LARGE SCALE SCIENTIFIC COMPUTATION VIA MINICOMPUTER

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Abstract—A program of research designed to test the suitability of minicomputers for large scale scientific computations is described. The scientific problems to be attacked are those traditionally reserved for the largest and fastest commercially available electronic computers: the calculation of potential energy surfaces and subsequent evaluation of the dynamics of chemical reactions.

INTRODUCTION

Theoretical chemists have traditionally been among the heaviest users of electronic computers. The earliest (Parr & Crawford, 1952; Boys et al., 1956), and still the most extensive (Schaefer, 1972), use of computers by theoretical chemists was in the calculation of electronic wave functions for atoms and molecules. A somewhat more recently developed (Wall et al., 1958), but equally important, area of research is the study of the dynamics of chemical reactions using classical trajectories (Bunker, 1971), semi-classical methods (Miller, 1971), or even fully quantum mechanical approaches (Light, 1971). The relation between the two fields is clear; while the potential energy surface is frequently the goal of the electronic wave function computations, the same surface is the most important prerequisite to the study of the reaction dynamics. The above discussion is particularly pertinent to the present time, since it is only during the past year that the first computations of the type we refer to (Bender et al., 1972; George & Miller, 1972; Doll et al., 1973) have been carried out.

It can be argued that the above areas are part of a new branch of chemistry, computational chemistry. In any event, the emerging importance of computation in theoretical chemistry will demand the availability of large amounts of relatively inexpensive machine time during the next decade. It has customarily been assumed that such large scale scientific computations require the use of the largest and fastest computers available. In the present paper we raise some questions concerning the economic feasibility of using machines such as the CDC 8600 for theoretical chemistry. We propose an experiment to determine the feasibility of an alternative route for large scale scientific computation—the use of minicomputers.

THE LARGE MACHINE FOR THEORETICAL CHEMISTRY

Our discussion must begin with the enormous complexity of the numerical problems facing theoretical chemists. In this light, it is not surprising that theoretical chemists have traditionally assumed that, at any given period in time, only the most powerful available computers would be appropriate for the solution of their problems. This attitude is grounded in experience, since each new series of machines has made possible the attack of a broader and more interesting range of chemical problems. To use the CDC machines as an example, the 3600, 6600, and 7600 computers each in turn opened up new areas of endeavor to the theoretician. Further, we do not claim to have been uninterested observers of this trend—one of us was the first (Schaefer & Heil, 1970) to use the CDC 7600 (as a consultant to UC Livermore in early 1970) for electronic structure computations. More recently, both authors have relied almost exclusively on continually smaller amounts of machine time on the Lawrence Berkeley Laboratory CDC 7600.

The Lawrence Berkeley Laboratory (LBL) has been designated a national center for computation, its 7600 is generally available to NSF grantees, and the rate structure is at the very least competitive† with other installations. Therefore it is convenient to base our economic discussion in terms of the LBL system. One hour of 7600 central processor (CPU) time costs $720 at LBL. However, input/output (IO) charges are made separately, and in many cases the IO charges exceed the CPU cost. For example, in self-consistent-field electronic structure computations, $720 in CPU time typically carries with it an additional $1080 in IO charges. Thus, in this case the actual cost of 1 h of machine time is $1800. This is a most important consideration, as it means that the true cost of computing is 2.5 times the apparent cost. More generally, let us assume that the average cost of 1 h of CDC 7600 time is $1500.

We feel that a modest yearly computing budget for a theoretical computational chemist, with perhaps seven graduate students and postdoctorals, is $24,000. In terms of the cost analysis of our previous paragraph, then, our modest theoretician will have 16 h-yr⁻¹ of 7600 machine time. We leave it to the reader to form his own opinion as to whether this is an adequate allocation of computing. It may be worth noting that there are presently about 15 theoretical research groups in the country with computing allocations this size, and perhaps eight additional groups with significantly larger budgets, most of them funded internally.

