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How can we effectively improve the mathematical capabilities of students of chemistry?

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Abstract:

We describe our extensive collective experience in the conduct of courses based on the use of advanced mathematical software to enhance the capabilities of students of chemistry to solve problems with a mathematical component. These courses have been based on an interactive electronic textbook *Mathematics for Chemistry with Symbolic Computation* that has been concurrently developed and expanded. The admirable performance of the students who have benefited from our courses leaves no doubt that mathematical software is an invaluable tool for the teaching, learning and practice of mathematics in a chemical context.

Keywords: mathematical software, mathematics for chemistry, symbolic computation

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Introduction

Chemistry is the natural and physical science that treats matter and its transformations. As a physical science, chemistry has a strong quantitative mathematical component, from the stoichiometric proportions applied in chemical reactions to the physical models in its theoretical bases (thermodynamics, kinetics, molecular interactions and spectra), passing through molecular structure (bond distances and angles as geometric attributes), to quantum theories and statistical thermodynamics. In most approaches to the teaching of chemistry, students learn how to handle chemical calculations performed with paper and pencil, some treatment of data using general software such as a spreadsheet, and perhaps also the use of *black-box* software for structural calculations. Those approaches are effective for introducing chemical concepts and for preparing the students for the future practice of their chemical profession, but chemical curricula in universities around the world typically lack the development of powerful mathematical capabilities using mathematical software on digital computers, in particular the capability of symbolic computation. We specify here symbolic computation because it allows the solution of problems arising in chemistry stated in the most natural way, beginning from basic equations applied to a particular situation. Harnessing the power of mathematical software in the form of computer algebra enables the students to become capable of solving complicated problems unfeasible by manual means or even with merely arithmetical computation. In this article we discuss the benefits of an interactive electronic textbook, of title *Mathematics for Chemistry with Symbolic Computation*, based on a particular mathematical program, *Maple*, to teach the mathematical skills that are applicable to chemistry.

Pedagogical basis of our approach and software selected for the delivery

To assist students of chemistry with the necessary mathematical knowledge and capability, during the past 18 years, one author has presented short courses, of duration up to 4 weeks, and full semester courses, and the two authors together have presented semester courses on other occasions; in each case these courses are based on an interactive electronic textbook, of title *Mathematics for Chemistry with Symbolic Computation*, that has been

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in concurrent development and is now in its fifth edition (Mathematics for Chemistry with Symbolic Computation, 2016). The objective of the course, and of the underlying textbook, is to provide students of chemistry with both an understanding of essential mathematical concepts and principles and a practical ability to solve mathematical problems over the entire range of chemistry – general, analytical, inorganic, organic, physical and theoretical – that a student might confront in an undergraduate programme. Both the textbook and the courses are based on advanced mathematical software, *Maple* (n.d.), that contains 5000 years of mathematical knowledge, that has a less steep learning curve than other mathematical software and that is freely available in many universities. Initiated in 1980, *Maple* was originally developed in University of Waterloo, Canada, for the purpose of assisting students of science and engineering to undertake mathematical calculations, analogously as previous compilers WATFOR and WATFIV, which were based on Fortran and are now obsolete, had been generated to assist calculations involving only arithmetical operations. These three programs became eventually released as commercial products that have been duly installed in universities around the world.

Interactive electronic textbook

Of two parts of the textbook *Mathematics for Chemistry*, the first is designed to encompass all mathematics that an instructor of chemistry might wish that his students would have learned in courses typically, but not exclusively, offered in departments of mathematics as a service to science students; the second part comprises chapters each of which is devoted to a particular area of mathematics, with its chemical applications, that might be taught within advanced courses in chemistry, including group theory, graph theory and dynamic chemical equilibrium. After a summary of various useful *Maple* commands, Part I hence has two chapters before the introduction of calculus, covering arithmetic in various forms and scientific notation, elementary functions, algebra, plotting, geometry, trigonometry, series and introductory complex analysis. Differential and integral infinitesimal calculus of one variable precedes multivariate calculus, linear algebra including matrices, vectors, eigenvalues, vector calculus and tensors, before differential and integral equations, and statistical aspects including probability, distribution and univariate statistics for the treatment of laboratory data, linear and non-linear regression and optimization.

