for example). Both these groups have developed packages for REDUCE written in the implementation language, rather than as user-level programs. One of these (Schwarz(1985)) now forms part of the distributed REDUCE.

Others using REDUCE here include Ito & Kako(1985) and Eliseev *et al.*(1985). MACSYMA has also been used in non-linear systems by Rosenau & Schwarzmeier(1986), Rosencrans(1985), Fuchssteiner, Oevel & Wiwianka(1987) and Armbruster(1987).

This area is expanding greatly, and in common with general relativity, analytical calculations are often preferred. We predict that this field will feature prominently in any future review of this general kind.

13. Theoretical Chemistry

Chemistry is in general outside the scope of this paper, but we saw that the number of papers appearing within chemical journals has been a significant feature of the last few years. At times the distinction between Chemistry and Physics is a little blurred. Here we comment on a few points; there is a general review in Ogilvie(1982).

μMATH was used by Hurley & Head(1987) to investigate the solubility of sextic equations, and in particular the method of power sums is used to calculate the algebraic resolvents. They also note that μMATH would take 11 years to do the calculation, but recent improvements in μMATH by Head has meant that this time is reduced to only 11 days. They do not hazard a guess at the time needed to perform the manipulations by hand. The application is to crystal elasticity. μMATH was also used by Trindle(1987) for chemical kinetical differential equations.

Jones has written much on quantum chemistry (for example Jones(1986)) where he has developed his own system, and while he does not make great claims for it, he clearly finds the algebraic techniques a major help. ALTRAN is also still in use by Rudowicz(1986) for chemical physics. In general we find that chemistry is some years behind physics in the use of computer algebra, but workers are beginning to realise the potential. The process is just beginning in chemical engineering as well (Atkinson *et al.*(1982)).

14. Other Applications

In looking at the literature for this paper it became apparent that there are a number of enthusiasts in new areas. For example Garrad & Quarton (1986) discuss the use of REDUCE as a tool in wind turbine dynamics, and in particular present a program for part of a stability analysis for a turbine tower. A more detailed description of the algebra involved in such a calculation is given in Quarton & Garrad(1984). There are others working in similar areas, such as helicopter rotor design, but there is a high degree of commercial significance in this work, and as yet there is no publication in the open literature.

Computer algebra and hand calculation formed a major partnership in the work of Broughan(1982) where REDUCE was used to perform substitutions while the integrations were done by hand. The results were thirteen moments of the collision term in a certain hot plasma, and judging by the computing times reported this constitutes a large calculation.

Gilbert & Wood(1986) used MACSYMA to evaluate a number of recursion equations with integrals in considering sound propagation under water. They present the programs as an appendix, in order to show how easy these operations are.

A very common sentiment expressed in papers is how tedious doing algebra is, and so typically REDUCE was used for part of the calculation. As well as the places above where we have remarked on this, it is found in such diverse topics as magnetohydrodynamics (Schrüfer & Heintzmann(1981), Maurer et al.(1986)), molecular physics (Greenland(1984), Tallents(1984)), statistical mechanics (Dhar & Maillard(1985)), numerical analysis (Alfeld(1982)), geodesy (Krack(1982)), special functions (Kölbig(1982,1983a,1983b), Piessens(1984)), accelerator storage rings (Adams(1983)), atmospheric tides (Aso et al.(1981)) and chemical physics·(Janssen et al.(1987)).

Other algebra systems are used in these contexts, such as CAMAL in molecular physics (Chidichimo(1981)), MACSYMA in magnetohydrodynamics (Coppi et al.(1981)), numerical analysis (Bjørstad(1983)), and heat transfer (Himasekhar & Bau(1987)), and FORMAC in heat transfer (Griffiths & Morrison(1983)).

