Symbolic calculation in chemistry: selected examples

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Abstract: A selective classified bibliography of symbolic computation in some areas of chemistry is provided together with some examples of computer algebra algorithms and techniques, to facilitate future joint work of chemists and computer scientists.

keywords: Computer algebra, Symbolic computation.

1 Introduction

Although only one of us (MPB) knew Herbert Jones personally, all four of us join in honouring his memory as a prolific author of papers that applied symbolic computation to chemistry during the 1990s. These include [48, 162, 163, 164, 165, 166, 167, 168, 169]. As such, he helped in the building of the field at large, besides developing his specific areas of interest in molecular integrals over Slater orbitals and the chemistry of small molecules. This paper addresses the larger issue accordingly, by (1) illustrating the range of chemical topics that symbolic computation has supported in recent years and (2) explaining some ideas of computer algebra that have vast potential in many branches of chemistry but are little known, as yet, to the majority of chemists. This information is intended to help computational chemists and computer scientists establish further commonalities of interest and the paper is, in part, a follow up to to MPB's talk [28] and a workshop at the International Symposium on Symbolic and Algebraic Computation 2003. Now that the level of cooperation between chemists and computer algebraists seems about to expand rapidly, note should be taken again of earlier papers by chemists that sought to bring the fields together, such as [65, 66] by Čížek, Vinette and Weniger. A recent survey of computer algebra in the life sciences [27] included many topics that overlap chemistry. The examples of basic computer algebra concepts that are included here are adapted from the recent monograph [113] by JvzG and JG. MPB has collected over 700 references to research papers that used symbolic calculation in chemistry, chemical physics and chemical engineering [30].

All the work cited in this survey used symbolic calculation unless it is included only to provide background and this is stated explicitly.

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2 Atomic energy levels

Fernández *et al.* developed high-order perturbation formulas that use moments and applied these to the Stark effect in hydrogen and to 2D hydrogen (a model of systems such as highly anisotropic crystals — see *e.g.* [191]), and to the Zeeman effect [96, 99, 100]. He and Ogilvie have used symbolic computation in studies of many other atomic and spectroscopic problems that were reported without explicit mention of this aspect [97].

Guiasu computed the ground state energies of H, He, Li, Be and B by a novel probabilistic approach to quantum mechanics in work that is summarized in [125] and given in detail in [126].

Adams used Lie algebras in a high-order perturbation calculation of the Stark effect in hydrogen and 2D hydrogen and the Zeeman effect [2]. Also, with Arteca, he derived a high order perturbation theory from the Hellman-Feynman and hypervirial theorems and made use of it [3].

Barnett *et al.* reworked the Pekeris treatment of two-electron atoms using MATHEMATICA and solved the secular equation as a power series in atomic number to show consistency with Moseley's law [31]. Analogous methods seem possible for a multitude of problems that involve parameterized matrix elements in a secular equation. Cox, Smith and Sutcliffe also repeated the basic Pekeris calculation using MAPLE [72].

Vinette *et al.* based a perturbation expansion of the energy of the N-dimensional H atom in a spherically symmetrical field on the hypervirial theorem [303]. Delhalle *et al.* tested an iteration-variation method to solve the Schrödinger equation on the H atom [80]. Work on quantum dots is discussed in §10.

Dubey, Khandelwal and Pritchard constructed asymptotic formulas for the hydrogenic radial dipole integral and computed transitions probabilities analytically using REDUCE [85].

Harris computed 3-electron atomic integrals over Slater orbitals, to investigate correlation effects [133].

3 Molecular dynamics

Harmonic oscillator: Korsch applied the position and momentum matrix method for handling eigenvalue problems to the harmonic oscillator as a simple example [181]. Several instructional modules based on the harmonic and other simple oscillators are included in the Symbolic Mathematics Documents for Physical Chemistry web site [327].

Quartic, sextic and octic oscillators: Hadinger *et al.* computed Yun-Dunham coefficients for the quartic oscillator by recurrence, applied these to the rotation-vibration spectra of diatomic molecules and compared the results with experimental data for CO, HBr, HCl in [129] and earlier papers. They used REDUCE.

The ground state energies of models up to octic have been considered by Čížek, Vinette and Weniger using inner projection methods [66], and by Weniger using Rayleigh-Schrödinger perturbation series and renormalized strong coupling [309, 310, 269]. In related work, effective characteristic polynomials are used in [67], and evidence of the Stieltjes nature of a perturbation expansion is discussed in [36]. Many more papers on the n-ic oscillators by Čížek, Vinette and Weniger with Bludský, Bracken, Dvorak, Kapsa, Skála, Špirko, Vrscay and Zamastil are listed in [30]. All these papers depend on unrestricted precision arithmetic and/or resources for mechanized differentiation.

Meißner and Steinborn computed the ground and excited states of the anharmonic oscillator by an iteration scheme based on the Bloch equation using 70-digit precision in MAPLE [219].

Morse oscillator: Bancewicz computed matrix elements of powers of the momentum to support investigations of the dependence of the density of vibrational levels on the coupling between bonds in a molecule [25]. He used MATHEMATICA to manipulate special functions. Sage applied van Vleck transformations using REDUCE to compute vibrational-rotational interaction [258]. Skála *et al.* computed the behavior of generalized Morse oscillators, using MAPLE [269].

Other diatomic models: Bouanich, Ogilvie and Tipping performed early symbolic computations of vibrational and vibrational-rotational matrix elements for diatomic molecules [46, 47].

Herbert and Ermler studied vibrational-rotational levels of diatomics using a Taylor series

expansion of the potential [139]. They produced formulas using MATHEMATICA and applied these to H_2, HD, N_2, CO and HF.

Polyatomic vibrations: The benefits and needs of flexible representation of molecular geometry in the expressions for the potential energy and kinetic energy operator have been considered by several authors who have applied symbolic computation to the problem.

Handy constructed separable KE operators for triatomic molecules and for HCHO-like and C_2H_2-like tetratomic molecules by a change of coordinates and showed how this simplifies the computation of matrix elements [130]. His subsequent work with several coauthors dealt with

1. anharmonic corrections to vibrational transition intensities, using 2nd order perturbation theory for the dipole matrix elements with application to H_2O [314],
2. another kinetic energy operator, with application to C_2H_2-like tetratomics, a rigorous symmetry analysis and singularities [53],
3. pentatomic molecules [76],
4. ammonia [131].

This work used REDUCE and MATHEMATICA.

Gatti, Iung and coauthors developed a matrix representation based on Jacobi position vectors for N-atom molecules [114, 152] and extended this work to use polyspherical coordinates [115, 152].

Rempe and Watts analyzed the vibrations of a hexatomic molecule [251].

Wang and Kupperman used hyperspherical harmonics for the mechanics of a four-atom molecule [305].

Bessis and Bessis considered the subtle effects of space curvature on the energy levels of the isotropic oscillator via a high order perturbation treatment of the Ricatti equation using MATHEMATICA [40].

4 Molecular electronic energy and spectra

Molecular integrals: The analytical evaluation of one-center Slater integrals by Gray, Pritchard and Sumner [118] and two-center Gaussian integrals by Turner and Boys, described in [49], are amongst the earliest examples of symbolic calculation in any field. Barnett used the idea of array manipulation, learned from Boys, to calculate auxiliary functions [304] and he used MATHEMATICA more recently in [29] and in papers that it cites.

In recent work on Gaussian integrals, Bracken and Bartlett used MAPLE [51] and Schwegler and Challacombe used MATHEMATICA [265].

For integrals over Slater orbitals, Jones and his coworkers used in-house software and MATHEMATICA in extensive work on two, three and four-center cases. Their earliest and most recent papers include [162] and [48], respectively. Righi and Kuhnen used REDUCE for 2-center integrals in [254]. Safouhi, Pinchon and Hoggan used the unrestricted precision of AXIOM for 2 and 3-center integrals in [257]. Harris used MAPLE for 2-center exhange integrals in [135].

Density functional theory: Jemmer and Knowles developed a MATHEMATICA package to obtain (1) functional derivatives in terms of the density and its gradients, and (2) position when the density is specified [157, 158]. They described applications to the Dirac-Slater local exchange, and to the Becke and Lee-Yang-Parr correlation functionals.

Strange, Manby and Knowles developed a MAPLE program to convert an expression for a density functional into FORTRAN code to evaluate the exchange-correlation kernel numerically [274]. Their program also produces the LaTeX file to document the functional. The code produced for two functionals of Tozer and Handy illustrates the action.