Implementation of the course

The recommended duration of a course to present all that material in Part I within the sole instruction in mathematics to undergraduate students of chemistry is at least three semesters, but our courses so far have occupied only one semester, based on prerequisite differential and integral calculus taught elsewhere. Under the latter conditions, the first half of the course, before multivariate calculus, serves as a review of mathematics that students are supposed to have learned, which serves as a valuable vehicle for learning the *Maple* language, which in turn serves as a foundation to enable a rapid progress through the succeeding material. Each such course consists of lecture demonstrations of the particular concepts and principles of mathematics and their implementation with the *Maple* program, and supervised practical sessions, of total duration per week consistent with the length of the course, the course load of the students and the availability of appropriate space and resources.

As explained with examples in a preceding report (Ogilvie & Monagan, 2007), the objective of our courses is to enable the students to solve problems with a mathematical component on applying their mathematical knowledge so as to direct their effort and their acquaintance with the computer program to implement the required calculations. When one has acquired an overview of the entire content of mathematics deemed useful for students of chemistry, one appreciates that the actual extent of mathematical knowledge of a particular topic is small: for instance, differential calculus is based nearly entirely on a definition of a derivative as a limit of a ratio of two quantities. A combination of an explanation in words, an algebraic formulation, some numerical examples and the use of a graphical animation that demonstrates how a secant to a curve becomes a tangent in the limit illustrates this concept far better than is practicable on even many printed pages or with drawings and scribbling on a blackboard. The mathematical program hence presents a basis to display text in an appropriate and conventional notation, an interactive algebraic derivation, a few appropriately selected critical numerical examples and, especially, powerful graphical capabilities to produce diagrams in two or three dimensions and with practical animation. Once a student understands that principle, its application is mere detail, but the instruction about the topic naturally includes not only a few examples, based on the algebraic properties of the selected formulae, but also pertinent exceptions such as what occurs at a discontinuity, again illustrated with appropriate live plots. In contrast, a typical textbook exhibits more or less crude and static plots with much

verbiage in an attempt to convey the dynamic aspect of impracticable animation, and hundreds of exercises that a student is supposed to undertake in a mechanical manner. Einstein's advice was "never memorize anything that you can look up" ("What you can learn from Einstein's quirky habits", 2017). With a few judiciously chosen exercises that a student in our course is expected to undertake to illustrate the principles, that student is ready, with direct access to that software, to differentiate any formula, anytime and anywhere.

Likewise for integral calculus, our explanation of the principle comprises a definition in words accompanied by an animated display of the area under a curve as the number of rectangular subdivisions of the axis increases; the total area of the rectangles is simultaneously exhibited at each stage. When we authors were students before access to mathematical software, the advice given to us in the course on integral calculus was to learn standard methods, such as change of variables, integration by parts and trigonometric substitutions, and to memorize a list of common integrations; if such manual methods failed to yield a convincing answer in a particular application, we should find a similar expression in a table of integrals, but then we had to undertake whatever transformation was required into the particular variables in the problem at hand. With powerful mathematical software such as *Maple* that contains more knowledge about integrals than any single printed table ever, one need not be concerned about typographical or other errors that have been prevalent in static printed tables; in any case one should directly differentiate the result of an unfamiliar indefinite integration to prove its correctness. The emphasis in our course is to encourage the student to think about the solution of a problem, and then to let the software, according to the subset of total commands and instructions included in the course, undertake the tedious algebraic manipulations or prepare an illuminating graph. Some 70 years ago in advanced countries, pupils in schools were trained how to extract manually a square root of a number, with no explanation of the principle (actually a binomial expansion, but that was never stated); the flood of pocket calculators more than 40 years ago terminated that drudgery, and now even most professors of mathematics are unable to extract a square root of a number by hand. The use of computer software for symbolic mathematics is a natural progression that is consistent with the use of computers for manifold other routine or boring purposes. To replace the learning of mechanical sequences of manual operations, an enhanced understanding of the principles is a valuable dividend of symbolic computation, as incorporated in the design of our interactive electronic textbook and as proven in tests over nearly two decades.