Our most serious concern is that, using large-scale computers, it appears unlikely that the cost of computing will decrease significantly during the next decade. An example which particularly influenced us was the December, 1972 preliminary report of the LBL Computer

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*Alfred P. Sloan Fellow.
†Camille and Henry Dreyfus Teacher-Scholar.
‡The most obvious reason for the very attractive LBL rate structure is the fact that the 7600 was purchased outright by the Atomic Energy Commission. The rate structure reflects only the costs of operation, and not the 7600 purchase price.
Center, which forecast cost of computing for the next 5 yr. The LBL extrapolation is based on the acquisition of a second 7600 in 1975 and a machine of the CDC 8600 calibre in 1978. Although the 8600 will be significantly faster than the 7600, it will also be more expensive to purchase and operate. To be specific, the estimate is that if 1 h of 7600 time costs $1500 in January, 1973, 5 yr from now the price of the same amount of computation will be $1050. We feel that this is an unacceptable situation. The rise to relevance of theoretical chemistry has in large part been due to the availability of a rapidly expanding supply of machine time. Although some slowing of this rate of 'growth' is to be expected, a near halt would be a disaster. For example, such a halt would crush the exciting opportunities arising from the application of sophisticated theoretical models to organic and biological problems.

THE MINICOMPUTER: AN EXPERIMENT WORTH TRYING

Until 3 months ago (November, 1972) we were only aware of minicomputers in the broadest sense of the word 'aware'. That is, we only knew that minicomputers existed and were becoming simultaneously faster, larger and cheaper. This minimal knowledge, combined with our pessimism concerning the continued use of large machines, led us to seriously consider the use of minicomputers.

Inherent in the name of the minicomputer is one of its real strengths—its small size. The minicomputer described in this proposal will sit comfortably in a 10 ft × 12 ft room and require little or no air conditioning.

The machines given serious consideration in our study were the Datacraft 6024/4, Data General Nova 800, Digital Equipment Corporation PDP-11/45, Texas Instruments 980, Varian 73, and Xerox 530. 'Serious consideration' included talks with one or more salesmen for each machine and careful examination of machine specifications and price. These six machines satisfy the following requirements:

(a) small size mentioned above;
(b) adequately configured, each machine sells in the neighborhood of $125,000;
(c) sufficient speed to make theoretical chemistry a real possibility.

Some pertinent characteristics of the six machines are given in Table 1.

Of the six minicomputers, the Datacraft 6024/4 was found to be qualitatively superior (for theoretical chemistry) to the other five. The reasons for this superiority are:

(1) The 6024/4 can directly address (through COM-MON) 32K (32,768) floating point words. We define a 'floating point word' to be a word long enough to provide the number of significant figures required in theoretical chemistry computations. The Datacraft's 48 bit floating point word (39 bit mantissa) is nearly ideal, as it provides 11 significant figures, just about optimum for our purposes. In this regard, the Xerox 530's 32 bit mantissa (9 significant figures) represents the bare minimum adequate for theoretical chemistry. As will be seen in the next section, the 32,768 words of floating point memory are absolutely necessary for our research. Among the other five machines, the maximum available floating point memory is 21,845 words.

(2) The Datacraft is more than a factor of 2 faster than the other minicomputers. Worst case floating point multiplication requires 5.25 μs. The nearest competitor, the PDP 11/45 requires 11.2 μs for the same operation. Although information is not yet available on either the Varian 73 or Xerox 530 floating point hardware, preliminary indications are that neither is likely to be faster than the PDP 11/45.

For theoretical chemistry in 1973, the Datacraft 6024/4 seems to be the only sensible choice among minicomputers. It should be pointed out, however, that within 2 yr there should be several machines capable of meeting our requirements. Furthermore, we anticipate that in 5 yr minicomputers 10 times the speed of the 6024/4 will be available for the current price of the 6024/4. Therefore, if our experiment is able to prove that in 1973 the 6024/4 is competitive with the 7600 for theoretical chemistry, minicomputers may in truth be the wave of the future for scientific computing.

Table 2 indicates the equipment suggested in the present study. The disk specified has a capacity of 28 million bytes, or for our purposes 41 million 48 bit words. Our intention is to keep the system plus all frequently used programs resident on the disk. In addition, the 50 ms average seek time makes direct access operations feasible. The tape specified is industry compatible, with a capacity of roughly 3 million 48 bit words.