15. Pedagogical Tracts

A few books and articles have been published with the aim of stimulating computer algebra applications. Some have been written ostensibly for a particular audience, but in practice they have all been written in the form of a series of applications surrounded by explanatory texts, which would be of interest to users in any field in the physical sciences. Probably, at present, the most sophisticated work, aimed at researchers, is that by Rand & Armbruster(1987). Rand has also written a simpler textbook (Rand(1984)). Another recent book designed for the unsophisticated user is that by Rayna(1987), which should be an invaluable help to people devising introductory courses for potential users, especially, we should imagine, in non-university environments. There are a number of well-written propaganda articles in existence, such as Rehak et al.(1987). On a more negative note, there are also many articles where the authors have generated expressions which extend far beyond any physical interest and where the main motivation of the paper seems to be "spreading knowledge about computer algebra". Unfortunately, this often produces a negative reaction among senior researchers in the said field.

16. Observations and Conclusions

If we look at the situation today, at one end of the spectrum we have the areas of General Relativity and QED where computer algebra has become an integral part of the fields and, at the other, areas like fluid mechanics where it is mainly used for assistance in mathematical methods or like chemistry where most workers seem to be unaware of its existence. Nonetheless the signs are hopeful and probably in the next few years even these areas will have research groups of high quality who are producing important results using computer algebra.

Applications of computer algebra are numerous. Many different research areas are represented, and use ranges from total dependence to small calculations as part of a larger whole. As was the case in the 1979 review REDUCE dominates applications, but MACSYMA now has a strong showing; amongst the specialist systems relativity and celestial mechanics continue to use their own systems, SHEEP, CAMAL and TRIGMAN. Other systems are found, such as the new MAPLE and the older FORMAC and ALTRAN, and there are a few publications which quote the microprocessor system μMATH. Perhaps the largest surprise was the lack of SMP references. However our methods of surveying the literature may be deficient. In our own work we frequently use automated algebra to investigate the problem, but there is no explicit acknowledgement of this in the published work. We suspect that this lack of acknowledgement is becoming a common phenomenon. It would be a sign of our success if it were accepted that algebraic calculation is as natural as numerical calculation, and references to REDUCE or MACSYMA were as uncommon as to FORTRAN and ADA in physics publications. Already workers are commenting that a particular new method is suitable for use by computer algebra, which show how our field is becoming accepted.

Many of the more exciting algorithms developed for integration, algebraic numbers and Gröbner bases have not yet reached the users, but we must expect a time lag. There are still new systems being constructed, but the evidence is that this is usually because of desperation. As the microprocessor implementations of REDUCE and MAPLE for example become more available this need will diminish, and new packages will more likely be built on top of one of the existing systems.

Lest the message of this paper should be too optimistic, we should state that not all the applications reported are successful. The chemical paper by Chinnick et al.(1986) contains the words "Although it [a Jacobian matrix] portrays the complete analytical form the algebraic solution derived for the isothermal 8

× 8 matrix, by using the algebraic programming system REDUCE is formidably complicated and does not yield immediate structural insight. Accordingly, we illustrate the principles ... through a simplified example".

Techniques and Acknowledgements

This survey has largely been based on a selection from papers collected by using Citation Index to trace forwards from key papers and also by doing a large database search on keywords. We have also collected several papers through the years. In the interests of brevity we have not included papers appearing in the Journal of Symbolic Computation, SIGSAM Bulletin, nor in the proceedings of the various conferences which have taken place in the computer algebra field in the past nine years. We feel the present audience will almost certainly have access to these and will probably at least have glanced through them. We have also avoided technical reports, as in general they are not easy for many people to consult. Our method of working will almost certainly have caused us to miss some works of importance. We were forced, also, to select from the large number of papers we identified. We gratefully acknowledge financial support from STU and an SERC project on industrial uses of computer algebra during which our desire to write this paper was kindled. The fuller data base of references on applications is being maintained as a general service; the authors would be grateful to receive new references. The references list is available from the second author, with the REDUCE component being distributed via the REDUCE net-library.

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