Further density matrix work is mentioned under nuclear magnetic resonance in §8 [255] and lasers in §10 [281, 282].

Coupled cluster theory: Bittl considered protein bound tetrameric metal clusters that occur in photosynthesis and other biological processes [42]. He evaluated matrix elements of single spin operators needed to calculate ground state energies and effective hyperfine coupling observed in EPR spectra.

Crawford, Lee and Schaefer used MATHEMATICA to solve 2nd quantized equations in coupled cluster calculations that included a spin restricted triple

excitation correction CCSDT [74]. They listed analytical results. Crawford gave the complete scripts [73].

Harris developed an algorithm to construct Feynman diagrams for a cluster of arbitrary size and reported a MAPLE implementation with a simple application[134].

J. Martin *et al.* computed the anharmonic potential surface of NH_2 to determine the spectroscopic constants and thermodynamic properties, using MATHEMATICA [210].

Piecuch *et al.* corrected quadruply excited clusters in single reference theory, using projected unrestricted Hartree-Fock wave functions [244]. They used MAPLE to compute matrix elements and to explore the energy surface. Piecuch and Paldus studied the convergence of energy expansions for molecules in electrostatic fields, in part to help calculate intermolecular potentials. MAPLE was used to solve the polynomial equations that arose [243].

Vinette [302] derived the coupled cluster equations for the Hubbard model of benzene using MAPLE.

Williams *et al.* [315] computed dispersion energies for He_2, ArH_2, ArHF, $(HF)_2$ and HeF^- in coupled pair approximation. They constructed spin free equations using the MATHEMATICA implementation of algorithms to manipulate orbital replacement operators (OROs) based on recursion schemes.

Electronic transitions: Boens *et al.* found the combinations of excitation wavelengths, emission wavelengths and co-reactant concentrations that allowed unique solutions for the spectral parameters related to absorption and emission and the rate constants in reversible intermolecular two-state excited state processes, using compartmental analysis [45]. This methodology is explained in [27], which comments on further applications in kinetics (see above) and gives references to background material.

D'yachenko and Petukhov computed overlap integrals for electronic vibration spectra of molecules, using Matlab [86].

V. Martin and Robledo developed a MATHEMATICA package to compute multipole matrix elements in the axial and triaxial harmonic oscillator basis [211]. The user can select an algorithm that produces analytical results recursively or gives numerical efficiency. The package includes a function to compute selection rules.

5 Long range forces and multipole expansions

Hadinger *et al.* developed an asymptotic scheme for the exchange interaction between open *s, p, d* and *f* valence shells and used MAPLE to construct and to check formulas for the exchange integrals by manipulating special functions [127]. They applied these to the ground states of the alkali dimers in [128].

Lustig, Rastogi and Wagner used Chebyshev economization to telescope both the far field multipole expansions and near field Taylor expansions used to solve N-body geometry optimization problems by fast multipole methods [202]. They gave a MATHEMATICA script to perform the calculation.

McDowell described the construction of general multipole expansions using MAPLE in [214] and applied the methodology to the H_2 trimer in [213], to the O_2 trimer in [217], and to the H_2, N_2, and O_2 trimers in [215]. He used 2nd order perturbation theory and spherical tensor formalism.

Novak defined a descriptor of coordination that involves the bond angles [232]. He used MATHEMATICA to expand small symbolic determinants that are then plotted for geometry optimization in a VSEPR model.

Piecuch and Paldus studied energy expansions for molecules in electrostatic fields [243], and Piecuch *et al.* computed the interaction of two atoms and a linear molecule using MAPLE [242].

Rérat *et al.* computed the critical points on the surface of the potential function of the long range interaction of several dipoles, using Morse inequalities of topology theory [253].

Xantheas and Sutcliffe considered the Hamiltonian of weakly interacting trimers, with special reference to water, and put the calculation in a form suited to symbolic calculation [318].

6 Collisions and scattering

Bancewicz constructed an analytical expression for the scattered light intensity corresponding to the interaction of a dipole with a multipole of arbitrary

order [26]. Teboul and Bancewicz considered the scattering of light by CO_2 induced by intermolecular collisions [287]. They used MATHEMATICA to tabulate formulas for the coefficients in the spherical harmonic expansion of the excess pair polarizability.

Bartschat and coworkers constructed movies to simulate collisionally excited atomic states [201].

Blackett and Stelbovics developed a MAPLE package to compute scattering amplitudes and differential and total cross-sections in electron-hydrogenic ion scattering using the 1st Born approximation [44].

Johnston and Sarkar used quantum transport theory to analyze inelastic scattering with optical phonons [160].

Noble evaluated exchange integrals for the impact parameter formulation of atomic charge-transfer collisions, using REDUCE [231].

Wang and Kupperman tabulated formulas for about 43.8 million hyperspherical harmonics with hyperangular momentum quantum numbers up to 30, to support calculations of the scattering theory of diatomic collisions [305]. They implemented a recurrence scheme in MATHEMATICA.

7 Conformational analysis

The treatment of ring closure by Go and Scheraga [116] that essentially follows the inverse kinematic methods used in robotics provides the infrastructure for some of the most dramatic applications of computer algebra to chemistry, with far reaching potential in the understanding of biomolecular processes and the development of drug design and discovery. The algebraic demonstration that cyclohexane can exist in boat and chair forms is given in detail in [113]. Geometrical reasoning based on fixed bond lengths and bond angles leads to an overdetermined set of equations and then, via a Gram determinant, to a set of multinomial equations that are solved using Gröbner bases. The corresponding analysis of cycloheptane was presented as a challenge to computer algebra by Levelt [193].

Manocha reported the early stages of a major study of ligand-protein docking in [205, 206] that he is pursuing actively at present. Emiris and Mourrain focus on the conformations of cyclic molecules in [89]. These authors all use the standard Denavit-Hartenburg formulation of robot linkage problems that is described in many texts *e.g.* [226] and they discuss the solution of the multinomial equations using Gröbner bases and resultant methods.

Finn and Kavraki provided an overview of this type of investigation [101]. Lewis and Bridgett [195] discussed docking from the standpoint of the Apollonius problem of tangents to sets of circles.

8 Nuclear magnetic resonance

Calucci and Geppi analyzed ^{2}H Zeeman and quadrupolar spin-lattice relaxation measurements in liquid crystals [56]. They used symbolic expressions generated by MATHEMATICA to explore trends in the computed effects of the diffusional and Arrhenius coefficients.

Gasparovic *et al.* discussed the design of a shielded gradient probe for high resolution work *in vivo* [111]. They used MATHEMATICA.

Grotendorst *et al.* analyzed NMR work on transport and diffusion across living cell membranes using MAPLE [123]. They solved a linear inhomogeneous system of ODEs with constant coefficients (the McConnell equations) by use of matrix exponentials. This REDUCEd the problem to symbolic matrix manipulation.

Jang and Han constructed formulas for spin-echo positions and amplitudes as functions of the pulse flop and phase angles and delay times for several pulse sequences [153]. They computed Zeeman and 1st and 2nd order quadrupole interactions for spins 1/2(1/2)3.

Kanters *et al.* published some prototype MAPLE procedures to manipulate product-operator expressions for spins under pulses and during chemical shift and coupling evolutions [173].

Kim *et al.* described an NMR study of hindered amide in an organometallic salt [178]. They solved a small set of linear equations symbolically.

Kuchel and his co-workers explored the biochemistry and physiology of erythrocytes with NMR. They used MATHEMATICA to deal with

1. spin-echo measurement of the diffusion of spins in a sphere [186],

2. the permeability of cell membranes from q-space data [183],

3. the shape of erythrocytes [185],

4. 2,3-biphosphoglycerate metabolism,

5. shape and movement in red cell alignment [184], and

6. time evolution computed from a tensor operator product basis for the density function [174].

Levitt produced hundreds of diagrams algorithmically that depict spin states, using MATHEMATICA for a text on spin dynamics [194] and developed a notebook to teach the subject.

Majumdar explored the structure of ^{13}C labeled proteins and nucleic acids. He computed magnetization transfers analytically, under the assumption of isotropic mixing in [203]. This led to a system of linear equations, that he solved symbolically with MATHEMATICA for 3 and 4-spin systems.