It is worth pointing out that, for the theoretical chemistry computations we carry out, the central processor might be five times faster before creating an input/output bound system. Further, it is not inconceivable that a central processor five times the speed of the 6024/4, but at the same cost, will appear in perhaps 3 yr. In

Table 1. Comparison of some features of six minicomputers

<table>
<thead>
<tr>
<th></th>
<th>Datacraft 6024/4</th>
<th>Data General Nova 800</th>
<th>Digital Equipment Corporation PDP-11/45</th>
<th>Texas Instruments 980</th>
<th>Varian 73</th>
<th>Xerox 530</th>
</tr>
</thead>
<tbody>
<tr>
<td>Word length (bits)</td>
<td>24</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>16</td>
</tr>
<tr>
<td>Single-block addressable memory (words)</td>
<td>65,536</td>
<td>32,768</td>
<td>32,768</td>
<td>65,536</td>
<td>65,536</td>
<td>65,536</td>
</tr>
<tr>
<td>Length of floating point words (bits)</td>
<td>48</td>
<td>64</td>
<td>64</td>
<td>48</td>
<td>64</td>
<td>48</td>
</tr>
<tr>
<td>Mantissa of floating point word (bits)</td>
<td>39</td>
<td>56</td>
<td>55</td>
<td>40</td>
<td>45</td>
<td>32</td>
</tr>
<tr>
<td>Single-block addressable memory (floating point words)</td>
<td>32,768</td>
<td>8,192</td>
<td>8,192</td>
<td>21,845</td>
<td>16,384</td>
<td>21,845</td>
</tr>
<tr>
<td>Cycle time (μs)</td>
<td>750</td>
<td>800</td>
<td>850</td>
<td>750</td>
<td>660</td>
<td>800</td>
</tr>
<tr>
<td>Floating point multiply time (μs)</td>
<td>5.25</td>
<td>19.3</td>
<td>11.2</td>
<td>~18</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>
Theoretical chemist three times the computing-power-per-
quiry 5 min/day of each associated student's time. Therefore the only new
paper supply, replacing the printer ribbon, mounting
this point we remind the reader that, unlike the LBL
minicomputers today appear capable of giving the
cost of $4156, one would be able to purchase the equival-
ed of 0.3125 h/day of 7600 time. In light of the monthly
discussion. Assuming the machine can be utilized an
that the 6024 will be less than 64 times slower than the
mentioned in the next section, certain jobs will be able to
Appendix. To reduce the possibility of future embarrass-
ments for the Diels-Adler reaction

This table 2. Proposed minicomputer system for theoretical chemis-
try. All equipment specified is manufactured by the Datacraft
Corporation.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Description</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Central processor with 8K memory</td>
<td>19.900</td>
</tr>
<tr>
<td>1</td>
<td>8K additional memory</td>
<td>52.500</td>
</tr>
<tr>
<td>1</td>
<td>Floating point hardware</td>
<td>11.100</td>
</tr>
<tr>
<td>1</td>
<td>Clock</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>Hardware bootstrap</td>
<td>600</td>
</tr>
<tr>
<td>1</td>
<td>Priority interrupt</td>
<td>200</td>
</tr>
<tr>
<td>1</td>
<td>24 bit input/output channel</td>
<td>850</td>
</tr>
<tr>
<td>2</td>
<td>Automatic block controller</td>
<td>3000</td>
</tr>
<tr>
<td>1</td>
<td>Teletype and controller</td>
<td>1450</td>
</tr>
<tr>
<td>1</td>
<td>Card reader, 300 cards per minute</td>
<td>4500</td>
</tr>
<tr>
<td>1</td>
<td>Line printer, 200 lines per minute</td>
<td>6800</td>
</tr>
<tr>
<td>1</td>
<td>Controller and magnetic tape drive,</td>
<td></td>
</tr>
<tr>
<td>9 track, 800 bpi, 45 ips</td>
<td>10,000</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>Disc controller: 28,000,000 bytes</td>
<td>8500</td>
</tr>
<tr>
<td>1</td>
<td>Disc unit: 28,000,000 bytes</td>
<td>17,000</td>
</tr>
<tr>
<td>1</td>
<td>FORTRAN IV compiler</td>
<td>800</td>
</tr>
<tr>
<td>1</td>
<td>Disc operating system</td>
<td>750</td>
</tr>
<tr>
<td></td>
<td>Subtotal</td>
<td>140,050</td>
</tr>
<tr>
<td></td>
<td>Educational discount (10%)</td>
<td>-14,005</td>
</tr>
<tr>
<td></td>
<td>Demonstration time, 50 h at $75/h</td>
<td>3750</td>
</tr>
<tr>
<td></td>
<td>Subtotal</td>
<td>122,255</td>
</tr>
<tr>
<td></td>
<td>California State sales tax (6%)</td>
<td>7338</td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>129,633</td>
</tr>
</tbody>
</table>

dollar of the largest available machines and (b) the modest
budgets of two theoretical chemists are very nearly
sufficient to support a properly configured minicomputer.

