letters

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.

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The contribution of such people, although 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 becomingly 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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11/28/78 *Nedlands, Australia*

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 undersupported. 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

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lead to a reduced budget for NSF. Should this happen, then a number of the creative and socially aware scientists who feel that the only—albeit little—effect they have in their professional lives to counteract the continuing self-destructive, militaristic trend in the world by not working on any project administered by a military agency will be squeezed out of areas of basic science to its detriment.

I therefore recommend that more vigorous and stronger basic-science programs be adopted and administered by NSF, NIH, NASA and similar civilian agencies.

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10/30/78

Pauli remembered

Laurie Brown's article "The Idea of the Neutrino" in September (page 23), I found both informative and delightful.

It was my privilege to have been a postdoctoral student of Wolfgang Pauli in Zurich during the years 1953–55. There I learned at first hand the truth of a remark R. A. Millikan made in a course he gave at Caltech on the history of physics: "Physicists are more interesting than Physics."

In the fall of 1953, just before the Christmas recess, word came through that Fred Reines and Clyde Cowan (Phys. Rev. **92,** 830, 1953) had successfully detected the free neutrino in experiments at Los Alamos. This provided conclusive proof of Pauli's idea of the neutrino—an idea that underwent significant evolutionary developments (as discussed by Brown) from the time of Pauli's original suggestion in December 1930 to the parity nonconservation experiments in 1957.

To celebrate, a number of us from ETH and the University of Zurich climbed the Utilberg near Zurich, where we had dinner. On the way down, Bleuler and I noticed that Pauli was a little wobbly from the red wine we had at dinner. (He had graciously responded to many individual toasts.) Bleuler said to me: "Take his left arm—I'll take his right arm, we can't afford to lose him now." Later when we were about midway, Pauli turned to me with a comment I shall always treasure, "Remember, Barker," he said, "all good things come to the man who is patient."

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11/17/78

Non-university research

The report of the NSF Subcommittee on Job-Related Issues, described in August (page 69) raises issues that deserve wider discussion.

The Subcommittee concluded the US should create at least 400–500 jobs in physics, and it recommended the creation of two categories of temporary jobs within university physics departments. It is obvious that the large departments would benefit greatly, but it is not so obvious that the recipients of the proposed jobs would benefit in equal measure. Many might prefer real jobs to 5–10 years of a not-quite-faculty limbo; if they are the outstanding people the Subcommittee would have them be, perhaps they deserve better.

If the Subcommittee's objective was revivication of basic research, why did it not give more attention to industry, the civil service and the national laboratories? The Subcommittee, in concluding that firm data are lacking to substantiate the claim that the employment situation in national laboratories is as bad as in the universities, behaved as if existing data *disprove* the claim. Moreover, the PHYSICS TODAY report does not indicate that the Subcommittee interested itself in the available documentation concerning the erosion of basic research in industry and the civil service.

Recently a number of articles have appeared claiming to voice concern about the state of basic research in the US (examples are cited at the end of this letter[1]). In fact the articles were concerned primarily about basic research in the universities, and in some cases they virtually made one-to-one identification between the two. One might have wondered whether basic research was being used merely as a vehicle for special pleading on behalf of academic science. The NSF Subcommittee's seeming indifference to the welfare of basic research outside the academy is another example of this selective concern.

Though most US basic research is performed in universities (plus national laboratories), even a glance at the list of Nobel Prize winners shows that very important basic research also has been performed in both the civil service and industry. It is a perversion of history to talk of "traditional opportunities" in basic science, as the Subcommittee does, and refer only to universities and national laboratories. Since repeated assertion of a proposition often convinces people of its truth, might such talk contribute to *alteration* of traditional patterns in basic research?

Even in the consideration of such a narrow issue as replacing the large number of faculty who will retire in 10–15 years, a broader view of research might have aided the Subcommittee. Many current faculty members first worked in industry, the civil service, or the national laboratories—and in jobs that, unlike the ones proposed by the Subcommittee, were "permanent." Future faculty could be drawn from such nonacademic institutions—and in great quantity if such or-