Sanctuary, Man and their coworkers published several papers on the analysis of quadrupolar interactions in single-spin solid state systems using MAPLE. They computed density matrices

1. for spin 5/2 excited by spin-lock sequences [204],

2. for spins 1, 3/2, 2 and 5/2 with RF excitation, using the Baker-Campbell-Hausdorff equation [151],

3. for spins 7/2 and 3/2 under 1st-order quadrupole interaction and RF pulse excitation [7, 8], and

4. Solomon echoes for spin 7/2 by soft pulse excitation [5].

Related work includes [4, 5, 6, 7, 8, 9]. Also, they developed pattern recognition algorithms CAPRI to analyze complicated 2D and 3D NMR spectra of proteins using graph theory and fuzzy mathematics. This was first reported in [319]. Back references to several other papers are given in the most recent account [197].

Mercier studied the relationship between the relaxivity and the molecular structure of paramagnetic coordination complexes, using MATHEMATICA to compute molecular electrostatic potentials in porphyrins as a basis for molecular modeling studies [220].

Nielsen and his co-workers published a survey of solid state NMR work on the characterization of membrane proteins [43] that cited their earlier work on the Baker-Campbell-Hausdorff problem [297] which used MATHEMATICA and is supported by a downloadable notebook.

Ouvrard *et al.* computed 2D NMR spectra of degenerate spin systems dissolved in liquid crystal media using product operator formalism and spherical tensor basis for the time evolution of the density matrix, using MATHEMATICA [236].

Rodriguez and Ruiz-Cabello developed a MATHEMATICA package to simulate the effect of RF coupling, J-coupling and precession in a space-varying magnetic field, via the use of density matrices and product operators [255].

Straubinger *et al.* extended the theory of pulse-angle dependence of double-spin-echo proton NMR [275]. They evaluated the time evolution of the density operator using MAPLE for comparison with the integral of the spectral signals. They compared theoretical and experimental results in [276].

9 Lattice spin models

Čížek, Vinette, Weniger and Bracken, in different combinations

1. applied the inner projection method to lattice spin [66],

2. showed that for finite cycles the energy of the anisotropic spin Hamiltonian is the root of a characteristic polynomial that they constructed using Gröbner bases [64],

3. combined the Lieb-Wu formulation and the configuration interaction approach to the Hubbard model in an application to cyclic polyenes [52],

4. constructed secular polynomials (containing coefficients that are functions of the coupling constant) for small cycles in the XY, Heisenberg and double Ising models [50],

5. used coupled cluster models [302].

In related work, Delhalle *et al.* used a Fourier method to evaluate lattice sums [81]. Further papers by these authors on symbolic spin lattice calculations are listed in [30].

Further work on the Hubbard model was reported in papers by Angelescu and Bhatt [16], Bartkowiak *et al.* [32] and Steeb *et al.* [132]. Taneri and Paldus [286], and Bishop *et al.* [41] considered Heisenberg and Ising models.

10 Lasers and electronic behavior of nanosystems

This area is dominated mathematically by nonlinear Schrödinger equations (nlSe). Software to deal with solitary waves and solitons and with coupled nlSe (cnlSe) is discussed later §15. Symbolic calculations for specific phenomena span a range of topics.

Bajer and Perina computed photon statistics and quadrature squeezing of second and higher harmonics generation using power series decompositions [23].

Bajer and Lisonek predicted laser pump dynamics for three- and four-wave mixing, developing Taylor series for the Hamiltonians in the time dependent Heisenberg formulation [22]. They computed the mean number of sub-harmonic photons under classical and chaotic pumping and squeezing.

Bancewicz interpreted low intensity scattered radiation signals by using a MATHEMATICA script to compute the interaction of a dipole with higher order multipoles, and deriving polarizability tensors for linear and tetrahedral molecules [26].

Beskrovnyi also approached three-wave mixing via the Heisenberg equations, generating second harmonics by mixing orthogonally polarized fundamental waves in a quadratic nonlinear medium [39].

Chow considered four coupled non-linear Schrödinger equations in relation to the propagation of light along birefringent optical fibers [63].

Dick calculated

1. the nonlinear optical response function and
2. the susceptibility of a molecule,

that correspond to

1. a given time sequence of light pulses and
2. a given combination of light fields,

respectively, using the Markov approximation to model molecular relaxation [83]. Radiation propagation steps and feeding were specified at run time.

Falloon and Wang computed the dynamic behavior of a single electron in a nanoelectronic device, using a time dependent propagation scheme for one-dimensional potential scattering, based on a Chebyshev expansion for the propagator $\exp(-2\mathcal{H}t)$ and a wavefront splitting algorithm coded in MATHEMATICA [91].

Janssen *et al.* computed the effect of saturation on the distribution of molecular angular momentum distribution in laser-induced fluorescence [154].

Javanainen and Yoo developed a semiclassical theory of the laser cooling of a trapped multistate ion, relevant to quantum jumps and frequency standards [156]. They used an anisotropic harmonic oscillator Hamiltonian and the Fokker-Planck equation for center of mass motion coded in MATHEMATICA. They dealt with closely related problems in [155, 322].

Johnston and Sarkar considered an electron trapped in a sub-micron device and used the concept of trajectories to construct a master equation for the single particle density matrix in a device with a driving field and inelastic phonon scattering [161]. They used MATHEMATICA to solve this for the tunneling diode.

Joyce, Pike and Sarkar constructed asymptotic expressions for laser line width by considering the time evolution of second order photon correlation functions of the radial field based on the Scully-Lamb master equation [171].

Kuchiev and Ostrovsky computed the dependence of angular asymmetry of photoionization and other observables of the multi-electron detachment from negative ions in a bichromatic laser field on the difference of field phases, using the Keldysh model and MATHEMATICA [187].

McCarthy, Wang and Abbott studied quantum dots [212] — electrons trapped between two layers of semiconductor that display many properties of 2D atoms that make them potential components of very efficient and precise lasers, nanodevices and quantum computers [306]. They described HF SCF calculations of the electronic states of N-electron quantum dots using MATHEMATICA [212].

Ng and Bhattacharjee extended the Ginzburg-Landau equation for a free-electron laser oscillator to the long-pulse low-gain region [229]. They devel-

oped a small amplitude expansion of the radiation field using MATHEMATICA and got excellent agreement between theory and experiment.

Nguyen and Nguyen-Dang derived the equations linking the time evolution operator for a laser driven oscillator to the operator for the corresponding free field system, as an example of the usage of a MATHEMATICA package for calculations that involve unitary transformations in quantum dynamics [230].

Orlowski and Wódkiewicz approached approximate laser theory, linear amplifiers and attenuators, correlated emissions lasers, two-photon lasers, amplifiers and related phenomena, using dynamical ordering of quantum quasiprobability functions to transform a Fokker-Planck type equation using MATHEMATICA [235].

Perinova *et al.* considered the quantum phase properties of a cubically behaved second-order nonlinear medium [241].

Pulov, Uzunov and Chacarov studied the propagation of

1. two waves at different carrier wavelengths in two-mode optical fibers,

2. two modes in fibers with strong birefringence [248].

They solved the cnlSe pair using the Lie symmetry approach to differential equations discussed in §15.

Sanchez *et al.* computed the steady state of the erbium laser model for 2-wavelength operation [261].

Schuermann and Schmoldt computed reflectivity and transmissivity of a lossless nonlinear dielectric slab when the dielectric function is linear in the intensity [263].

Senthilvelan *et al.* discussed the formation of a self-written waveguide, produced by light propagating through a photosensitive medium [267]. They solved the partial differential equations using the Lie symmetry software package LIE [136].

Tadić *et al.* discussed continuum (free-state) wavefunctions for ultrathin quantum confining structures. They avoided errors in the prior literature by using the WKB (Liouville-Green) approximation and asymptotic boundary conditions and unrestricted precision in MATHEMATICA [283].

Ueta considered the dynamics of an electron-wave packet in a quantum dot subjected to magnetic fields [296].

Yu *et al.* computed the quasi-discrete Hankel transform [323].

Yura *et al.* considered Laser-Doppler velocimetry [324].

11 Crystals, solids, surfaces

Achim *et al.* studied electron transfer in a mixed valence Fe^{2+}/Fe^{3+} complex [1]. Evidence of low symmetry components in the crystal field at the iron site prompted the inclusion of off-diagonal interactions in the simulation of the relaxation spectra. This used MATHEMATICA.

Anstis studied the reflection of fast electrons from a crystal surface and a decrease in depth of penetration when diffraction sets up a wave just beneath the crystal surface [17]. The three-beam approximation required eigenvalues of a 6×6 matrix, that were expressed as a power series in the Fourier components of the potential. MATHEMATICA was used to compute the leading terms.

