

The Computational Perspective

NETWORKS

It is by now axiomatic that if you change the way people communicate you will change the world. The fabric of computer networks which is springing up as one even now contemplates the idea is a clear example of this going on before us. An excellent example of the axiom with which we started is the telephone system.

The international telephone network is familiar to us all and by now is taken for granted. There can be no doubt that the speed of communications has increased dramatically but there have also been certain side effects that most people are unaware of. These are the sort of side effects which will always attend any change in human communications.

Consider what happens when a small box called a fax machine is added to the telephone network. In fact, it might be even more interesting if the fax machine had been invented before the telephone. But this subject strays too far from my point. One small side effect in the United States, and probably in many other countries as well, has been to cause any piece of communication with perhaps no more than marginal importance to be sent by fax. These are pieces of communication which had formerly gone by post. As a consequence, the actual volume of mail carried by the U.S. Postal Service has dropped and continues to drop. It has dropped so much that the Postal Service is now in the process of laying off 37,000 workers. This is but one example of those little surprises which such changes can produce. From a postal worker's viewpoint it is not a nice surprise but it will inevitably occur.

Just as inevitably, the proliferation and interlinking of an almost uncountable number of computer networks will take place. What little surprises this may ultimately visit on society can hardly be predicted. It will render almost impossible the control of information flow across international boundaries. This, as many of you may recall, was a very popular pastime only a few short years ago. It may also render impractical the total monitoring of information that crosses certain international borders. This remains, even today, a very popular pastime. The point is that there will be an awful lot of electromagnetic information flying around and there will be a great number of people who have ready access to it.

At the moment, the use of the many national networks seems to be essentially free of charge. This fact has undoubtedly contributed to the growth we are now experiencing. At the moment some relatively unknown government agency is paying the bill in many countries. It is doubtful that this will continue far into the future. As we are all aware, the telephone and fax do cost money to use, albeit not much.

The development of high quality networks makes it feasible for an organization such as QCPE to contemplate heavy use of these resources in transferring information. We are, however, concerned not to put all our eggs in one basket. We always have the question with us about exactly what these charges will be when these networks are being charged for in the manner the telephone now is. To put this point in perspective, consider for a moment how long it takes to ship a large program to a remote destination. In a recent conversation with Dr. Michael Schmidt, the gentleman who so kindly ships the GAMESS Ab Initio system throughout the world, I discovered that it requires about two hours to ship the entire system. If one were being charged at the current telephone rate of something as high as \$60.00 per hour in prime time, you can appreciate our concern.

Would a client be willing to pay this sort of shipping cost and receive a program instantly or perhaps pay a third of this cost and receive it in 10 days. Clearly there will be both types of clients but the ability to carry out the above sort of operation will force yet additional economic choices on everyone.

Another aspect of networks which will become of even greater concern as their use becomes commonplace is their ability to distribute faulty as well as accurate information. We have had very little concern about this problem in the past simply because we could control the situation. However, in today's world of networks, it is completely possible to set up an anonymous ftp account on a computer somewhere in the world and tell people that they can have a free copy of some important software system. The little surprise would be that the software was faulty. I use this example because it has already occurred in the United States. We have seen at least in microcosm what can happen.

Someone put up a software system that was supposed to be a UNIX version of the MOPAC 6.0 system. He then sent out an announcement which essentially said that a *free* Unix MOPAC was available. This happened at a time when no such system was available from MOPAC's author. Many unsuspecting users around the world assumed that the system had been thoroughly certified and took for granted that it was the author who was putting up the system. They were wrong on both counts and a form of electromagnetic chaos followed almost immediately. We really have no practice in place which will protect us from this sort of little surprise.

Before the field of computational chemistry reaches the maturity to deal with these sorts of situations, we will probably experience many other little surprises. For example, there is an entire bookful of questions about ownership of software and what constitutes ownership in an environment such as we are discussing, as well as what constitutes violation of ownership rights and how one might prove violation. What we may find is that our neverending electronic frontier, as some have chosen to call it, may restructure our whole society.

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