

The Computational Perspective

NEW PRODUCTS AND RUMORS OF NEW PRODUCTS

In the United States today — and probably throughout the world — the people who practice computational chemistry are genuinely confused. On all sides there are computer manufacturers eager to sell their products. There are computers which can sit on or under your desk and execute truly large-scale calculations at blinding speeds. There are computers which are larger and may need their own air-conditioned rooms — and can also execute truly large-scale calculations at blinding speeds. Yet again, there are supercomputers and supercomputer centers which dedicate entire buildings to a single machine which can execute truly large-scale calculations at blinding speeds...

One can invest anywhere from \$20,000 to \$25 million — and buy a computer that runs at truly blinding speeds. What one must do is ask the question, what is one really buying exactly? Are there gradations of blinding speed of which one needs to be aware?

The answer to this question appears, unfortunately, to be both yes and no. As one looks beneath the manufacturer's brochures, one finds that it is possible to achieve 'blinding' speed by using relatively low-performance components and arranging them in highly original ways, such as is done in the Multiflow TRACE series of computers. Or one could take fairly capable components, such as the INTEL 80386 chips, and have dozens of them operate in parallel. Then again, one could use state-of-the-art components and drive them with vast amounts of power at liquid nitrogen temperatures as is done in the CRAY and ETA/10 series of computers. One must remember that 'blinding speed' can be achieved in any of these ways and in several variations thereof. One is, however, left with the question of the meaning of 'blinding speed'. Further, one still needs an approach for sorting through the vast array of offerings. Many of the products coming on the market today are possible because a few electronics firms manufacture individual chips or chip sets which can be routinely purchased at rather nominal prices to become the heart of a new product.

As everyone is aware, the Motorola 68000, 68020 and now the 68030 chip powers many computers. More recently, MIPS R2000 and R3000 chip sets are powering very high-speed systems. It is, in fact, only the very large computer manufacturers who can and still do develop their own chips; and even many of them are seriously considering the MIPS technology. What we have is a lot of product based on not all that much original technology. In fact, if one looks carefully at the largest display screens available from literally all manufacturers today, they all seem to say SONY somewhere inside. Similarly, smaller tape drives and very large disk systems are likely to have been made by the Control Data Corporation. The message is that not everything is what it seems, yet all the brochures advertise 'blinding speed'.

Adding to this muddle is the fact that a number of the companies who are selling these marvelous machines have no idea whatsoever what one does in computational chemistry, thereby creating a situation in which everyone becomes reluctant to buy — and computer sales begin to decline.

Computer companies are, of course, prepared with a stock response when their sales stagnate. They simply introduce an entirely new line of equipment — usually based on a wholly new technol-

ogy (RISC architecture) — and then claim even more blindingly superior speeds of execution for things which they really do not understand. At this point, the cycle of confusion is bound to be repeated.

We are now on the verge of massive new product introductions by an uncounted number of manufacturers. Will this cycle end eventually? Yes, it must. What will be the result? Probably the largest shakeout that the computer industry has yet seen. Will everyone learn a lesson from this? Doubtful! Is this what we mean when we talk about progress? I'm afraid so. Has the field of computational chemistry been advanced? Maybe, to some small degree.

The confusion caused by the large number of manufacturers and their advertising will undoubtedly continue to be with us, caused as much by their own ignorance as by any conscious attempt to create confusion. After all, confusion is the great enemy of product sales.

For those of us who must invest our finite resources in some computing capabilities, there is some guidance. We must know very thoroughly what our real computing needs are today. We must try to formulate in some organized fashion what our computing needs are likely to be into the near future (possibly 18 to 24 months ahead). With this planning firmly in mind, we must find the most effective way of providing for today's needs, with the ability to evolve into providing for tomorrow's. By having an accurate fix on one's true needs, it is possible to pick and choose among the many similar claims.

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