Angelescu and Bhatt computed the ferromagnetic interaction of polarons in dilute magnetic semiconductors [16]. They used overlap integrals between hydrogenic atoms, in a Hubbard model, that had been computed using MATHEMATICA for K, L and M shell orbitals.

Bartkowiak used a single band Hubbard model to compute the grand canonical potential, staggered and charge ordered magnetic susceptibilities and compressibility from a series expansion in $1/T$ using diagrammatic perturbation theory [32]. He used MATHEMATICA to generate and to collect formulas.

Barvik *et al.* studied exciton transfer between molecules in a dimer using a dichotomic stochastic model in [33] and earlier papers. They used MAPLE to solve the time development of the site occupation probabilities and then the memory functions entering the generalized master equation.

Bishop, Hale and Xian computed ground state energy, anisotropic susceptibility and staggered magnetization as functions of anisotropy parameters using microscopic coupled cluster methods [41].

Bittl worked on protein bound tetrameric metal clusters that occur in photosynthesis and other biological processes [42]. He evaluated matrix ele-

ments of single spin operators needed to calculate ground state energies and effective hyperfine coupling observed in EPR spectra.

Coffey considered the magnetic interaction of type-II superconductors and point dipoles using London theory for work on magnetic force microscopy and low temperature imaging [69].

Folcia *et al.* studied systematic errors in high-accuracy universal polarimeter (HAUP) measurements [102]. They used MATHEMATICA to construct transmitted intensities.

Hergert and Dane simplified group theoretical studies of photonic crystals and applied the results to 2D examples [142]. They described a MATHEMATICA package that can be downloaded.

Kristoffersen studied the quantum Hall effect using high order perturbation via a Green's function and the density of states of electrons in a high magnetic field in 2D crystals [182]. He used MATHEMATICA to handle a combinatorial problem involving representations of Feynman diagrams.

Larsen and Thorkildsen computed the primary extinction factors for a perfect non-absorbing spherical crystal in the Bragg limit [190]. They computed absorption, weighted path lengths and extinction coefficients in cylinders and spheres in [289] and earlier papers.

Repetowicz *et al.* computed the eigenvalues of the tight binding models of quasi-crystals on 2D rhombic tiling structures for particular values of the hopping parameters [252].

Sobral *et al.* constucted formulas for the magnetic moments of intermallic compounds from the characteristic polynomial (CP) of the model Hamiltonian containing molecular and crystal field components using MATHEMATICA and applied these to $PrAl_2$ and $NdAl_2$ [271]. They discussed the magnetic properties corresponding to hexagonally symmetrical crystal fields, showed that the CP factorizes and computed high temperature susceptibility expressions [272].

Szöcs and coworkers used a generalization of coherence observation by interference noise (COIN) to explore electron excitation energy transfer (ET) that affects optical relaxation pathways between molecular aggregates, multichromophoric polymers and photosynthetic complexes [280, 282]. They used MATHEMATICA and MAPLE to compute the elements of large density matrices. Also, they studied nonlinear subsystem dynamics induced by a reaction field coupled to a quantum heat bath by applying projection techniques to the Liouville equation [281].

van Eijck and Kroon dealt with Coulomb energy in polar crystals [300].

Crystallographic group theory is discussed below in §15.1. The crystallographic aspects of combinatorial tiling theory are included in the short account of the topic by Huson [146]. This provides references to work of Dress, Huson, Molnar and others.

12 Kinetics

The earlier survey of life science applications of symbolic calculations [27] mentioned papers on

1. (pseudo-)steady state enzyme kinetics by Bennett, Dewar *et al.* [37], Bayram [34]–[35] and Yildirim [320]–[321],

2. compartmental analysis and identifiability methods in metabolic systems and pharmacokinetics by Raksanyi *et al.* [249], Chappell, Godfrey and Vajda [61], Ljung and Glad [200], Margaria *et al.* [209], Cobelli's group [19, 20] and Zheng [326],

3. affinity binding relations by Grinfeld, Bennett and Hubble [38, 120],

4. models of animal digestion by Jumars [172],

5. abortive complexes and random substrate binding by Schulz and Südi [264],

6. on-line estimation in bioprocess engineering by Farza and Chéruy [93].

Most of the papers in items 1–3 involve the solution of simultaneous multinomial equations using Gröbner bases and resultants. The survey [27] also includes a section on population dynamics that refers to several papers on Volterra-Lotka systems and related mathematical problems that are paralleled in chemical kinetics. In further work on symbolic computations in kinetics:

Ajbar delineated the behavior of bioreactors by a straightforward analysis to find pitchfork singularities using MATHEMATICA [10].

Alberty studied the thermodynamics of biochemical reactions involving water. He found the number of apparent components (independent reactions) at specified pH by row reduction of the apparent conservation matrix of stoichiometric numbers [11] and he computed Gibbs free energy [12]. He used MATHEMATICA for matrix operations and differentiation.

Fraser studied the steady state kinetics of enzyme mechanisms. He related the standard treatment to (1) slow manifold theory and (2) singular and ordinary perturbation theory applied to ODEs [103]. He gave formulas generated by MAPLE.

Grotendorst and Dornseiffer determined the mass and energy balance of a steam reformer that turns organic waste into hydrogen rich gases [122]. They computed the dependence of the extent of the reaction on temperature and pressure. They included a FORTRAN code generator.

Ratkiewicz and Truong generated reaction mechanisms mechanically [250] discussed in §13 below.

Gatermann investigated polynomial systems apropos kinetic studies based on Clarke's cone and stoichiometric network analysis [68], using toric varieties in an account that addressed a mathematical audience [112].

13 Chemical graph theory

The structural formulas of molecules are treated as graphs — weighted or unweighted, directed or undirected — in chemical investigations that require the number of possible structures, the actual list of these alternatives, the ranking of the alternatives by reference to a set of criteria, and pattern matching to test for overall identity and for substructural commonalities.

The mathematical infrastructure dates back to the isomer enumerations of Cayley in the nineteenth century. It led to the concept of isomorphism in graphs, to Pólya theory [247], and to related work in group theory [175]. In recent years, the chemical and pharmaceutical industries have been driving forces in the development of structure search algorithms and, for drug discovery and design, combinatorial chemistry. An extensive literature involves software that was implemented in general purpose languages using standard kinds of data structure representation and manipulation. The journal MATCH is devoted largely to this topic. Trinajstić gives the general background [295].

The MOLGEN system of Kerber, Laue and their associates is a powerful resource for research, industry and education. An early account was given in [15] and a recent application to patents is described in [177]. The web site [124] provides further extensive information, including links to several online journal articles about the system and its applications.

In other projects, Cash developed programs to compute the characteristic polynomial based on several different algorithms and pointed out the benefit of unrestricted precision arithmetic in this work [58]. He reported a new algorithm to compute the permanent polynomial and its implementation [59]. Dias and Cash developed a program to find the number of resonance structures in concealed non-Kekuléan benzenoid hydrocarbons [82].

Salvador *et al.* computed matching polynomials of fullerene graphs for C_{60-100} by an algorithm that uses partial differential edge operators [259].

Pisanski, Plavšić and Randić proposed a new characterization of cyclicity that involves the distance and detour matrices, and developed a computational algorithm that overcomes problems of slow convergence [245].

Ratkiewicz and Truong developed representations and combinatorial algorithms to generate mechanisms for complex combustion reactions and implemented these in a program COMGEN that was written in FORTRAN 90 to support the graph operations and pattern matching to eliminate redundancies [250]. Their COMGEN system uses the SMILES chemical notation [270].

van Almsick *et al.* developed an algorithm to enumerate isomers and diamutamers (same central skeleton but different arrangements of ligands) and wrote an implementation. They used the Cauchy-Frobenius lemma and Pólya polynomials [298, 299].

14 Other

Debye-Huckel theory: Sushkin and Phillies used MATHEMATICA to evaluate some integrals in a Silverstone-Moats expansion of electrostatic interaction of a pair of polyelectrolytes [278].

Dielectric properties of proteins: Simon-

son and Perahia used MATHEMATICA to solve some algebraic equations in a Charmm simulation of TMV [268].

Liquid films: Rubenstein and Leshansky considered the dynamics of thin liquid films with nonsoluble surfactants. They computed the film rupture time analytically from amplitude equations for Turing instabilities. They used MATHEMATICA to perform bifurcation analysis [256].

Polymers: Nakao *et al.* reported calculations on the cascade theory of substitution effects in non-equilibrium polymerization [227]. The kinetic equations give rise to polynomial equations which were solved using Gröbner bases.

