SCIENCE OR TECHNOLOGY?

The computational chemistry world is confronted with what is perceived by many as a major public policy question. The question focuses on the tools of the trade, namely pieces of computer software. The question is simple enough at first glance. Is computer software a manifestation of science or is it technology?

The reason for this question involves one immediately in a question of public policy. In our society there is a general conviction that for the society to progress, scientific information should be shared. In the case of technology, which many view as simply an application of scientific ideas, we tend to patent it with the intent of enriching the developers.

There are many opinions today as to what should be done with computer software. As all of you are aware, we are uncertain enough about what computer software actually is, so that we do not always share it nor do we always patent it. In fact, in the United States today it is usually copyrighted much as intellectual property such as a book is.

One has to look very carefully at what is held in a piece of computer software. It is possible to argue on very general grounds that all the science contained in computational chemistry was published years ago, and is generally known as quantum mechanics. On the other hand, quantum mechanics is a very general theory, and the business of reducing it to a useful form even by computer must be viewed as some form of science. A technique for more accurately representing what is contained under the general title of quantum mechanics must certainly add to our science. One might assume that once this new result is published in the open literature, any social responsibility has been taken care of.

The implementation of this new science in a computer-executable form must certainly be considered to be simple technology under the definition given above. By the same token, it is feasible that in the process of such an implementation, one discovers yet another aspect of the science which was previously not reported. Here, we have new science intermixed with technology. Can one really ever separate science from technology in major computer systems? This is a question which I will not attempt to answer.

A belief which is generally held is that it is to everyone's benefit to make immediate disclosure of new science, but that it is perfectly acceptable to lock new technology away under patents and other sorts of protections. There is no loss to society by this act. It is based on this sort of analysis that we now have a public policy and numerous laws regarding patents and copyrights. These sorts of ideas certainly made some sense in the early days of the Industrial Revolution, as technology and science were so remote from one another that there was really no possibility of any cross-fertilization. If one checks back, I think that it will become obvious that the laws which are with us today had their beginnings in the thinking of this era.

An old maxim which I suspect is also rooted in this same thinking says 'Build a better mousetrap and the world will beat a path to your door'. The obvious flaw in this thinking is that the world will not beat a path to your door unless they somehow find out about your better mousetrap. It is possible to overprotect a piece of technology, which might also contain some new science, to such an extent that the world never finds out about it or perhaps to price it so high that the world is unwilling to go to the trouble to find out about it. There are countless ideas and inventions which people have lost track of over the years and which may never serve mankind.

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In the case of computer software, there are examples of potentially useful approximations and systems which could have been of major use to computational chemistry, but which have been so guarded that they have never come into broad availability. Without broad use of such software, it is impossible for the field, in general, to ever judge whether or not this work is of any value. Overprotected work might well have been more than simply useful; it might well have been the source of new research directions. How much has been lost we can never know. There is, however, a nagging suspicion that our losses have been and may be substantial.

In the case of overprotected or overpriced software, there is a loss to the individual developer as well as to the society. New software is worth very little until it has been worked with extensively. New software does not emerge as a perfected whole. It usually becomes useful through careful maintenace and development over a period of years, as the result of the work of many people. A major part of any evaluation of software requires continuity by the research community over a period of years. If there is no access, there can be no evaluation, and the best ideas may pass by unexploited.

There is much conversation about patent laws and copyright in the industrial world today. There is also considerable political tension, as many developing countries do not concern themselves with such matters at all. There is an awareness that our existing laws do not recognize enough different gradations of ownership to possibly serve the needs of a complex civilization adequately. Unfortunately recognition is not sufficient guidance for people to move forward and reform the existing laws. In the absence of any action, the laws which now exist will remain in force. It is from this situation that a very serious threat now exists.

Computational chemistry has developed to the point at which we find it today because so many people simply felt that new software should be evaluated by the community at large. Their basic instincts told them this without resort to any sort of legalistic reasoning. Should people cease to feel this way, it may well be that computational chemistry will fall prey to the same force which brought ancient Athens to social gridlock – a litigious society.

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