

The Computational Perspective

TO BUY OR NOT TO BUY?

Until 1978, computational chemistry belonged to the few who had sufficient access to a main-frame computer to permit the use of large amounts of CPU time and large amounts of data storage, usually on magnetic tape. In this year, the Digital Equipment Corporation (DEC) introduced their VAX 11/780.

While this piece of hardware did not create computational chemistry, it went a long way toward making it a viable field and providing the type of routine access to computational power which proved to be the needed ingredient for growth.

In the early 1980s the IBM-PC appeared. Chemists quickly discovered the virtue of the open architecture on this piece of hardware and began to exploit its potentials to the point at which these machines are now integral to the field of computational chemistry.

Almost concomitant with the IBM-PC development was that of the workstation. Early on, the workstation, as pioneered by people like Apollo Computer, made large inroads into the market for engineering computation but had little impact on computational chemistry. The reasons for this lack of a presence are not clear but probably related to the major position which DEC established in the field with its VAX line of computers. In spite of their earlier absence, our field is now confronted with several major corporations offering their products (workstations) to the field with an ever increasing desire for a piece of the chemistry market.

For a brief period of time it was possible to mentally segregate manufacturers' offerings based on a series of inequalities which said that supercomputers (CRAYS) were greater than mainframes and these were in turn greater than workstations which were, of course, greater than IBM-PCs in computational capabilities.

The predictable occurred and these neat distinctions blurred. The PC manufacturers (now including the Apple MACINTOSH II) upgraded their offerings to compete with the workstations. Workstation manufacturers making use of networking concepts began to nibble at the market for mainframe computers. The mainframers then entertained visions of becoming supercomputer manufacturers.

Most people in positions of responsibility threw up their hands in dismay as they were bombarded by claim and counterclaim as to what computer hardware would be the most useful now and in the future for any particular problem. On the surface, there appeared to be very little guidance as to how to proceed in a hardware purchase.

Today, in computational chemistry at least, there appears to be emerging a fairly simple picture as to what hardware will be most useful. The picture seems to be based on a simple look at the type of activities which most characterize the field.

Stated simplistically, a computational chemist will probably be using a computer to either develop new code and modify existing code or he will be carrying out studies on ever larger and larger structures.

If you accept this premise, such a person will need a relatively modest computer on which he can modify and develop code and in many cases do smaller studies as well as prepare input for

larger studies. He will also need access to if not actual possession of a supercomputer to do the ever more large scale studies which have by now become routine.

The workstation with its high quality graphics and good communications capabilities as well as adequate computational capabilities and low maintenance cost will probably emerge as the individual computer used by the chemists. This offers a working environment which each person can control and adapt to individual needs. Work which is too large for these machines can then be shipped to centers which are remote for processing.

The implications of this model for computing which I have developed for entities such as university or corporate computer centers would seem fairly clear. Their role will change.

In some situations they may be bypassed altogether. Funding shifts will occur. Their earlier positions as arbiters of any research which required computing will be all but forgotten. Change, the force which moves mankind, will have once again exhibited its awesome power.

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