

Computer programs for crystallography and chemistry

I must draw attention to the poor judgment shown by an overwhelming majority of research funding agencies in allocating funds for computing in crystal-structure analysis and in theoretical chemistry. If the funds available were redistributed to give greater emphasis to high-quality general-purpose routines it would improve research productivity substantially. This may at first appear to be a trivial issue, but the costs incurred because of poor use of computational facilities, of pointless duplication of effort and unproductive man-hours spent wrestling with programming errors and wretched program documentation are enormous.

In crystallography there are gallant attempts to produce general-purpose systems, but the funding for these is miserable when compared with that spent on other research in this field.

The distribution of programs for theoretical chemists is taken care of by the Quantum Chemistry Program Exchange, but the desirable goal of a set of machine-independent programs has not been achieved. If a proposal to develop such a set were put forward the chances are that it would not be funded.

The attitude of funding agencies reflects the views of the senior scientists who advise them. By and large the understanding of this question by these scientists is limited. My criticism is directed at that deficiency.

The value of crystallography and of theoretical calculations of the properties of molecules as scientific tools is generally acknowledged. It is neither possible nor desirable for all those wishing to use those tools to acquire a detailed understanding of the computational procedures involved. For many purposes a general understanding is sufficient. While the principles underlying the procedures are straightforward, their practical application presents some of the more demanding computational problems known to science. Very few people are capable of solving these problems in a satisfactory way, that is, producing programs which (a) are error free (b) may be applied to a wide range of problems and (c) do not require an inordinate amount of care or detailed understanding by the users themselves.

The contribution of such people, al-



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though widely acknowledged in the computing field, is almost totally ignored in science. Citation of a system of computer programs in some hundreds of publications is likely to produce benign approval and no support.

It would be invidious for individuals if I were to quote specific examples but I have collected sufficient case histories to show that this is a universal problem, and not just a parochial one. In non-computational areas it is relatively straightforward to obtain support for a worthwhile project. An outstanding project involving the solution of a specific computational problem may be funded. Development of a set of high-quality general-purpose programs will either be dismissed as not being research, or else given a Z rating, and that only because there are no more letters in the alphabet. But such a set of programs can make a major contribution to tens and perhaps hundreds of individual projects.

Work on such sets progresses because of dedicated and at times heroic efforts by a few people, but it is becoming increasingly difficult to sustain that effort when faced with continued lack of support. It is time for funding agencies to ensure that their referees understand the

economic and scientific consequences of such systems.

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Basic research and DOD

Your news story on page 93 in October discusses the recommendation of the Galt panel on support of basic research by the DOD.

I wholeheartedly agree with the panel's diagnosis that a national problem exists in this area, namely that basic research in the US is presently significantly under-supported. Various indicators such as the percentage of US publications in the world scientific literature and the percentage of US patents have shown a steady decline *vis-à-vis* the rest of the scientifically developed world. In much of the world a larger percentage of the economy is devoted to basic science. It is a recognized fact that basic science fosters applications and patents.

My reason for writing this letter is, however, to take issue with the conclusion and recommendation of that panel, namely that the DOD should step up its efforts in the area of basic research.

I believe it to be a dangerous threat for the scientific community if it would acquiesce to proposals that tax money for basic research would be controlled by the DOD rather than the NSF. Most members of the political community have seen this danger clearly when they accepted the Mansfield amendment, which essentially gave the NSF, not the DOD, the mandate to administer basic research in the USA.

One might make the argument that the money DOD could spend on basic research would otherwise not be available to NSF, and thus that more basic research would result.

However, I believe it to be more likely that the usual tendency of any large bureaucracy to grow, unless checked, would lead in this case—if the recommendations of the Galt panel are to be followed—simply to a shift in programs supported by NSF to DOD and would in the long run