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Publication Date
1980-07-01

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COMPARISON OF NUMERICAL METHODS FOR SOLVING THE SECOND-ORDER DIFFERENTIAL EQUATIONS OF MOLECULAR SCATTERING THEORY*
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*This work was supported in part by the U. S. Department of Energy under Contract W-7405-ENG-48 and the National Science Foundation under Interagency Agreement CHE-7721305.

## Comparison of Numerical Methods

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## ABSTRACT

The numerical solution of coupled, second-order differential equations is a fundamental problem in theoretical physics and chemistry. There are presently over 20 commonly used methods. Unbiased comparisons of the methods are difficult to make and few have been attempted. Here we report a comparison of 11 different methods applied to three different test problems. The test problems have been constructed to approximate chemical systems of current research interest and to be representative of the state of the art in inelastic molecular collisions. All calculations were done on the same computer and the attempt was made to do all calculations to the same level of accuracy. The results of the initial tests indicated that an improved method might be obtained by using different methods in different integration regions. Such a hybrid program was developed and found to be at least 1.5 to 2.0 times faster than any inidividual method.

## 1. INTRODUCTION

State-to-state chemistry is currently one of the forefront fields of chemical physics. In the past 10 years the ability to study the microscopic behavior of single collision events, both experimental and theoretically, has developed rapidly. A common feature of nearly all quantum-mechanical methods for studying molecular collisions, whether elastic, inelastic or reactive, is the need to solve coupled sets of linear second-order differential equations.

In the past 15 years there has been a rapid proliferation of methods for solving these equations. Meaningful comparisons of the methods are very difficult to make because of the number and intangibility of the parameters which should be explored. These include for example, the computer and compiler used, the accuracy of the solution and the efficiency of the computer codes. The few comparisons which have been made[1-4] usually involved only two or a few methods. Sometimes the calculations were done on different computers, and possibly worst of all, the tests were done on simple model problems. The collinear vibrational problem of Secrest and Johnson[5] and the 9-, and 16-channel rotational problems of Lester and Bernstein [6,7] are commonly used test cases. These problems, however, reflect the status of research in this field ten years ago. Methods which perform well on those problems may very well not be optimal for problems which are typical of current research in molecular collision theory.

Because of the large number of new methods, the lack of good bases for comparisons and the importance of solving these coupled equations in many branches of molecular collision theory, the National Resource for Computation in Chemistry (NRCC) sponsored a workshop on this topic. The goals of the workshop were to identify the methods and computer codes commonly in use, compare their performance on a fixed set of problems and make tested versions
of them available to the scientific community. Volume I of the workshop proceedings[8] contains presentations of 12 different methods and a discussion of the problems used here. Volume II of the proceedings[9] provides a detailed analys is of the test results for eleven different computer codes. All of the codes tested are now available from the NRCC[10-22].

The main result of these testsis the development of a new hybrid program which typically runs twice as fast as any individual program and in many cases even faster for a given accuracy. In this paper we briefly describe the methods and test problems, present the main findings of the tests, and describe the new hybrid program.

## 2. COUPLED EQUATIONS

The equations to be solved are:

$$
\begin{equation*}
\left(\frac{d^{2}}{d r^{2}}-\frac{e_{i}\left(\ell_{i}+1\right)}{r^{2}}+k_{i}^{2}\right) u_{i j}=\sum_{i \prime} v_{i j}(r) u_{i \prime j}(r) . \tag{1}
\end{equation*}
$$

The boundary conditions imposed on the solutions are,

$$
\begin{equation*}
u_{i j}(0)=0 \tag{2}
\end{equation*}
$$

and

$$
\begin{equation*}
\lim _{r \rightarrow \infty} u_{i j}(r)=k_{i}^{-1 / 2} j_{\ell}\left(k_{i} r\right) \delta_{i j}+k_{i}^{-1 / 2} n_{\ell}\left(k_{i} r\right) k_{i j} \tag{3}
\end{equation*}
$$

where, $j_{l}(k r)$ and $n_{\ell}(k r)$ are spherical Bessel functions. It should be emphasized that these equations apply to many different types of collisions and many approximate formulations of close-coupling theory. Different systems and
approximations differ only in the definitions of the potential matrix elements $V_{i j}$.

