It is argued that a computer algebra system should replace the FORTRAN-like languages in the undergraduate and graduate programs in chemistry. To support the argument, example applications from physical chemistry are used to display the symbolic, numerical, and graphical capabilities of one such system. The code for the more complex applications is given in an appendix.

Introduction

Many colleges and universities have a computer literacy component as part of the degree requirements for their Chemistry Major. The question that must be answered is what constitutes computer literacy. The answer has been ever-changing because of dramatic changes in the computing technology and its availability and, more recently, in the type of computer programs
available. Certainly, word processing and graphics tools are required. Presently, both of these skills are possessed by more than ninety percent of the third-year students in my physical chemistry course. Requirements can and should build on the background of the student population. Until a few years ago most physical chemists thought that computer literacy meant some form of computational programming: BASIC, FORTRAN, and, more recently, Pascal and C. It is the thesis of this paper that the advent of the computer algebra system (CAS) requires that this view be changed.

There is and will continue to be a need for programmers versed in the “old tongues” to maintain and extend the current holdings in computational chemistry. The number of programmers required for this maintenance role is a small minority of the chemistry degree candidates and their needs should not be the focus of any general computer literacy requirement. The time required to learn a useful set of tools in any of these languages is just too great to be useful in the learning of physical chemistry. At the end of a typical introductory programming course a student cannot integrate a simple differential equation let alone the Schrödinger equation.

The spreadsheet program has a large and loyal following of users. Nearly every issue of The Journal of Chemical Education has an example of some problem that can be solved using a spreadsheet template. My chief argument against the spreadsheet is that the logic flow is hidden in cells that are invisible to the user unless special actions are taken. If the problem can be solved using a spreadsheet, it can be solved as well using a CAS, but the converse is not true. Learning the details of spreadsheet programming is not significantly easier than learning a CAS. Given the limited time available in students’ undergraduate lives we should expend their time on the most useful computer programs.

If we are to replace the FORTRAN-like languages, we need to specify the requirements for the replacement. Whatever we institute, it must provide in fact the numerical tools we hoped for from FORTRAN but did not acquire. This requirement is amazingly easy to satisfy with any modern CAS. Probably the most pressing requirement is in the area of mathematical assistance both for our students and for ourselves; it allows for more sophisticated applications and eliminates trivial errors. When users need to integrate a differential equation, they should be able to give a command to do so. They should not have to worry about the implementation, whether the equations are stiff, or even what stiff means. Someone should worry about such things, but not third-year students. The student should know that it is necessary or important to integrate the equation and that