Computer Algebra Systems as Tools for Chemical Education

A NEW DIMENSION IN PROBLEM SOLVING TECHNIQUES

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In recent years a number of exciting developments have emerged in the area of scientific computational tools for classroom use. Computer Algebra Systems (CASs), for example, Maple, are at the forefront of this arena. Such tools have been long sought by teachers of physical chemistry, inherently a mathematics intensive subject. With a CAS at hand, students can look forward to taking college science courses, like physical chemistry, without the usual mathematics anxiety. These tools can be used to do numerical and symbolic mathematics including calculus and linear algebra. In addition, they have wonderful graphics capabilities that include three-dimensional plots, contour plots, and animations. This paper describes the implementation of Maple in two junior-level physical...
chemistry courses. The materials used for beginning workshops are presented here and additional examples of Maple’s graphic and algebraic capabilities are described.

Introduction
An area of the undergraduate chemistry curriculum, that requires mathematical versatility of students, is physical chemistry. Experience shows that a vast majority of students who take this course feel intimidated by the mathematics required to understand the principles. As one author recently stated [1]: “There is a suspicion among students that physical chemistry is the Great White Whale of the chemistry curriculum.” Mathematics is the language of physical chemistry. Students need to understand this language well enough to appreciate the formulations of the principles and the techniques used to apply them for solving model problems. It is generally agreed that the frightful reputation of physical chemistry courses is, in part, due to students’ lack of fluency in basic symbolic (algebra and calculus) and numeric mathematics. Today, numerical calculations and other data manipulations are routinely performed on desk-top computers and sophisticated pocket calculators [2, 3]. This has alleviated some of the difficulty that students traditionally have had in physical chemistry courses. Until recently, however, there was little affordable computational help available to students to deal with the algebra, calculus, and graphical aspects of physical chemistry. Fortunately, there now are a number of symbolic, as well as numeric, computational packages available for desk-top computers. These programs help take away the mathematical fear for students enrolled in physical chemistry courses. Comparative reviews of the earlier versions of a few of these programs have been reported previously [4].

Maple represents an exciting development in scientific computational software for desktop computers [5]. This interactive command-line driven program not only does commonly encountered numerical computations to any desired degree of accuracy, but it is also a powerful symbolic processor that can be used to solve algebra, calculus, and other advanced mathematics problems with ease. Maple contains more than 2500 routines and has a built-in programming language that “allows the flexibility to extend existing routines or create new ones” [6]. Powerful graphing capabilities are available for representing data. These include two- and three-dimensional graphing with animation. CASs have the potential for revolutionizing the way we teach science and mathematics and the way we analyze and approach problems. Practical problems that