The number of coupled equations which must be solved ranges from one, for elastic scattering from spherically symmetric potentials, to many thousands for large molecules with many closely-spaced energy levels. At the present time, up to about 100 coupled equations can be solved routinely and as many as 210 coupled equations have been solved[23]. With improving computer technology and numerical techniques, these numbers will undoubtedly increase significantly in the near future.

## 3. METHODS

Almost as important as the number of equations which must be solved, however, is the number of numerical methods one must chose from for solving them. Table I presents a list of the most commonly used methods for solving differential equations. Those which have an abbreviation or acronym were tested in the present study. Although the development of these methods spans nearly 100 years, most have been developed since 1965. It was about this time that high-speed, digital computers became widely available as research tools, and chemists and physicists began developing specialized techniques for the solution of Eq. (1).

The methods in Table I fall into two broad categories - approximate solution methods and approximate potential methods. With the approximate solution methods, some functional form, usually a polynomial in $r$, is assigned to the solution, $u$, and/or its derivatives, over an interval $\Delta r$. The parameters of that functional form are then chosen to best satisfy Eq. (1). These methods tend to be numerically simple, but require stepsizes 10 to 20 times smaller than the wavelength of the solution. They are usually advantageous when the wavelength is long compared to the range of the potential. The
approximate potential methods assign a functional form to the potential over an interval $\Delta r$, usually constant or linear in $r$, for which exact solutions are known. The solutions are then matched at the interval boundaries to propagate over the entire region. These methods are advantageous when the potential is slowly varying and when the wavelength is small compared to the range of the potential. They also have the advantage that much of the intermediate computational information for a given potential and basis set is energy independent. Therefore, if the potential is energy independent and calculations are done for more than one collision energy, the information from the first calculation can be saved and reused with considerable savings in computation time for other energies. The approximate potential methods in Table 1 are the methods of piecewise analytic reference potentials, the R-matrix propagator methods and the variable-interval, variable-step method. The others can all be classified as approximate solution methods. For further classification and discussion of the relative advantages and disadvantages of these methods the reader is referred to the articles of Secrest[8,45].

A very brief description of each of the programs used in the tests follows.

Approximate Solution Methods
$P C[10]$ - Predictor-corrector methods are among the oldest in use, but have been significantly improved in recent years[32,33,46]. This program uses the variable-order, variable-stepsize predictor-corrector method of Shampine and Gordon[46].

DEVOG[11] - The DeVogeleare algorithm was introduced to close-coupling calculations by Lester[47]. It is efficient, simple to program, and stepsize changes of arbitrary value are easy to introduce.

MNN[12] - The Numerov method has been widely used in many problems in theoretical physics. Recent modifications to it have been given by Allison[3] and Johnson[38]. The program used in these tests was the Minnesota Numerov (MNN) program of Brandt, Truhlar, Onda, and Thirumalai.
$\operatorname{LOGD}[13,17]$ - The log derivative method [34] uses a special invariant imbedding technique to propagate $u^{\prime} u^{-1}$ rather than the wavefunction, $u$, itself. This program also has an option for using a multi-channel WKB approximation[48]. This is useful for very long range problems where the potential is slowly varying over several wavelengths. In this region the WKB approximation is both accurate and efficient.

SAMS[14] - Sams and Kouri[30] transformed Eq. (1) into a Volterra integral equation and then developed a numerical technique by introducing an equallyspaced quadrature formula. The program used in these tests employs a trapezoidal integration.

INSCAT[15] - This is an integral equation formulation of the piecewise analytic potential method[35]. The differential equations are converted to Volterra integral equations, but a constant potential approximation is made over each integration step. Since the potential is not diagonalized, however, this method is intermediate between the approximate solution and potential methods.

Approximate Potential Methods
GORDON[16] - The piecewise analytic reference potential method of Gordon[31] was the first approximate potential method. This is a modified version of the original Gordon code[49].

VIVS[17] - This new variable-interval, variable-step method[42] uses piecewise constant potentials and a fixed basis within each interval.

Analytic perturbation corrections to the solutions are summed over the steps in an interval and the solutions are carried in R-matrix form.

RMAT[18] - This is a modification[50] of the R-matrix propagation method $[36,37]$ in which the analytic $R$-matrices are perturbatively corrected in each sector, but propagated as in the original method $[36,37]$.