Demonstration of the validity and utility of our approach

How effective have these courses and their underlying interactive electronic textbook been in improving the ability of students of chemistry to solve problems with a mathematical component? One measure of the efficacy arises from a direct comparison of the performance of students in a given course, for instance physical chemistry that has a significant mathematical element, as we describe below. Another measure is what the students have accomplished that could not have been done without this capability acquired through such a course as we have presented. What a student feels, on completing this course, is a tremendous *power* to attack chemical problems with a strong mathematical component. This power has resulted in its spontaneous application to undertake original calculations for some purpose or other, or perhaps for no particular purpose at all – just curiosity to prove that a calculation is feasible. Several cases of such calculations have resulted in submissions to the Maple Application Centre (n.d.), of which we note the following instances. A procedure for optimization with sequential simplex was originally developed separately, but became incorporated in *Mathematics for Chemistry* with the permission of the author (Ogilvie & Romero-Blanco, 2002). Likewise some admirable examples of chemical equilibrium involved in titration curves (Hidalgo, 2012) now constitute a major part of chapter 9 in *Mathematics for Chemistry*. Two other former students, completely independently of us instructors of their courses, submitted programs to treat the equations of states of non-ideal gases (Viales-Montero, 2012a, 2012b) and the density of probability of an electron near a nucleus (Hercules, 2010b) and the magnetic field and inductance of a torus (Hercules, 2010a). Other students have contributed valued content, particularly animated plots to illuminate some aspect of the content of *Mathematics for Chemistry* at a germane point, which is duly acknowledged within the present fifth edition. Such material was clearly devised by imaginative and superior students in our courses, but even more pedestrian applications of their mathematical knowledge and capability acquired in the same manner have contributed to the academic experience and performance of many other students beyond the particular course for which they received credit. The fraction of submissions to the chemistry category in the Maple Application Centre contributed from students in our courses is astonishing in view of the limited number, less than 100 in total, who have completed our semester courses over the years.

Benefits to the students

The following observations about our past students enable a comparison of the performance in courses of physical chemistry of both lecture and laboratory type between the students who enrolled in our course and other students. The major advantages that students gain on learning to use mathematical software for symbolic and numeric computation are rapid solving of assigned problems, improved presentation of information in producing plots of high quality, animations, three-dimensional plots – most students are amazed when they apply rotations to an object in a 3D-plot, and those who are able to produce such a plot are certainly proud of that achievement – and the ability to perform non-linear regression on experimental data.

Among the benefits acquired by students with skills in mathematical computation is notably the loss of fear about facing elaborate calculations. In many situations a complicated physical or chemical model is based on a statement of systems of equations. Each such equation is typically not difficult to set based on a knowledge of the underlying physics and chemistry; the difficult part of solving many problems is finding the solution for the mathematical system (algebraic or differential), because that task is tedious and commonly difficult to perform with merely *paper and pencil*. In other cases a problem can be correctly stated equation by equation, but the knowledge to solve the problem lies beyond the expected mathematical preparation of a student of chemistry. That barrier disappears on learning how to use software for symbolic and numeric computation: the student does the thinking and makes the statement, and the computer undertakes the slave labour that yields the answer. In this respect we recall the superb performance of a student in the physical-chemistry laboratory who undertook a special experimental project on the chemical kinetics of oscillating reactions; this student was able to model his experimental data on solving the system of differential equations that described the variation of concentration of each involved substance with time; the demonstration of his results inspired awe in the other students watching the presentation. Another instance was solving the Schroedinger equation for the hydrogen atom, which can be readily effected in several coordinate systems simply on translating the laplacian operator from one system to another.

