WATCHING OUR NUMBERS DOUBLE

As we go about our daily tasks we should afford ourselves a few brief minutes to reflect on the fact that the number of people in the world who are actively involved in computational chemistry has probably just about doubled in recent months. Recent political events in the nations which comprised the former Soviet Union and its trading partners have brought into contact with many of us the very large number of scientists who have been working in this field as best they could in their laboratories and academies for the past twenty to twenty five years. In addition to this significant group, the decline of the defense industries in many European countries and the United States also appears to be contributing to an upsurge in the amount of computational chemistry going on as many very sophisticated computer users now turn their talents to more commercial research ventures in chemistry.

In the case of the new practitioners from the defense sector of the economy they seem to require very little assistance. They are now primarily reorienting themselves into this field and discovering the jargon and the standard pieces of software which everyone seems to have a copy of. They will be productive almost immediately. They may even be in a better position to get something done than many of us are as the defense industries have computer facilities which go far beyond what most of us are accustomed to. In a short period of time we may be following them rather than they following us.

The problem is quite different in the case of the scientists in new countries. The only common ground which we have with these people is the PC-DOS operating system. Generally speaking, these scientists are not familiar with operating systems such as Digital's VMS or any versions of UNIX, as government policy in many of our countries has systematically denied these people access to the hardware, and therefore the software, with which all of us are so familiar. In fact, in the United States today, all the laws and regulations left over from that earlier time are still in force. None has been repealed and, as things go, it is doubtful that anyone will ever get around to doing this. However, there appears to be little interest in enforcing these laws now and it would seem that we can do business as we need to. This is the point on which I wish to dwell.

Business as usual can not be expected to be the order of the day. The problem which will prevent this is that the currencies of many of these countries, such as the ruble, are not convertible into currencies such as German marks or British pounds sterling. This fact will prevent them from buying modern computing equipment or commercially available software. Yet they will be aware of what is going on from the printed journals which have been available historically and they will have a very strong desire to participate in this field. At least this has been QCPE's experience during the last year.

Many of us will receive requests for software from many countries with which we have had little contact. We may find that these requests often exceed our ability to meet them and yet I am certain that everyone will do their best. I am aware of many individuals who have personally shipped a vast amount of software to researchers whom they have never met before. It is encouraging to see that this community of scientists can respond as effectively as they have to the events of the past few months. Unfortunately the greatest amount of goodwill in the world will probably not get the job done. It is simply too large.

The problem is currency convertibility. We must develop a mechanism to avoid this impediment and yet not damage commerce on the international scale on which it must take place. The simplest approach is barter. It has been used before and may once again be useful in a somewhat sophisticated form until time eventually solves the problem of currency convertibility.

Let us consider for a moment a fictional company such as the Digital Computation Corporation (DCC) for lack of a better name. Let us assume additionally that DCC has a very large production capacity for workstations and would desperately like to sell these to researchers in Russia perhaps. However, DCC does not know how to account for rubles on its quarterly reports. What can they do?

Rubles are still a useful currency in Russia but DCC does all its business in US dollars. One possibility is for DCC to open an office in Moscow and offer to sell its workstations at a price of so many barrels of oil per workstation. If a research organization in Russia wants to buy a workstation they take the rubles which they have in their budgets and go to the people who have the oil and buy so much of it for their rubles. They then have the oil delivered to whatever location DCC wants to receive it at and the transaction within Russia is over. As oil is a saleable commodity on the open market, DCC pools all of the oil which it takes in and becomes a major dealer in crude oil for which it can obtain German marks, US dollars, etc. The same sort of approach can be used for all commodities such as gold, chromium, and many other items. In fact, one could set up an organization to handle the interchange of one commodity for the other so that a company like DCC which is already set up to market oil could accept payment in terms of any commodity and convert it to oil for convenience of marketing. An entire economy of a nation, such as Russia, can not be operated in this fashion forever but you could probably boot-strap trade to life in such a manner. Things of this nature must certainly be going on with some of the companies now operating in these countries.

Many US companies are excessively worried about their vulnerabilities in doing business in such environments but in reality how much downside vulnerability can there be when one is being paid in commodities for which there are readymade markets? I would expect that the rewards will be dramatic for the companies which are willing to take the trouble to work through the details of any such arrangements. I, personally, anticipate that the rewards to the field of computational chemistry will be dramatic.

Richard W. Counts
QCPE
Indiana University
Bloomington, IN 47405
U.S.A.