L2RMAT[19] - This is a modification of the R-matrix propagation method which uses an $L^{2}$ expansion of the wavefunction in the region of rapidly varying potential[41]. The original R-matrix propagation method[36,37] is then used for the remainder of the integration range.

VIVAS[17] - This is a hybrid program[43,44] which uses the $\log$ derivative method in the inner region where the potential is rapidly varying, and uses the variable-interval, variable-step method for the outer region.

## 4. TEST PROBLEMS

In constructing the test problems, an attempt was made to pick only realistic, three-dimensional problems of current research interest. With this in mind, three chemical systems -- $\mathrm{He}-\mathrm{H}_{2}, \mathrm{Li}^{+}-\mathrm{CO}$, and $\mathrm{e}^{-}-\mathrm{N}_{2}-$ were chosen.

Test 1. This is the problem of rotational and vibrational excitation of $\mathrm{H}_{2}$ by He impact. An accurate configuration-interaction (CI) potential energy surface is available and converged close-coupling calculations of the inelastic transitions probabilities have been done[51]. The study of this system is therefore representative of the present state of the art in inelastic collision studies. The case we report here is an 18-channel problem for total angular momentum, $J=4$, and relative kinetic energy, $E=0.0224$ Hartree atomic units. When $\mathrm{H}_{2}$ is in its ground state, this corresponds to an asymptotic impact parameter of $b=0.38$ and $a$ wavelength of 0.6 Bohr. Table II gives the complete set of basis quantum numbers.

Test 2. This is the problem of rotational excitation of rigid-rotor C0 molecules by $\mathrm{Li}^{+}$impact. The problem was chosen because of the extremely long range of the interaction potential. The charge-dipole interaction leads to off-diagonal coupling matrix elements which asymptotically are proportional to $r^{-2}$. A high quality CI potential energy surface is available[52] and experimental measurements of the differential cross sections in the energy range $4.0-7.0 \mathrm{eV}$. have been done[53,54]. Because of the close spacing of the $C 0$ rotational energy levels, converged close-coupling calculations at these energies are not possible with existing methods. Therefore, the full cross section problem is really beyond the scope of exact present day methods. However, we can still test the speed and performance of the methods on unconverged basis sets. The problem we chose is a 22 channel problem with $\mathrm{J}=25$ and $E=0.00195$ Hartrees. For $C 0$ in its ground state, this corresponds to an asymptotic impact parameter $b=4.0$ and a wavelength of 1.0 Bohr. The complete basis set used is shown in Table II.

Test 3. This is the problem of rotational excitation of $N_{2}$ by electron impact. We wanted to test the codes on an electron-molecule system, but without the complications of the exchange interaction. For this reason we used the potential energy surface of Onda and Truhlar[55] which employs, a local approximation to the exchange potential, valid only for a collision energy of 1.1025 Hartrees. The total angular momentum is $\mathrm{J}=5$. The asymptotic impact parameter is $\mathrm{b}=3.37$ and the wavelength is 4.23 Bohr. The complete basis set for this test is contained in Table II.

Table III summarizes most of the physical attributes which are important in molecular collision calculations. For the tested group, we list the range of the attribute covered by the tests. Tests $1-3$ do not cover the full ranges listed in Table III. They are only a representative subset of the 24 test
problems studied[9]. However, examination of the full set of results does not change the conclusions reached here based on the above three tests.
5. RESULTS AND DISCUSSION

In order to get a meaningful comparison, all calculations were done on the same computer (LBL's CDC 7600), and all programs were compiled on the same compiler. The programs were all written in fairly portable FORTRAN. No assembly language routines were used.

Possibly the most difficult quantity to assess in a comparison such as this is the accuracy of the solution. For any given method, the difference between two- and three-significant-figure accuracy is often a factor of two or three in computer time. Therefore, it is important to compare times only for calculations which result in similar accuracy. Unfortunately, precise accuracy control is very difficult to obtain - especially when the exact answer is not known ahead of time as with these test problems. An attempt was made in each case to achieve two-significant-figure accuracy in one specified transition probability for each test. The actual values computed and the correct values are shown in Table IV. It can be seen that while the results are reasonably uniform, there are differences in the accuracies achieved. Therefore, it is quite possible that the times reported for specific methods could be improved by a factor of two or three on some tests by fine tuning. Nonetheless, we believe the comparisons are meaningful for two reasons. First, as we show below, the spread in computer times over all methods for each test is a factor between 20 and 50. This is a significant difference which could not be eliminated by refining the accuracy. Second, the accuracies and times reported here are typical of those which would be chosen for a new research problem where the accuracy of each partial wave could not be individually fine tuned.