Breaking the mathematical barrier in solving end-of-chapter problems and modeling experimental data using symbolic and numerical computation have opened a new knowledge perspective for some students who embraced the enterprise of learning about programming, to create their own algorithms. In this regard, the built-in *help* documentation of software, such as in *Maple*, provides effective guidance to assist self-learning. In this way, some students applied powerful utilities such as programming routines and image analysis for their post-graduate studies.

Holistic design of the textbook and the courses

In practical terms, an instructor of a course in chemistry requires a textbook for each course, which he or she follows to a lesser or greater extent. Even before 1950, printed textbooks were published with the stated aim to assist students of chemistry to undertake various calculations. Different in concept from any printed textbook, *Mathematics for Chemistry with Symbolic Computation* (2016) is an interactive electronic textbook that is operated on a computer with the *Maple* program simply on executing the computer files that it comprises; it is interactive in the sense that all calculations contained and discussed within the text are directly executed at the reader's instigation, simply on depressing the key to enter a selected command, which can be modified at will. The approach to the preparation of the composition of this textbook has been holistic: although its chapters might have names reminiscent of conventional courses, the total content has been designed to include material that is both valuable for chemical applications and lacking from conventional courses of constrained content; the entire Part I of the textbook is the objective of fulfillment, not merely the individual chapters thereof. This textbook is intended to be sufficient for all purposes involving the included topics, but traditional printed textbooks or material from internet might usefully supplement the descriptive content and explanation, no matter how comprehensive is that content or its exposition.

As an alternative to a traditional course such as we present in computer laboratories or classrooms with either computers provided or facilities for students to use their own portable computers, *Mathematics for Chemistry* is, by its nature, highly appropriate for self instruction. For the purpose of preparing to offer a course based on this textbook, a present instructor of chemistry can readily and rapidly progress through this textbook, learning to use *Maple* in the process as appropriate, to remind himself or herself of the mathematics that he once studied in traditional courses – or that was lacking from those courses because of their inadequate scope. Despite the extent and nature of the explanation and the explicit examples in this textbook, after a dozen years of school in one form or another, most university students are inured to more of the same style of teaching and learning; after our lecture demonstrations, we have found that the supervised practical sessions, in which the students

are encouraged to ask questions and to request hints for the solution of assigned exercises, play a major role in the acquisition of competence by the students. Our students have naturally had, and availed themselves of the opportunities, to extend their practice of *Maple* and the concerned mathematics beyond those supervised sessions, as desired and appropriate in each individual case, with the option to explore unresolved questions in the next practical session.

Many instructors of chemistry have developed and tested myriad devices and techniques to try to assist their students to cope with some mathematical component of chemistry in their courses. Our experience indicates that a truly successful achievement of the desired results necessitates a completely fresh and inclusive approach, namely to embrace a thorough application of symbolic computation in the teaching and practice of mathematics for students of chemistry. The availability, gratis, of textbook *Mathematics for Chemistry with Symbolic Computation* combined with powerful and easily learned *Maple* software can cause that successful achievement to materialize. Once a student has learned to use one particular program for symbolic computation, it is not difficult to learn the language of an alternative program. Free software for computer algebra, such as *Maxima* or *Reduce* each of which is commendable, lacks, however, the pedagogical aids that are incorporated in *Maple*, and that are applied to great advantage in *Mathematics for Chemistry*; as the free software is naturally being developed less rapidly than commercial software, it is much less powerful for various aspects of higher mathematics, such as the solution of differential equations or group theory. By dint of its interactive nature and electronic format, *Mathematics for Chemistry* must be embedded in a particular software, but the least steep learning curve of *Maple* and the abundant *Student* packages provided within this software are inestimable assets. For these reasons *Maple* is particularly pedagogically valuable for teaching mathematics in general, and for chemistry in particular, even though some packages in *Maple* for higher mathematics, such as for general relativity in physics, are unlikely ever to be engaged for chemical purposes.