Thermodynamics: J. Martin *et al.* computed thermodynamic properties of NH_2 [210] as mentioned under density functional theory in §4.

Levelt derived the equation of the critical curve of a binary mixture by converting the problem to a polynomial system that he solved using Gröbner bases [192].

Transport phenomena: Galceran *et al.* developed methods to analyze steady state currents of the scanning electrochemical microscope based on a theory of diffusion of an electroactive species through a multi-layered medium [107]. The MATHEMATICA code was included. It manipulates special functions and performs symbolic linear algebra.

Grotendorst *et al.* analyzed NMR work on transport and diffusion across living cell membranes using MAPLE [123].

Metzler and Comte solved the fractional diffusion equation to deal with advection processes [222]. They used MATHEMATICA to compute Fox functions.

15 Mathematical methods

15.1 Group theory

Classical applications of group theory to chemistry and materials science were aimed primarily at spectroscopy, crystallography and solid state physics. The development of software to compute properties of groups had grown sufficiently by 1967 to warrant the survey talk by Neubüser [228]. The numerous papers that he and other authors wrote in the years that followed have built computational group theory into a major activity. This affects many subjects besides chemistry and chemical physics. The monograph [54] explains the role of the mathematical objects that underly point group calculations and gives references to a wide range of computational schemes. Further background will be provided in [143].

Crystallographic groups: The GAP system that was initiated by Neubüser in 1986 addresses a wide range of topics in computational algebra and discrete mathematics [110]. It is a major source of algorithms for computing with groups in general. Most of these are performed by packages with individual authorship. CRYST [88] implements algorithms for work with crystallographic groups that include the computation of Wyckoff positions and maximal subgroups [87] and CRYSTCAT [95] contains a library that gives access to all crystallographic groups up to dimension 4. Gähler has also considered density of states on tilings [106]. Souvignier considered the enantiomorphism of crystallographic groups in higher dimensions with results in dimensions up to 6 [273].

The CARAT project of Plesken *et al.* handles enumeration, construction, recognition and comparison for crystallographic groups up to dimension 6 — see [57, 234] and further papers cited in [57]. It was coded in C and it can be used as a standalone package or within GAP together with CRYST and CRYSTCAT that, in combination, constitute a very powerful resource.

Tools of this kind, that

1. regenerate data which had to be transcribed from printed tables in the past, and
2. which will generate data for new groups that arise in the course of future work on quasicrystals and structures of kinds that have not been anticipated,

transform the nature of crystallographic computing.

Altmann and Herzig constructed the extensive Point Group Theory Tables [14] using general purpose programming methods. They included char-

acter and multiplication tables, irreducible representations, subductions, direct products and other properties of proper and improper point groups. Besides crystallographic work, these tables are cited in scores of papers that relate to topics as diverse as quantum wires, magnetic properties of CoO, π-electron theory of 2D and 3D conjugated systems, fullerenes, phosphomolybdates and many other topics (found in an online search using Science Citation Index). Pokorny and the authors of the compendium [14] extended its methods in [246].

Altermatt and Brown reported a computer-based symmetry algebra to reconstruct an infinite bond network without *a priori* knowledge of atomic coordinates [13].

Arteca and Mezey computed a hierarchy of homologous shape groups of algebraic topology to represent and characterize potential surfaces, conformations and other shapes of chemical interest [18].

Chen, Ping and their coworkers reported point group calculations in [62] and earlier papers.

Grosse-Kunstleve presented algorithms for crystallographic space group information and described tests using the SgInfo library [121].

Thiers *et al.* discussed incommensurably modulated crystals and quasicrystals and used superspace groups to describe them [288].

van Almsick *et al.* used point group calculations to enumerate isomers and diamutamers [299].

For combinatorial tiling theory that applies to crystallography, see [146].

Spectroscopic applications of point groups supported by symbolic computation include the work on CO_2 [75] and tetratomic molecules [53] that were mentioned under molecular vibrations.

Symmetry groups: These were used by Fripertinger [104] and Kerber and Kohnert [176] in work related to chemical graph theory discussed in an earlier section, and by Li and Pauncz [196] in an evaluation of valence bond matrix elements based on algebrants (generalized matrices).

Pseudo orthogonal groups: Taneri and Paldus constructed dimensional information concerning the irreducible representations needed in a Hubbard model of cyclic polyenes, using MAPLE [286]

Lie groups: This term has double meaning. In one usage that occurs in the titles of several monographs and texts, *e.g.* [149, 233, 262], the commonplace usage of "symmetry" is generalized to a very large class of local transformations that are used to solve differential equations by Lie symmetry analysis. The Russian literature also uses the term Ovsiannikov group [237]. The methods are discussed under Lie algebras below. Recent accounts of symbolic calculations of chemical interest that mention Lie groups with this connotation report the work of Ayari on supersymmetric two bosons equations [21] and the work of Pulov *et al.* on optical fibers discussed earlier [248].

The other usage, found in titles that include [199] and in monographs that include [2, 98, 79] refers to unitary and orthogonal groups of operators that satisfy the Jacobi anticommutation identity, used in studies of spin and angular momentum and in models that create and annihilate particles.

As regards this double usage, Hydon has commented "The main focus in quantum physics is on the groups and algebras themselves; tools such as representation theory are particularly useful in applications. By contrast, symmetry methods focus on the role of symmetries as transformations of a given differential equation. Once the symmetries have been found, they can be used to construct exact solutions. Although the structure of the underlying Lie group or Lie algebra is important (particularly when one looks for discrete symmetries), many applications do not require this structure to be stated explicitly." [148]

Unitary Lie groups were used by Paldus for many-electron correlation calculations [238]. The relation between these Lie groups, *e.g.* SU(3) and SO(3), and the corresponding Lie algebras su(3) and so(3) is explained in [2, 79].

15.2 Lie symmetry analysis

Hydon provided a very clear introduction [147]. Further accounts include [149, 233, 262, 237]. "Symmetries" in this context can be regarded as changes of variable that permit the simplification of differential equations, in part by converting high order equations to sets of lower order equations, and separating PDEs into sets of ODEs. Hydon explained the ideas of diffeomorphisms, symmetries, infinitesimal generators, orbits, invariant points, REDUCEd characteristics, canonical coordi-

nates, prolongations and other terms that are taken for granted in some of the software documentation.

A recent literature search by MPB has found (1) an extensive literature that applies these methods using "pencil and paper" (or at least makes no mention of symbolic software), (2) accounts of numerous software packages to solve differential equations using these methods that do not have published applications which could be found using a variety of search strategies, and (3) a few packages written for particular applications that did, in each case, receive wider published use.

Hereman provided an extensive survey of software through 1994 to support the mathematical reduction of cnlS systems using Lie algebras [140]. Mansfield, Reid and Clarkson included references to software for Lie algebra work on cnlS systems through 1998 [207]. The Symbolic Analysis Focus Group website provides further updates [279]. Carminati and coworkers reported a detailed comparison of the performance of several packages in applications to test examples of the Boltzmann, Fokker-Planck, magneto-gas-dynamic, Navier-Stokes and nonlinear Schrödinger equations [55].

Symmetries for the stationary Schrödinger equation, and for numerous problems in fluid dynamics, nonlinear optics and properties of liquid crystals are among the results in [149], which contains further material for a wide range of physical problems. Many of these symmetries were derived using Russian symbolic computation software [148].

Wittkopf listed symmetries for numerous differential equations that came from physical problems in the account of the MAPLE package `rif` [316].

Wolf developed the packages Crack, LiePDE (Refs. 205 and 207 in [140]) and ConLaw (for the related computation of conservation laws) and applied these to his work in the theory of relativity and the classification of integrable systems. He discussed his general methodology in [317].

Head developed the package LIE for his own work in materials science and extended it to BIGLIE [136, 137, 138]. These have been used in several further applications in science and engineering [138] including work on a self-writing waveguide [267].

Hereman developed the Macsyma package `symmgrp.max` that was the basis of numerous papers in plasma physics, fluidics and other natural phenomena (Ref. 30 in [140]).

15.3 Lie operator algebras

Adams used these in symbolic calculations to manipulate expressions containing angular momentum operators and the matrix elements in high order perturbation calculations of the Zeeman effect [2].

Fernández reported similar work and further symbolic Lie algebra computations to construct functions of square matrices, and to manipulate expressions that contain operators to create and annihilate particles [98]. Examples include calculations of the vibration-rotation spectra of diatomic molecules. Fernández and coworkers reported related symbolic calculations in several other papers — see §2.