Most workers in this field have realized that the computational effort to integrate Eq. (1) is different in different regions of the integration variable, $r$. For example, when $r$ is near the origin the potential is often large and rapidly varying. The solutions have exponential behavior requiring small stepsizes. When $r$ is large, the potential is small and slowly varying. The solutions are oscillatory and numerically stable to integrate. Therefore, rather than simply compare the total integration times for all of the methods, it is much more revealing to see which methods are fastest in different regions of $r$. We do this in the following fashion. By dividing the total time by the total number of integration steps we get the average computer time per step. Then by dividing the entire integration range into smaller intervals and counting the number of steps taken in each interval, we get an histographic approximation to $\mathrm{dt} / \mathrm{dr}$, the computer time to integrate a unit of distance, i.e.;

$$
\begin{equation*}
\frac{d t}{d r} \cong \frac{T_{\text {total }}}{N_{\text {total }}} \frac{N(r+\Delta r)-N(r)}{\Delta r} \tag{4}
\end{equation*}
$$

where $N(r)$ is the number of steps required to integrate from $r_{\text {min }}$ to $r$. Note that the reciprocal of this, $\mathrm{dr} / \mathrm{dt}$, is the "velocity" at each point, $r$, with which the computer is integrating the coupled equations.

The results from all the methods tested are shown in Tables V-VII and selected results in Figs. 1-3. It was not convenient to compute $\mathrm{dt} / \mathrm{dr}$ at exactly the same points, $r$, for all methods. Therefore, linear interpolation was used to calculate the numbers in Tables V-VII. The time at the bottom of each table is the total time for the region bounded by the first and last values of $r$ listed.

Figure 1 and Table $V$ show the results for Test 1. High absolute accuracy is required on this problem because the transition probability being calculated is very small. For many of the programs this was the most difficult problem to solve. For small $r$, LOGD is most efficient by a fairly wide margin, and VIVS at the second energy is best for large $r$. For first energy calculations, however, INSCAT has the smallest total time.

Figure 2 and Table VI show the results for Test 2. This is a long range problem and the total times are dominated by the value of $d t / d r$ at large $r$. The results are only shown for $r \leq 150.00$ even though $r_{\max }=800.0$ was necessary for the correct answer. For first energy calculations, LOGD is still best at small $r$. However, several of the approximate potential methods, especially GORDON, are faster at second energies in this region. For large $r$, VIVS at the second energy is again the fastest. Because of the long range of the potential and the large number of oscillations over this range, the approximate solution methods are impractical for this problem.

Figure 3 and Table VII show the results for Test 3. Although the collision energy is much higher for this problem than for the others, the asymptotic wavelength is still quite long - 4.2 Bohr - because of the small mass of the electron. Consequently, the approximate solution methods do much better than one might at first expect. For most of the programs, getting the correct answer for this problem presented the fewest difficulties. The potential energy function for the $e-N_{2}$ interaction at small $r$ is quite small in contrast to the large barriers which are typical of atom-molecule potentials. In the non-classical region the interaction is dominated by the centrifugal terms. Since these terms are already included without approximation in the SAMS program, SAMS excels on this problem. Its total time is best of all the individual programs, even bettering the approximate potential methods on the
second energy. LOGD and SAMS perform equally well at small $r$ and are best in this region. VIVS, at the second energy, is again best for large $r$. However, we should emphasize that when the potential depends on the collision energy, as is the case for local approximations to the electron exchange potential, the second energy calculations of the approximate potential methods are not valid for comparison. The advantage these methods normally have for additional collision energies is lost in this case.

Overall, one is struck by the widely varying performances of the individual programs on the different physical problems. For example, INSCAT is the best performer for first energy calculations on Test 1 and a factor of 6 faster than SAMS. On Test 3, nearly the opposite is true. It is also quite clear that the best program would be a hybrid which followed the lowest $\mathrm{dt} / \mathrm{dr}$ curve in all regions. Although no single method is best for all tests in any region, the $\log$ derivative method is nearly always best for small $r$ and the variable-interval, variable-step method is nearly always best for large $r$. It therefore was desirable to combine these methods and form a new hybrid program. This is not the ideal combination for all problems, but this hybrid is always better than any individual method. This is evident in Table VIII.