APPLICABILITY OF THE MINICOMPUTER TO SPECIFIC
PROBLEMS IN THEORETICAL CHEMISTRY

The previous section demonstrated that the central
processor of the 6024/4 is sufficiently fast, and the price
sufficiently low, to suggest that large scale scientific
computation may be very economical. The only serious
question remaining is whether the relatively small mem-
ory of the 6024/4 is capable of handling the specific
problems of interest to us as theoretical chemists.
More specifically, we have configured the 6024/4 with a
memory of 32,768 double precision (48 bit) words, as
opposed to the 64,000 word (60 bit) memory of the 7600.
Our longest computer program not amenable to subdivi-
sion consists of about 3000 FORTRAN statements. The
machine language instructions generated by this FOR-
TRAN will unfortunately occupy a sizeable fraction of
the 6024/4 memory. Specifically, it can be estimated that
the part of the system which must reside in core plus the
instructions generated by 3000 FORTRAN statements
might usurp as many as 12,768 floating point words from
the memory. That is, the sum of the dimensions of the
unique arrays used in any program cannot exceed 20,000.
In the following paragraphs, we discuss the ramifications
of this and other limitations of the 6024/4 as regards
the solution of selected important problems in computational
chemistry.

(a) Two-electron integrals. The traditional bottleneck
(Mulliken & Roothaan, 1959) in molecular electronic
structure calculations has been the computation of two-
electron integrals arising from the Coulomb repulsion
between pairs of electrons. For the most part, this bott-
leneck has been broken; for linear molecules using Slater
functions (McLean, 1971), and for general molecules
using Gaussian functions (Ciszmadia et al., 1966). In our
work at Berkeley, we are now using contracted gaussian
functions almost exclusively, and accordingly, integral
computation, although quite time-consuming, will put no
strain on the memory limitations of the Datacraft. The
practical limit of the 6024/4 at the integral stage would be
a series of 'double-zeta' basis set (Schaefer, 1972) calcula-
tions for the Diels–Adler reaction

\[
\begin{align*}
& \text{C} = & \text{C} & + & \text{CN} \\
& \text{C} & & \rightarrow & \text{C} & \text{CN}
\end{align*}
\]

Computation of the integrals required for a single point on
this potential surface would require about 3 days of 6024/4
time. Note that we have assumed no elements of sym-
metry for the above reaction. An analogous computation
on the comparable, but highly regular, cyc-
looctatetraene dianion would require less than 1 day.

(b) Self-consistent-field procedures. Most of our elec-
tronic structure studies involve the computation of SCF
and/or small multiconfiguration SCF wave functions. For
a general open-shell case, the methods (Hunt et al., 1972)
we are currently using require the simultaneous residence
in memory of one \(N^2\) array and four \(N^2/2\) arrays, where \(N\)
is the number of contracted gaussian functions in the basis set. For the Diels–Adler system described in (a), \(N\) is 98, and thus the minimum memory requirement is 28,812 words, considerably more than is available with the 6024/4. Nevertheless, we feel that it is possible to carry out such calculations on the 6024/4. Briefly, we must either alter the existing algorithms or adopt new algorithms (Wilkinson, 1965) to carry out the necessary matrix operations using a minimum amount of core storage. The Nesbet–Shavitt algorithm (Nesbet, 1965; Shavitt, 1970) is a shining example of the sort of insight needed to solve this problem. The 44 million word disk specified with the system will make such ‘out-of-core’ matrix manipulations possible. However, it is clear that large sections of the presently functioning programs will have to be completely rewritten. The estimated time for the SCF part of a calculation on \(\text{C}_6\text{H}_5\text{CN}\) is 1.5 days.