Conclusion

Our answer to the question in the title of this essay is, not astonishingly, to teach students of chemistry more mathematics, specifically in the form of a course based on a particular textbook with a broad coverage. When one of us was an undergraduate in a Canadian university, a student of chemistry there was required to enroll in 5 year courses, equivalent to 10 semester courses, in mathematics to complete the degree. The average requirement in Canadian universities is now three semester courses, despite the increasingly mathematical nature of at least analytical and physical chemistry in recent decades. In other countries the situation might be even worse. What matters, however, is not just *more* mathematics but a *greater capability* in mathematics, which naturally arises, as we have endeavoured to demonstrate above, from instructing the students to apply symbolic computation with powerful mathematical software. Lord Kelvin stated that the human mind is never performing its highest function when it is doing the work of a calculating machine. With even just three semester courses each based on symbolic computation, or a single semester course extending traditional courses up to and including integral calculus, the results can be outstanding. With such resources at their fingertips on a computer keyboard, the mathematical achievement of chemistry students is nearly unlimited. For chemistry, mathematics is no end in itself but a tool to be applied in attacking chemical problems. The rate-determining step in implementing the appropriate courses that offer and implement the requisite tools is the rate at which instructors of chemistry themselves make the effort to learn to use symbolic computation; instructors should not expect a student to do what they have not done.

This paper was part of an online discussion hosted by the Chemical Education Division of the American Chemical Society (ACS CHED) and organised by the Committee on Computers in Chemical Education (CCCE). These are free online conferences with no requirement to be a member of ACS or CHED to participate. Further information is available at the website, <https://confchem.cce.divched.org/>.

References

- Hercules, D. A. (2010a). Toroids: magnetic field and inductance. Retrieved May 17, 2018 from <https://www.maplesoft.com/applications/view.aspx?SID=89944>.
- Hercules, D. A. (2010b). Density of probability of an electron near the nucleus. Retrieved May 17, 2018 from <https://www.maplesoft.com/applications/view.aspx?SID=95272>.
- Hidalgo, R. (2012). Chemical equilibrium. Retrieved May 17, 2018 from <https://www.maplesoft.com/applications/view.aspx?SID=129394>.
- Maple Application Centre. (n.d.). Retrieved May 17, 2018 from <http://www.maplesoft.com/applications/>.
- Maple: software for symbolic computation. (n.d.). Retrieved May 17, 2018 from <http://www.maplesoft.com>.

- Mathematics for Chemistry with Symbolic Computation. (2016). Retrieved May 17, 2018 from <http://www.cecm.sfu.ca/research/chemistry.html>.
- Ogilvie, J. F. & Romero-Blanco, E. (2002). Optimization with sequential simplex of variable size. Retrieved May 17, 2018 from <https://www.maplesoft.com/applications/view.aspx?SID=4289>.
- Ogilvie, J. F., & Monagan, M. B. (2007). Teaching mathematics to chemistry students with symbolic computation. *Journal of Chemical Education*, 84(5), 889–896. <http://www.cecm.sfu.ca/CAG/papers/ChemEdPaper.pdf>.
- Viales-Montero, C. (2012a). van der Waals equation of state (I). Retrieved May 17, 2018 from <https://www.maplesoft.com/applications/view.aspx?SID=134131>.
- Viales-Montero, C. (2012b). Analysis of basic equations of state (II). Retrieved May 17, 2018 from <https://www.maplesoft.com/applications/view.aspx?SID=134136>.
- “What you can learn from Einstein’s quirky habits”. (2017). Retrieved May 17, 2018 from <http://www.bbc.com/future/story/20170612-what-you-can-learn-from-einsteins-quirky-habits>.