Table VIII summarizes the total times from Tables V-VII, with the methods ordered according to computer time. The HYBRID entry is not from an actual program. It was hand calculated by integrating $d t / d r$ from $r_{m i n}$ to $r_{0}$ for LOGD and from $r_{0}$ to $r_{\text {max }}$ for VIVS. It can be seen that the second energy HYBRID time is always smaller than any individual method. For the short range problems the HYBRID result is 1.5 to 2.0 times faster than either of the two methods individually. For the long range problem of Test 2 , the improvement is minimal because the total time is dominated by the long range region.

Based on these findings a hybrid program, VIVAS, has been developed [17,43, 44], which combines the variable-interval, variable-step and the $\log$ derivative methods. In addition, this program includes significant improvements to the original variable-interval, variable-step program, VIVS. It can be seen in Table VIII that the new program is significantly faster than any of the individual programs.

Finally, regarding Table VIII, we return to the discussion of accuracy. As stated before, factors of two or three improvement can often be made and probably could be made here by refining the input parameters to each program. This means that the ordering of the methods in Table VIII should not be taken literally. However, factors of 20 to 50 are observed between the smallest and largest times. These differences are significant and it is believed doubtful that they could be eliminated by refinements in the accuracy of the calculation.

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TABLE I. Numerical methods for integrating differential equations.

| Year | Method Name | Library Name ${ }^{\text {a }}$ | Author(s) |
| :---: | :---: | :---: | :---: |
| 1883 | predictor-corrector |  | Bashforth and Adams [24] |
| 1895 | Runge-Kutta |  | $\begin{aligned} & \text { Runge (1895) }[24] \\ & \text { Kutta }(1901)[24] \end{aligned}$ |
| 1933 | Numerov | MNN | Numerov [25] |
| 1955 | DeVogelaere | DEVOG | DeVogelaere [26] |
| 1966 | amplitude density |  | Johnson and Secrest [27] |
| 1966 | exponential |  | Pechukas and Light (1966) [28] Chang and Light (1969) [29] |
| 1969 | integral equations | SAMS | Sams and Kouri [30] |
| 1969 | piecewise analytic reference potentials | GORDON | Gordon [31] |
| 1969 | variable-order, variable-step predictor-corrector | PC | $\begin{aligned} & \text { Krogh (1969) [32] } \\ & \text { Gear (1971) [33] } \end{aligned}$ |
| 1970 | iterative Numerov |  | Allison [3] |
| 1973 | log derivative | LOGD | Johnson [34] |
| 1974 | integral equations with piecewise analytic reference potential | INSCAT | Redmon and Micha [35] |
| 1976 | R-matrix propagator | RMAT | Light and Walker [36] <br> Stechel, Walker, and Light [37] |
| 1977 | renormalized Numerov |  | Johnson [38] |
| 1978 | exponential fitting |  | Raptis and Allison [39] |
| 1978 | finite element method |  | Rabitz, Askar, and Cakmak [40] |
| 1979 | $L^{2}$ approach to R-matrix propagator | L2RMAT | Schneider and Walker [41] |

Table I. Continued

1979 \begin{tabular}{lll}

\& | iterative method for a |
| :--- |
| single vector of solutions | \& Thomas [23] <br>

1979 \& | variable-interval, |
| :--- |
| variable-step method | \& VIVS

\end{tabular}$\quad$ Parker, Schmalz, and Light [42]

a Library name, when given, indicates that the method was tested in this work and the entry is the program name in the NRCC software library.