The work on nuclear magnetic resonance, mentioned earlier, that is based on the Baker-Campbell-Hausdorff equation [151, 297] does, in effect, use Lie algebra methods (see, *e.g.* [98]).

Several of the symbolic calculations in nonlinear optics, mentioned earlier, manipulate expressions containing creation and annihilation operators using the methods of Lie algebras, without using the term explicitly. Bajer and Lisoneck coded in TURBOPASCAL [22]. Beskrovnyi wrote simple MATHEMATICA scripts [39]. Dick used a diagrammatic perturbation theory, represented operators and observables by lists, and coded in REDUCE. Nguyen wrote MATHEMATICA modules for a substantial class of unitary transformations [230].

15.4 Solitons

Solitons play an important role in several areas of chemistry and allied fields that involve nonlinear differential equations. Many of the papers that discuss symbolic calculation in relation to solitons deal in general mathematical terms. The connection with potential applications that address specific chemical, physical and biological properties and phenomena has to be made largely through further literature that does not mention symbolic calculation. Among the monographs that made these connections

1. Davydov addressed the behaviour of proteins, muscles and other biological systems [78],

2. Kishvar and Agrawal considered optical solitons in a wide range of contexts [180],

3. Ihn considered electronic properties of nanosystems [150], and
4. Wegener and Schafer dealt with both optical solitons and nanosystems [308].

A recent search of the online archives of the International Journal of Quantum Chemistry, using "solitons" as the key, found 46 papers, and the corresponding search of the Journal of Chemical Physics found 76 papers. Most dealt with electronic and dynamic properties of conducting polymers, a subject surveyed by Chandrasekhar [60].

Other topics included

1. metal-polymer interfaces [77],
2. lattice relaxation [159],
3. surface catalysis [90],
4. liquid films [170],
5. Raman processes in molecular liquids [179],
6. carcinogenic radiation [188],
7. fullerene superconductivity [208],
8. Langevin equations [216],
9. coherent biosystem excitation [221],
10. geometry optimization [224],
11. hydrogen bonded molecular chain solids [225],
12. vibron dynamics [239],
13. polyelectrolyte light scattering [266],
14. inorganic complexes [277].

The papers just cited did not use symbolic computation but they all suggest fertile fields for applying software that supports soliton theory.

Hereman and Zhuang provided a very convenient explanation of the computational basis of some of the key methods, and commented on a few of the early Macsyma and MATHEMATICA packages [141].

Gao and Tian have published over 60 papers on the mathematics of soliton theory, both in general terms and in relation to specific applications to plasmas, fluid dynamics, hydrology, optics, and topics in chemistry and biology.

The reports of their software include accounts of

1. a generalized hyperbolic function method [290, 291],
2. a variable coefficient balancing act method for NLEEs [108],
3. a direct method for non linear Schrödinger equations [292],
4. Bäcklund transformations and soliton-like solutions via the truncated Painlevé expansion, applied to coupled KdV equations [293],
5. the Clarkson-Kruskal direct reduction method extended to variable coefficient and coupled NLEEs [294].

The five papers just cited refer back to the considerable earlier work of the authors. They have application, respectively, to

1. non-linear chemical kinetics modeled by the Duffing equation, as in [260],
2. rotating fluids,
3. optical fibers,
4. liquid films as in [170], and phase separation as in [218],
5. the Brusselator problem.

Also, [109] relates to superconductivity.

In the further recent literature of symbolic computations that relate to single solitary waves and solitons

1. Fan discussed a generalized Hirota-Satsuma coupled KdV equation and a coupled MKdV equation [92],
2. Hong discussed dark solitary wave solutions for the higher order nonlinear Schrödinger equation with cubic-quintic terms [144],
3. Hu, Tam, Wang and co-workers discussed the Jimbo-Miwa and related equations [145] and the 2+1 dimensional Kaup-Kupershmidt equation [285],
4. Li and Liu described Rath, a MAPLE package for finding solitary wave solutions to nonlinear evolution equations [198],

5. Parkes and Duffy discussed a tanh method, with several illustrations [240],

6. G. Zhang *et al.* discussed the tanh method combined with Wu elimination or Gröbner basis reduction [325].

7. Baldwin, Hereman and their coauthors recently completed an extensive treatment of the tanh method for ODEs and PDEs which introduces several innovations, includes MATHEMATICA implementations and surveys earlier literature [24].

This literature cites extensive earlier work of the respective authors.

15.5 Convergence acceleration

Weniger summation was treated extensively in [311, 312] and earlier papers. These discussed sequence transformations and the related algorithms of Aitken, Wynn and Brezinski, and Padé approximants. Also, [311] gave references to applications that include the polarization expansion for the interaction energy of hydrogen atoms, the interaction of atomic hydrogen with an ultrashort laser pulse, a perturbational treatment of the triplet S even-parity ground state of helium, auxiliary functions for the evaluation of molecular integrals over Slater orbitals and Gaussian orbitals, scattering equations, SCF iterations, Fourier series in the evaluation of Green's functions, excluded volume problems of dilute polymer solutions, statistical systems, and electronic structure of stereoregular quasi-one-dimensional polymers such as undistorted and Peierls-distorted polyacenes, using both solid-state and crystal cluster approaches.

15.6 Coupling coefficients

Clebsch-Gordan, Wigner, $3j$, $6j$, Racah, Gaunt and related coefficients have been computed precisely by several authors, using a variety of formulas and the unrestricted precision rational arithmetic provisions of several computer algebra systems. Early work included Takada [284]. Wang and Williams [307] and Kocbach and coworkers [94] used MATHEMATICA. Lai used MAPLE [189]. Draeger used MACSYMA [84]. Recently, Fritzsche *et al.* developed a further powerful system in MAPLE using Racah algebra, reported in [105] and papers cited therein. Barnett has used a non-standard approach [29].

15.7 Statistics

Symbolic calculation has vast potential in its application via statistics to theoretical work in natural science and to data analysis. This has been discussed at length with extensive references in [27].

16 Modern computer algebra — fast multiplication

Symbolic calculation is supported by a panoply of algorithms that have evolved over the past half-century from an algebraic approach to mathematics. While linear algebra and group theory are used and understood very widely in the natural sciences, there is need for increased awareness and understanding of the methods of computer algebra. These have been brought together in two recent books [71, 113].

The manipulation of polynomials is a major focus of published results and ongoing research that impacts chemistry via many routes.

The multiplication of integers on a computer with fixed word length d and base r illustrates some of the key principles. Typically, an n-digit integer can be stored in an array of $\ell = \lceil n/d \rceil + 1$ words. The 1st word contains ℓ, the 2nd word contains the leading n mod d digits, and the 3rd through final words contain the successive blocks of d digits in decreasing order. Then, multiplication of two integers can be regarded as the multiplication of two polynomials of degree ℓ and argument $x = r^d$. The contents of the array comprise the coefficients. The use of symbolic calculation software to perform unrestricted precision arithmetic is being reported increasingly, even when formulas are not generated. The efficient multiplication of integers is supported by algorithms to multiply polynomials efficiently.

The multiplication of two polynomials of degree n with integer coefficients by the classical pencil and paper method requires $(n+1)^2$ integer multiplications and n^2 integer additions. For example, when $n = 1$, evaluating the formula $(a+bx)(c+dx) = ac+(ad+bc)x+bdx^2$ requires 4 integer multiplications and 1 integer addition, when

a, b, c, d are integers. However, by computing ac, bd, $u = (a+b)(c+d)$ and $ad+bc = u - ac - bd$ in turn, the number of multiplications is REDUCEd to 3, at the expense of increasing the number of additions and subtractions by 3. This principle is used in the Karatsuba algorithm. Two polynomials $f(x)$ and $g(x)$ of degree at most $n = 2m-1$ can be written $F_0 + F_1 x^m$ and $G_0 + G_1 x^m$, where F_0, F_1, G_0, G_1 are polynomials in x of degree $< m$. The product $f(x)g(x)$ can be written as

$$\begin{aligned} & F_1 G_1 x^{2m} + \\ & ((F_0+F_1)(G_0+G_1) - F_0G_0 - F_1G_1)x^m + \\ & F_0G_0 \end{aligned} \tag{1}$$

This requires one polynomial multiplication to form the first coefficient F_1G_1, another to form the third coefficient F_0G_0, and two additions, a multiplication, and two subtractions to compute the middle coefficient, because F_0G_0 and F_1G_1 have been formed already. Their degree is up to $2m-2$, and the two subtractions cost as much as four additions at degree less than m. Finally, there are two more additions of the "top half" of F_0G_0 (namely, at degrees $m \ldots 2m-2$) and the "bottom half" of F_1G_1, (at degrees $0 \ldots m-2$) to the middle coefficient. As an example with $m = 2$, we have

$$\begin{aligned} & ((2x+1) + (4x+3)x^2) \cdot ((6x+5) + (8x+7)x^2) \\ & \quad = (32x^2 + 52x + 21)x^4 + \\ & \qquad (40x^2 + 60x + 22)x^2 + 12x^2 + 16x + 5. \end{aligned} \tag{2}$$

Each of the three multiplications involves a pair of polynomials of degree less than m. By the classical method, this costs $3m^2$ integer multiplications instead of $(2m)^2$, at the expense of $3(m-1)^2 + 8m$ additions instead of $(2m-2)^2$, i.e., a saving of m^2 integer multiplications and $m^2 - 10m + 1$ additions.

