

Letters

Advanced Computing

John Walsh's article "NSF plans help with big computer problems" (News and Comment, 24 Feb., p. 797) struck a sympathetic chord. For the last 6 months, the National Cancer Institute (NCI) has been discussing, in parallel with the National Science Foundation (NSF), the role for advanced computing capacity in molecular biological sciences. The areas of consideration have been the rapidly expanding databases for nucleic acid and protein sequence comparisons, crystallographic structure refinements of complex biomolecules, molecular dynamics, multidimensional graphic analyses, and especially the molecular modeling of defined structure-target interactions.

For example, determination of the homologies of transforming gene sequences and their cellular counterparts have been among the most exciting recent developments (1). Future searches will require increasingly more computation time. Intuitive studies of amino acid substitution in the sequenced molecule of dihydrofolate reductase, the target for the chemotherapeutic agent methotrexate, have shown changes in the configuration and substrate affinities (Research News, 20 Jan., p. 269). It seems that rational drug design based on computational analyses should readily replace such empirical approaches. Analogous situations in several areas of molecular biology support the position of the NSF committee that advanced computing needs are essential to today's science.

In conjunction, NCI has planned for a newly expanded Laboratory of Mathematical Biology within the Division of Cancer Biology and Diagnosis. One of the functions of this laboratory would be to work on already identified problems in biomedicine that require advanced computing capabilities. With this in mind, NCI has tentatively budgeted for a "supercomputer" that could be operational in a relatively short time. Prospective users would not only be from NCI and NIH but from the entire biomedical community. The location of this laboratory would be at the NCI-Frederick Cancer Research Facility, where the necessary

support elements could come from the contractor operation already in place.

Because no such computer is presently dedicated to biomedicine, the subject was broached with a number of molecular biologists. The response was quite positive. Some were already considering the need for purchasing such equipment, while others were ready to present us with problems that require immediate advanced computational capacity.

It is recognized that alternative solutions, such as array processors involving available hardware, have been proposed and may be adequate for a number of problems. However, those options seem to be in their formative stages, while regular supercomputer use is an established fact. More important, because of the complexity of future questions, the depth to which they can be answered depends essentially on machines of extraordinary capacity.

NCI has been in contact with NSF's Advisory Committee for Advanced Scientific Computing Resources and strongly concurs with their recommendations. Although their potential users would come primarily from the physical and chemical sciences and engineering, we anticipate attracting a counterpart group in the biomedical area. Additional input and suggestions would be welcome.

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References

1. R. F. Doolittle *et al.*, *Science* **221**, 275 (1983); M. D. Waterfield *et al.*, *Nature (London)* **304**, 35 (1983); J. Downward *et al.*, *ibid.* **307**, 521 (1984).

Releasing the Fork

There is an additional lesson to be learned from Gina Kolata's article "Order out of chaos in computers" (Research News, 2 Mar., p. 917). As in the story of the philosophers and the forks, there are often win/win solutions to complex problems that could be reached through collaboration if only all of the participants could recognize that this is so. But so often when complex issues are

being debated, there is no common recognition that a win/win solution is possible; because of their cultural instincts, all of the participants become adversaries—to their respective loss—which leads to a lose/lose result.

We must find a better way to give a clear and irrefutable demonstration to the philosophers that each would be acting in his own self-interest, when one of the two forks is not available, if he were to release the fork in his hand and to start the whole process again. Such an attitude is counterintuitive and against the dominant adversarial behavior of our culture. We must learn that most of the big issues of our times require these seemingly altruistic and collaborative acts if we are to achieve an eventual "win" rather than a "loss." Sometimes it is better to give up one fork and thereby win a meal.

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Cooperation with Japan

It is refreshing to learn from Martin Goland's editorial (20 Jan., p. 241) that a respected authority in U.S. science and technology can look at the technological growth of Japan in a dispassionate way and recognize that, by maintaining a strong bilateral relationship, we can realize significant benefits. Regrettably, Goland's position is not reflected widely among politicians in Washington, either in Congress or the Executive Branch, where pressures from industry and labor are almost entirely in the direction of restricting the flow of even unclassified scientific and technical information to Japan.

While I cannot speak for the private sector in the United States, I have a good understanding of the bilateral technical relationship between the United States and Japan at the government level, not only from the years I spent as the senior science officer of the American Embassy in Tokyo, but also from studies I have conducted during the past year for the Department of State, the National Research Council, and the Department of Commerce. These studies show that technical cooperation through government channels is generally characterized by the American participants as healthy, productive, of good quality, and absolutely worthy of continuation.

Furthermore, it is not generally known that the Japanese government has committed itself to investing more than \$100