TABLE II. Basis set quantum numbers for Tests 1,2 , and 3 . Blank entries indicate a repeat of the above entry.

| Test 1 |  |  |  |  | Test 2 |  |  |  |  | Test 3 |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| No. | $n$ | j | $\ell$ | Target energy | No. | j | $\ell$ | Target energy | No. | j | $\ell$ | Target energy |
| 1 | 0 | 0 | 4 | 0.0 | 1 | 0 | 25 | 0.0 | 1 | 0 | 5 | 0.0 |
| 2 |  | 2 | 2 | 0.001616 | 2 | 1 | 24 | $1.76 \mathrm{E}-5$ | 2 | 2 | 3 | 5.46E-5 |
| 3 |  |  | 4 |  | 3 |  | 26 |  | 3 |  | 5 |  |
| 4 |  |  | 6 |  | 4 | 2 | 23 | 5.28E-5 | 4 |  | 7 |  |
| 5 |  | 4 | 0 | 0.005329 | 5 |  | 25 |  | 5 | 4 | 1 | 1.82E-4 |
| 6 |  |  | 2 |  | 6 |  | 27 |  | 6 |  | 3 |  |
| 7 |  |  | 4 |  | 7 | 3 | 22 | 1.06E-4 | 7 |  | 5 |  |
| 8 |  |  | 6 |  | 8 |  | 24 |  | 8 |  | 7 |  |
| 9 |  |  | 8 |  | 9 |  | 26 |  | 9 |  | 9 |  |
| 10 |  | 6 | 2 | 0.011009 | 10 |  | 28 |  | 10 | 6 | 1 | 3.82E-4 |
| 11 |  |  | 4 |  | 11 | 4 | 21 | 1.76E-4 | 11 |  | 3 |  |
| 12 |  |  | 6 |  | 12 |  | 23 |  | 12 |  | 5 |  |
| 13 |  |  | 8 |  | 13 |  | 25 |  | 13 |  | 7 |  |
| 14 |  |  | 10 |  | 14 |  | 27 |  | 14 |  | 9 |  |
| 15 | 1 | 0 | 4 | 0.018971 | 15 |  | 29 |  | 15 |  | 11 |  |
| 16 |  | 2 | 2 |  | 16 | 5 | 20 | $2.64 \mathrm{E}-4$ | 16 | 8 | 3 | 6.56E-4 |
| 17 |  |  | 4 |  | 17 |  | 22 |  | 17 |  | 5 |  |
| 18 |  |  | 6 |  | 18 |  | 24 |  | 18 |  | 7 |  |
|  |  |  |  |  | 19 |  | 26 |  | 19 |  | 9 |  |
|  |  |  |  |  | 20 | 6 | 19 | 3.70E-4 | 20 |  | 11 |  |
|  |  |  |  |  | 21 |  | 21 |  | 21 |  | 13 |  |
|  |  |  |  |  | 22 |  | 23 |  |  |  |  |  |

TABLE III. Most of the important physical attributes of molecular collision problems.

| Attribute | Range ${ }^{\text {a }}$ |
| :---: | :---: |
| Chemical systems | $\mathrm{H}_{\mathrm{e}}-\mathrm{H}_{2}, \mathrm{Li}^{+}-\mathrm{CO}, \mathrm{e}^{-}-\mathrm{N}_{2}$ |
| No. of channels | 2-32 |
| No. of closed channels | 0-21 |
| Integration range needed for convergence | 16-1000 Bohr |
| Collision energy | 0.779E-4 - 1.1025 Hartrees |
| Asymptotic wavelength | 0.6-5.0 Bohr |
| Transition probabilities | 0.91E-10-0.47 |
| Reactive scattering | not tested |
| Multiple electronic surfaces | not tested |
| Very high energy (very short wavelength) | not tested |
| Coulomb potentials | not tested |
| Large No. of channels (~100) | not tested |
| aThe range, when given, indicates the range covered by the test problems. |  |

TABLE IV. Selected transition probabilities, $\left|S_{i j}\right|^{2}$, for each test and method. The correct answers for Tests 1 and 3 are accurate to four significant figures. For Test 2, the correct answer is only guaranteed to two significant figures. $r_{\text {min }}$ and $r_{\text {max }}$ indicate the integration range used to calculate the correct answer.