The Karatsuba algorithm applies this principle recursively to each of the polynomial products in (1). The detailed analysis in pp. 221–223 of [113] showed that when n is a power of 2, polynomial multiplication can be performed with $9n^{\log 3} - 8n$ additions and multiplications instead of $2n^2 - 2n + 1$. This is a 1.7 fold improvement for $n = 128$ and a 4 fold improvement for $n = 1024$.

The same approach applies to the multiplication of long integers, except that one has to take care of carries as well. Thus one obtains an $O(n^{\log 3})$ algorithm for multiplication of n-word integers.

Further advances for polynomial and integer multiplication give $O(n \log n)$ and $O(n \log n \log\log n)$ performance. The latter are due to Schönhage and Strassen, Schönhage, and Cantor and Kaltofen. All of these were described and analyzed in Chapters 8 and 10 of [113].

The fast multiplication techniques described above can be employed not only for multiplication of integers and polynomials of arbitrary length, but also of multiprecision floating point numbers.

We now have a trio of multiplication methods: slow (classical), medium (Karatsuba), and fast. Experience shows that any implementation must use all three in a hybrid fashion, because typically the slow algorithm is the fastest for small inputs, at some input size the medium algorithm takes over, and large inputs are the domain of fast methods. Fortunately, the typical user of a computer algebra system need not give any thought to this, since this is one of the core functionalities provided by such systems.

Following the discovery of the Karatsuba algorithm in 1962, attention was directed to other multiplication processes. In particular, the conventional methods of linear algebra require $O(n^3)$ operations to multiply two $n \times n$ matrices. In 1969, Strassen developed a scheme for matrix multiplication that requires $O(n^{\log 7})$ ring operations (additions and subtractions). Each of the input matrices A and B "is divided into four $n/2 \times n/2$ blocks, and the computation of AB is REDUCEd to seven multiplications and 18 additions of $n/2 \times n/2$ matrices, in comparison to eight multiplications and four additions for the classical algorithm" (p. 327 of [113]).

The multiplications are handled recursively, as in the Karatsuba algorithm for polynomials. Matrix addition is much less costly than multiplication. Hence the asymptotically shorter running time. A slightly shorter variant was analyzed on p. 328 of [113], which also cited subroutine libraries that contain (1) implementations and (2) quotations concerning the range of practicality of the algorithm. Golub and van Loan gave a trivial example of the Strassen algorithm producing an incorrect numerical result [117]. Their argument depended entirely on fixed precision, and the rationalization of the matrix elements in their example leads to the correct result without intermediate swelling.

"Further computational problems in linear alge-

bra include matrix inversion, computing the determinant, the characteristic polynomial, or the LR-decomposition of a matrix, QR-decomposition and unitary transformation to upper Hessenberg form. It turns out that all these problems have the same asymptotic complexity as matrix multiplication (up to constant factors), so that a fast algorithm for one of immediately gives fast algorithms for all of them. ... The most fundamental consequence of Strassen's breakthrough was the development of *bilinear complexity theory* ... that is concerned with good and optimal algorithms for functions that depend linearly on each of two sets of variables" *e.g.* the coefficients (elements) in a pair of polynomials (matrices) — p. 329 in [113] — which went on to discuss fast modular composition of polynomials, "black box linear algebra", Wiedemann's algorithm for solving linear equations and sparse linear algebra.

Many chemical problems lead to vast, sparse matrices. The development of fast algorithms based on the methods of computer algebra, that benefit from structural features that are consequent on the underlying chemistry is an open field for research.

17 Modular arithmetic

Modular operations are used extensively in the theory and application of computer algebra. Checking the correctness of new algorithms for the rapid multiplication of long integers is one of the simplest applications. Assume that a and b are positive integers and c is supposedly the value of ab. Let p stand for a prime and let $a^* = a \bmod p$, $b^* = b \bmod p$, $c^* = c \bmod p$. Then if $(a^*b^*) \bmod p \neq c^*$, it follows that $c \neq ab$. As explained in [113], the converse $(a^*b^*) \bmod p = c^*$ only REDUCEs the probability that $c \neq ab$ to less than $1/2$. But the probability can be REDUCEd to any required tolerance by checking that the equality holds for a large enough number of primes.

This "fingerprinting" method is used to compare separate copies of large databases that have been updated independently by supposedly the same changes. Each copy is a bit string and viewed as a (possible huge) number, and with an exchange of a small (logarithmic) number of information bits one can quite reliably detect discrepancy. This might be applicable when molecules, sets of molecules, lengthy mathematical formulas, numerical reference data, sequencing information, or depictions of molecular properties in combinatorial chemistry are compared.

Many of the algorithms of computer algebra exploit the duality between "ordinary" and modular operations. In some cases, data is REDUCEd modulo a single prime integer or polynomial, operations are performed on the modular image, which is then "lifted" to an image modulo a sufficiently high power of the prime or polynomial, respectively, using an algebraic variant of the well known Newton iteration technique from numerical analysis. The final result of direct interest is reconstructed from its image that the lifting has produced.

In other cases, the same set of modular operations is performed with respect to several small primes and the modular results are combined to form a single end product. The formal recombination, called the Chinese Remainder Algorithm, is based on the extended Euclidean algorithm that is discussed below. This technique is analogous to the well known Lagrange interpolation from numerical analysis, which recovers the value of a function from its images at several points and, in fact, is also used in symbolic computation. Exercise 5.18 in [113] provides a lighthearted illustration of the recombination in the integer case.

The extended Euclid algorithm (EEA) follows the general path of the elementary Euclid algorithm but, additionally, constructs a set of intermediate results that the following table illustrates. It relates to the computation of the gcd of $r_0 = 126$ and $r_1 = 35$.

i	q_i	r_i	s_i	t_i
0		126	1	0
1	3	35	0	1
2	1	21	1	-3
3	1	14	-1	4
4	2	7	2	-7
5		0	-5	18

Reading down the r_i column we have the two starting numbers 126 and 35, and then the remainders of the successive divisions $126/35, 35/21, 21/14$ and $14/7$. Reading down the q_i column, the occupied slots 3, 1, 1, and 2 are the quotients of these divisions. The Bézout coefficients s_i and t_i satisfy $r_i = s_i f + g_i t$ leading to an expression in row 4

for $\gcd(r_0, r_1)$ as a linear combination of r_0 and r_1, namely $7 = 2 \cdot 126 + (-7) \cdot 35$.

The fast algorithms for multiplication, factoring, linear algebra and other processes based on modular arithmetic and algebra and the EEA comprise several chapters of [113]. The algorithm to evaluate a determinant, that is a staple of many software packages including the SACLIB system used in [31] provides a relatively simple example of the use of modular methods.

A determinant can be evaluated by Gaussian elimination, which costs at most $2n^3$ multiplications, additions and divisions. Edmonds and Bareiss have shown that the numerators and denominators in all intermediate results are of length $O(n)$, if the coefficients of the input matrix are word-size integers. Thus, using classical arithmetic, computing the determinant via straightforward Gaussian elimination takes $O(n^5)$ word operations. Using a modular approach, described below, the cost can be REDUCEd to $O(n^4)$.

The idea is to choose $O(n)$ word-size primes, compute the determinant independently modulo each prime via standard Gaussian elimination, and reconstruct the determinant from its modular images. The following toy example illustrates the process. Suppose we want to compute the determinant of the matrix

$$A = \begin{pmatrix} 4 & 5 \\ 6 & -7 \end{pmatrix}.$$

We choose the prime numbers 17 and 19 as moduli and obtain $\det A \equiv 10 \bmod 17$ and $\det A \equiv 18 \bmod 19$. The recombination yields $\det A \in 265 + 323\mathbb{Z}$, and in fact $\det A = -58$, the integer of least absolute value in this set.