(c) Configuration interaction. It now seems established (Bender et al., 1972) that in many cases the most crucial step in obtaining a potential surface of chemical accuracy will be the judicious use of configuration interaction (CI). Let us consider a surface of chemical importance, \(\text{O} + \text{C}_2\text{H}_4\text{.}\) A basis set of 68 contracted Gaussian functions will be required for chemical accuracy. From the above two paragraphs it is clear that the integral and SCF steps will each be modest, requiring a total of perhaps 0.5 6 day per point on the surface. ‘First-order’ wave functions (Schaefer, 1972), which appear well-suited for this type study, would include on the order of 3000 configurations. The most time-consuming step in the CI will probably be the transformation of two-electron integrals over basis functions to two-electron integrals over molecular orbitals. Although this transformation can be carried out faster using a larger memory, the Datacraft’s 20,000 words of storage is quite adequate for the large number of such operations on 32 bit (7 significant figures) floating point words. An equally important feature, which can be rather time-consuming, is the search for those trajectories with desired initial and final vibrational and rotational quantum numbers. Fortunately, the magnitude of the task can be greatly reduced by partial averaging (Doll & Miller, 1972), i.e. treating one or more degrees of freedom within a Monte Carlo framework. We estimate that a rather thorough study of tunneling in the \(\text{CH}_2 + \text{H}_2\) reaction would require about 30 days of 6024/4 time.

To conclude, most of the problems involved in the theoretical study of simple chemical reactions can be handled on the 6024/4 without major alteration of presently existing codes. It appears that the remaining problems, i.e. those involved in multi-configuration SCF calculations, can be solved using algorithms designed to optimally utilize the relatively small memory of the minicomputer.

REFERENCES


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Doll, J. D. & Miller, W. H. (1972), \(\text{J. Chem. Phys.}\ 57, 5019.\)


Light, C. C. (1971), \(\text{Adv. Chem. Phys.}\ 19, 1.\)


Large scale scientific computation via minicomputer

Schafer, H. F. & Hall, T. G. (1970), Lawrence Radiation Laboratory Report UCRL-199183, September. See footnote a to Table II.

APPENDIX

SPEED COMPARISONS BETWEEN THE DATACRAFT 6024/4 AND CONTROL DATA 7600

We stated earlier that the 7600 is not likely to perform more than a factor of 64 faster than the 6024/4. In this appendix we discuss the reasoning behind the factor of 64.

By means of 'pipelining', the 7600 achieves a cycle time of 27.5 ns. A register-to-register floating point multiplication requires 5 cycles and thus 137.5 ns. The 6024/4 cycle time is 750 ns. A floating point multiplication (including one memory reference) requires 7 cycles, and thus 5250 ns. This oversimplified comparison suggests that the 7600 is a factor of 38 faster than the 6024/4.

The main reasons this comparison is not completely valid are (a) the parallel processing feature of the 7600 makes one multiply every 5.5 ns feasible under special circumstances, and (b) the memory reference included in the 6024/4 multiplication time would require 8 cycles, or 220 ns of 7600 time. We suspect that these two features may just about cancel each other, implying that the quoted factor of 38 may be more realistic than could have been expected.

To remove this discussion from a purely theoretical plane, we have run five benchmark programs on a variety of machines. Since the Datacraft 6024/4 will not be available until July, 1973, the benchmarks were run on the 6024/1. The 6024/1 and 6024/4 are nearly identical (same FORTRAN compiler and assembler language) machines, except that the 6024/1 has a 600 ns cycle time. We also ran one benchmark on the 6024/3, which is a third similar machine and has a 1000 ns cycle time. To three significant figures, the 6024/3 required a factor of 5/3 longer time than the 6024/1. This test proved to us that the speeds of the 6024 series machines are in fact proportional to the cycle times. The 6024/4 times quoted were obtained by multiplying appropriate 6024/1 times by 1.25.

On each machine, the benchmarks were run using the current standard FORTRAN compiler. The first three benchmarks were those provided by Datacraft, and are seen in Fig. 1. Being skeptical of these first three benchmarks, we verified that the times quoted by Datacraft were legitimate, i.e. they were reproduced by the Datacraft machine available to us, using the standard FORTRAN compiler. The fourth benchmark was the repeated computation of simple dot product of two vector arrays, A(1000) and B(1000). The final benchmark was the set up and diagonalization of a 50 x 50 matrix. Although the program used, HDIAG (based on the Jacobi algorithm), is very slow, it has the virtue of being compatible with almost every FORTRAN compiler known.

