YESTERDAY, TODAY AND PERHAPS TOMORROW

It is probably safe to say that computational chemistry as a field has reached a certain level of acceptance. If one briefly glances through the some two thousand names which stand on the QCPE membership lists, it is clear that the techniques of the field have found acceptance in all aspects of chemistry and throughout our world. At the same time, our field exhibits a behavior which has been noted in many other computationally based disciplines. This behavior is the focusing of activity on a very small number of computational packages. A good example of this can be found in the almost total dependence of many engineering fields on a very few packages for finite element calculations. There are perhaps only three packages which can be considered as standards or can be thought to be widely used in the finite element world. Yet all aspects of engineering which require structural, thermal and fluid flow information depend on these few pieces of software.

To be sure these 'pieces of software' are often as not over a million lines of code in length and are maintained and extended by whole teams of very capable people. These packages, which are so critical to the modern fields of engineering that they are given special names, are referred to as production systems as opposed to just systems. The impact of these systems is so pervasive to modern society that an error in one of them could be responsible for literally billions of dollars in losses should it go undetected. For each such system there are teams of people working who are dedicated to simply insuring the integrity of these systems. Many of you have heard the names of some of these systems such as NASTRAN or ANSYS. These names are in fact now registered trademarks.

Consider for a moment what the state of things would be if all of these codes were suddenly no longer available or thought not to be reliable. Where would modern engineering find itself? While this is a somewhat farfetched supposition in the engineering world, it is not so farfetched a scenario when applied to the computational chemistry world. To be sure, there are now several different and well-established organizations in engineering that compete with one another. The conditions which would lead to the complete loss of a certain capability cannot be easily realized. If, for some reason, one of these firms were to go under, there would be another one available to pick up the new business and carry on. Unfortunately, the situation in computational chemistry is not identical.

Reflect for a moment on the type of code or codes on which you, as a computational chemist, are dependent. These codes fall into a few broad categories such as Semi-empirical, Molecular Mechanics-type codes and Ab Initio codes. Now think for a moment on how many codes of truly production quality there are in each one of these groups. The result is a little startling.

I need to remind you that a production code is one that you obtained from a reputable source and which has met some form of certification procedure. It is a code which would give the same answer to a given question anywhere in the world when used by any competent scientist. It is not a code that came to you through four different people and for which no one can find the original documentation.

In the area of Ab Initio systems, four, and perhaps a fifth system, can be truly called production quality. However, standing behind many of these codes is a single person or, at best, a very small

0920-654X/$5.00

organization. The situation becomes even more critical when one considers the Semi-empirical world. There are two systems that one can clearly call of production quality and which are heavily used. Behind one of these systems we have a single individual. Behind the other system we had a single person and a research group which he headed for many years. I use the word 'had' because that person is now retired and, to the best of my knowledge, the former research group has to some degree disbanded. In the case of Molecular Mechanics-type calculations, we now are confronted with perhaps a single system that can be viewed as a worthy production system and, as its guarantor, we have a single individual and the research group which he heads. This individual must also eventually retire.

The point which I want to make here is that computational chemistry is very vulnerable on this issue as opposed to the finite element world. It is conceivable that this field could be damaged significantly by something as simple and tragic as an airplane falling or an automobile accident. We are a field that has many appliers of the technology and, perhaps, too few developers of the technology. How has this situation developed?

There is no single, simple answer. In a sense we are victims of the manner in which the field developed and perhaps the times we live in. We are victims of a reality that has haunted this field since its beginnings. The reality is that there is little or perhaps no financial support of an ongoing nature for people who develop computational systems let alone support for those who develop raw computational systems into true production systems.

One might think that industry would be a productive place to seek such support. This is not the case! In the United States (and I suspect the rest of the world as well) major industries have no interest whatsoever in investing in research of this nature. By the very definition of the word 'research' there is some probability that the venture will not succeed. Industry will put no money into a venture that has a certain, a priori, possibility of failure. Their attitude is that they would rather wait for any new ideas to become part of some commercial system and then simply buy it. With everyone taking this attitude it is unlikely that many new ideas will see development.

Organizations such as the National Science Foundation (NSF) in the United States, and comparable organizations in other countries, have taken the attitude that they are in the business of funding science – at least in the sense which they understand it – and not software. They have consistently refused to fund such work for many years. In fact, if one were to write a history of how the systems which we now have actually came into existence, it would be a testimony to the determination and persistence of a few individuals.

The future of computational chemistry can probably not be assured as long as we are in a situation which can be so readily damaged. Where there is no investment in the research which underlies a field there can be no field. It is now time for the people who are benefiting from the field to give consideration to their own self interest and begin investing in that field.

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