In the determinant example, the size of the result of interest is about the same as the size of the coefficients in all intermediate results. There are, however, many examples in symbolic computation, the most prominent one being the greatest common divisor of two polynomials with integer coefficients, where the coefficients of the intermediate results are significantly larger than the coefficients of the final result. This phenonmenon is known as intermediate expression swell. The small primes modular approach described above is particularly useful in such a case, since the required number of primes depends only on the size of the final result.

18 Polynomial systems

Many computer algebraists regard the pinnacle of their field to be the theory of Gröbner bases started by Bruno Buchberger in the early 1950s. The solution of sets of simultaneous multinomial equations comprise the main practical application in the natural sciences. Gröbner bases were used for this purpose in

1. some of the stereochemical work of Manocha [205], Emiris and Mourrain [89] and Levelt [193],
2. the polymerization studies of Nakao *et al.* [227],
3. the enzyme kinetics work of Bayram [34]–[35] and Yildirim [320]–[321],
4. the compartmental analysis and identifiability work of Margaria *et al.* [209] and Cobelli's group [20, 19] on metabolic systems, and Boens work [45] on spectroscopic data analysis,
5. the transformation of the Bethe equation by Čížek and P. Bracken [64] and
6. Levelt's work on the thermodynamics of binary mixtures [192],

which have all been mentioned earlier in this survey.

Buchberger developed an algorithm to construct Gröbner bases. Refinements and extensions of this algorithm are the subject of ongoing research that has been the subject of entire books and conferences. Methods based on the classical theory of resultants in fact are used for polynomial equations to an increasing extent, but Gröbner bases will undoubtedly continue to command considerable attention. The literature of computer algebra tends to introduce these by reference to ideals and other mathematical concepts. A simple explanation that begins by sidestepping algebraic terminology is being provided separately [223].

For the present, we give a very simple example. Suppose that a piece of equipment must be installed in a rectangular box that has a capacity of 6 cubic centimeters, a surface area of 22 square centimeters, and a total edge length of 24 centimeters (because of some scenario involving the radiation or

absorption or catalytic properties of surfaces and edges). How long are the edges? Call the edge lengths x, y, z. Then the geometry is expressed by Eq. (3).

$$\begin{aligned} x\,y\,z &= 6, \\ 2\,x\,y + 2\,y\,z + 2\,z\,x &= 22, \\ 4\,x + 4\,y + 4\,z &= 24. \end{aligned} \tag{3}$$

In MATHEMATICA, the single command (4)

```
GroebnerBasis[
  {x y z - 6,
  2 x y + 2 y z + 2 z x - 22,
  4 x + 4 y + z - 24},
  {x, y, z} ]
```
(4)

converts the three equations (actually the polynomials that comprise the left hand sides, after the transpositions that make the right hand sides zero) to the triangular system Eq. (5).

$$\begin{aligned} &\{x + y + z - 6, \\ &-z^2 - z\,y + 6\,z - y^2 + 6\,y - 11, \\ &-z^3 + 6\,z^2 - 11\,z + 6\}. \end{aligned} \tag{5}$$

The third of the polynomials in Eq (5) factors to $(z-1)\,(z-2)\,(z-3)$. Substituting the root $z = 1$ in the second polynomial gives $-y^2 + 5\,y - 6$. This factors to $-(y-2)\,(y-3)$. Substituting the roots $z = 1, y = 2$, in the third polynomial gives $(y-3)$. So $\{x = 1,\ y = 2,\ z = 3\}$ is a solution of the original equations and, by symmetry, so are $\{x, y, z\}$ set to all permutations of $\{1, 2, 3\}$.

In this particular example the Gröbner basis provides a triangularization of the original set of equations. Many other sets of polynomials can be triangularized correspondingly to Gröbner bases. However, this does not always occur. Certain side conditions have been tacitly assumed that cannot be taken for granted in general. Triangularization of a set of polynomials does not always create a Gröbner basis. And the word "basis" in this context does not have the meaning that it usually conveys to chemists, that comes from linear algebra where it connotes the basis of a vector space. For a full explanation, see [223].

19 Discussion

This survey is, of necessity, incomplete. It has been spun off a bibliography that MPB compiled for an NSF workshop two years ago, that has since grown in a manner reminiscent of the broomstick of the Sorcerer's Apprentice. The survey [27] was an earlier spin-off. Here, the constraints of space and time have prevented the coverage of heat/mass transfer and several other topics that are important in chemical engineering and materials science. The many pieces in the educational resource maintained by Zelinski [327] have not been woven into the fabric of the survey. The Journal of Chemical Education has published numerous articles in recent years on the instructional use of symbolic calculation. For further citations that relate to these topics and to the topics in the present survey see [30].

The process of collecting material for the survey provided a dramatic experience of the power of current technology in the location, retrieval and organization of information. The process also has provided salutary insights into the limitations of some resources, and pointers to presentational tactics to facilitate future mechanized survey writing. Numerous papers of considerable relevance that slipped through the net of CAS and SCI searches were found by searching the websites of the journal publishers. Citation searches based on book titles can be rather incomplete. Macsyma and other acronyms that do not have multiple meanings are excellent search keys. "MAPLE" and other words that are in general usage are not.

Having the full text of articles online has expedited the inspection of recent papers (and older papers in some journals) enormously. But there is no substitute for expert knowledge and the collection of information by email has been essential and the key to many parts of this survey.

The citations to several workers do not show the full extent of their published work which uses symbolic computation. In some cases — notably Čížek and Weniger, the work was too voluminous to list here. We have tried to indicate this in the text. In some cases, the workers used symbolic computation in research without mentioning this in the published accounts. Férnandez has provided MPB with a list of over 20 papers which he and Ogilvie wrote individually and jointly, in which this hap-

pened. Pike has told MPB that he and several other members of the Wheatstone Laboratory used MATHEMATICA in work for dozens of papers over the past decade without mention.

While the authors believe that symbolic calculation will become commonplace in scientific research, they think that mention of its use can be beneficial, particularly when scripts are made available in the supplementary material which journals put in online archives to an increasing extent. It is to be hoped that these scripts will contribute to a growing body of material that builds on earlier work mechanically and, in turn, is built on correspondingly.

Looking to the infrastructure of symbolic computation, MAPLE and MATHEMATICA have featured most extensively in the material which has been surveyed. General purpose programming languages have been used effectively in several calculations, *e.g.* TURBOPASCAL in [22]. FORTRAN 90 contains features that are a major advance on the more commonly used FORTRAN 77, that proved very useful in [250].

FORM [301], SINGULAR [119], SACLIB [70] and other languages that were developed for special research environments are far more powerful for certain applications than MAPLE and MATHEMATICA. A partial comparison for one problem is given in [31]. The specification of future languages should take note of the varied needs of users that published accounts reflect. While some users need (or avail themselves of) the very varied features of MATHEMATICA, many users have very simple needs that are best addressed by relatively simple low cost systems with short learning curves and freedom from idiosyncratic behavior. The whole issue of learning *via* MAPLE worksheets and MATHEMATICA notebooks has been bypassed here, but it is very important. So is the combination of symbolic calculation with graphic display. Besides plotting continuous functions, this includes limitless possibilities of algorithmic generation of diagrams. Obvious examples include (1) Feynman diagrams, (2) reaction pathways, (3) transition schemes in laser systems, and (4) simple enumerations of chemical formulas and depictions of orientation, 3D structure, chirality and properties of atoms and bonds.

Future developments in hardware and in algorithms for parallel and grid computing are needed to increase the extent to which symbolic calculation can benefit society. Weniger has provided the following historical comparison. "As a simple test for the power of a computer, I like to compute 10000! — approximately $0.28 * 10^{35660}$ — with the help of MAPLE. On my old 486 PC, I needed something like 220 seconds, and older SUN workstations were actually not much faster. Under MAPLEV Release 5.1, my private laptop now needs 1.7 seconds, but under MAPLE 8 I need on the same machine only 0.14 seconds" [313].

Still further advances, however, are needed. Pharmaceutical/biomedical applications of CA is conspicuously limited by present compute power in Manocha's work on protein-ligand docking [206] and Cobelli's work on identifiability [19].

More than a dozen benefits of symbolic calculation were listed recently in [28]. Herbert Jones was probably the first user to observe and report several of these. The juggernaut rolls on. He was one of the drivers.

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