The benchmarks are summarized in Table 3. As expected the first three programs show the 6024/4 in a more favorable light. After all, these three benchmarks were almost undoubtedly designed to get the most from the Datacraft FORTRAN compiler and floating point hardware. The exceptional speed of the external functions is noteworthy, and is a feature emphasized by the Datacraft salesmen. The SIN, COS, EXP, and SQRT functions are particularly important in theoretical chemistry computations. The last two benchmarks probably show the 6024/4 in a more

Table 3. Speeds (in s) required for several computers to carry out specified benchmark calculations. See text for a description of the benchmarks

<table>
<thead>
<tr>
<th>Machine</th>
<th>CDC 7600</th>
<th>CDC 6600</th>
<th>Univac 1108</th>
<th>CDC 6400</th>
<th>Datacraft 6024/4</th>
<th>7600</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integer arithmetic</td>
<td>1.8</td>
<td>9.6</td>
<td>25</td>
<td>36</td>
<td>41</td>
<td>23</td>
</tr>
<tr>
<td>Floating point arithmetic</td>
<td>0.21</td>
<td>1.2</td>
<td>3.0</td>
<td>4.5</td>
<td>4.8</td>
<td>23</td>
</tr>
<tr>
<td>External functions</td>
<td>0.52</td>
<td>1.2</td>
<td>3.2</td>
<td>7.0</td>
<td>4.1</td>
<td>13</td>
</tr>
<tr>
<td>Dot product</td>
<td>0.70</td>
<td>2.1</td>
<td>7.3</td>
<td>19</td>
<td>30</td>
<td>43</td>
</tr>
<tr>
<td>Matrix diagonalization</td>
<td>1.2</td>
<td>6.2</td>
<td>13</td>
<td>53</td>
<td>59</td>
<td>49</td>
</tr>
</tbody>
</table>

(1) INTEGER ARITHMETIC

PAUSE 1
J = 0
DO 30 I = 1,100000
30 J = J + ((I**3)/(250*J - I) + 10000).
PAUSE 2
WRITE (6,300) J
300 FORMAT (6H ANS1 = 18)
STOP
END

(2) FLOATING POINT ADD, SUBTRACT, MULTIPLY AND DIVIDE

PAUSE 3
A = 0
DO 10 I = 1,100000
X = I
10 A = ((X - 1)/(X + 1))*X**39 + A
PAUSE 4
WRITE (6,100) A
100 FORMAT (6H ANS2 = E13.6)
STOP
END

(3) INTRINSIC AND BASIC EXTERNAL FUNCTIONS

PAUSE 5
A = 0
DO 20 I = 1,100000
X = I
20 A = A + SQRT(ABS(SIN(X)) + X***(IFIX(ALOG10(X)) + EXP(-ATAN(X/666)))+
PAUSE 6
WRITE (6,200) A
200 FORMAT (6H ANS3 = E13.6)
STOP
END

Fig. 1. Benchmark FORTRAN programs supplied by the Datacraft Corporation.
realistic light, while supporting our contention that the 7600 is no more than 64 times faster than the Datacraft machine.

Since it was feared that some of the simple benchmarks taken might not fairly reflect the parallel processing characteristics of the 7600, a final comparison was devised. The dot product benchmark was written in the respective optimized machine languages for the 7600 and 6024/4. The time on the 7600 was 0.34 s, an improvement of more than a factor of 2 over the FORTRAN version. However, the 6024/4 machine language time was 11 s, an even greater percentage improvement. We conclude that the benefits to be accrued by using optimized machine language programs on the 7600 are not likely to be greater than those obtained in an analogous manner on the 6024/4.

**Epilogue**

The present paper differs only in a few details from a proposal prepared in February, 1973 for submission to the National Science Foundation. Hence, all statements such as 'during the past few months' are not current.

The proposal was funded on 15 June, 1973. Computing equipment began to arrive in November 1973 and the system was complete by the end of March 1974. Since we intend to write a later paper describing the first year of our experiment, only a few interim remarks will be made here. Nevertheless, the machine is now (January 1975) fully operational, and both classical trajectory and self-consistent-field programs are running successfully. One significant departure from the original proposal is the fact that a 56,000,000 byte disk was obtained in the final package. The timing estimates given in the paper now appear to have been relatively conservative. That is, we have found the Datacraft 6024/4 to execute most typically at a speed 30 times slower than the CDC 7600. Thus we remain optimistic about the future of minicomputers in large scale scientific computation.