| Program | Test 1 <br> $(1,15)^{\mathrm{a}}$ | Test 2 <br> $(1,4)^{\mathrm{a}}$ | Test 3 <br> $(1,2)^{\mathrm{a}}$ |
| :--- | :--- | :--- | :--- |
| PC | $0.1184-8^{\mathrm{b}}$ | $0.2036-1^{\mathrm{b}}$ | $0.2864-2^{\mathrm{b}}$ |
| DEVOG | $0.1183-8$ | $0.1722-1$ | $0.2874-2$ |
| MNN | $0.1181-8$ | $0.1666-1$ | $0.2874-2$ |
| LOGD | $0.1185-8$ | $0.1715-1$ | $0.2868-2$ |
| SAMS | $0.1181-8$ | $0.1752-1$ | $0.2876-2$ |
| INSCAT | $0.1149-8$ | $0.2154-1$ | $0.2887-2$ |
| GORDON | $0.1278-8$ | $0.1702-1$ | $0.2860-2$ |
| VIVS | $0.1213-8$ | $0.1732-1$ | $0.2867-2$ |
| RMAT | $0.1193-8$ | $0.1709-1$ | $0.2885-2$ |
| L2RMAT | $0.1170-8$ | $0.1718-1$ | $0.2865-2$ |
| VIVAS | $0.1164-8$ | $0.1710-1$ | $0.2861-2$ |
| Correct | $0.1184-8$ | $0.1715-1$ | $0.2873-2$ |
| $r_{\text {min }}$ | 2.5 | 3.0 | 0.01 |
| rmin | 45.0 | 120.0 |  |

[^0]TABLE V. $d t / d r$ (sec/Bohr), computer time for integrating a unit distance vs. $r$ for Test 1. E1 and E2 refer to first and second energy calculations, respectively. Time (at bottom of table) is the total time for integrating between the first and last values of $r$ in column 1.

| $r$ | PC | DEVOG | MNN | LOGD | SAMS | INSCAT | $\begin{gathered} \text { GORDON } \\ \text { EI } \end{gathered}$ | $\begin{aligned} & \text { VIVS } \\ & \text { EI } \end{aligned}$ | $\begin{gathered} \text { RMAT } \\ \text { E1 } \end{gathered}$ | $\begin{gathered} \text { L2RMAT } \\ \text { E1 } \end{gathered}$ | $\begin{gathered} \text { GORDON } \\ \text { E2 } \end{gathered}$ | $\begin{gathered} \text { Vivs } \\ \text { E2 } \end{gathered}$ | $\begin{aligned} & \text { RMAT } \\ & \text { E2 } \end{aligned}$ | $\begin{gathered} \text { L2RMAT } \\ \text { E2 } \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.8 | 4.241 | 1.020 | . 810 | . 202 | 2.208 | 1.500 | 10.396 | 2.130 | 5.019 | 7.607 | 2.043 | . 542 | 1.920 | . 520 |
| 2.9 | 3.540 | . 912 | . 719 | . 202 | 2.211 | 1.196 | 12.184 | 2.354 | 4.988 | 6.966 | 2.394 | . 600 | 1.908 | . 580 |
| 3.0 | 2.839 | . 805 | . 628 | . 202 | 2.213 | 1.105 | 13.330 | 2.579 | 4.957 | 6.325 | 2.620 | . 657 | 1.896 | . 640 |
| 3.1 | 2.138 | . 698 | . 537 | . 202 | 2.213 | 1.040 | 14.202 | 3.000 | 4.927 | 5.684 | 2.792 | . 764 | 1.884 | . 700 |
| 3.2 | 1.438 | . 591 | . 446 | . 202 | 2.213 | . 979 | 15.074 | 3.532 | 4.896 | 5.043 | 2.964 | . 899 | 1.873 | . 760 |
| 3.3 | 1.013 | . 560 | . 391 | . 202 | 2.213 | . 932 | 14.943 | 4.064 | 4.865 | 4.403 | 2.938 | 1.033 | 1.861 | . 820 |
| 3.4 | 1.583 | . 635 | . 412 | . 202 | 2.213 | . 882 | 13.810 | 4.515 | 4.835 | 3.762 | 2.714 | 1.147 | 1.849 | . 880 |
| 3.5 | 2.154 | . 710 | . 434 | . 202 | 2.213 | . 820 | 12.677 | 4.945 | 4.804 | 3.121 | 2.489 | 1.256 | 1.837 | . 940 |
| 3.6 | 2.725 | . 786 | . 455 | . 202 | 2.211 | . 758 | 11.647 | 4.845 | 4.589 | 2.480 | 2.286 | 1.231 | 1.755 | 1.000 |
| 3.7 | 3.295 | . 861 | . 477 | . 202 | 2.208 | . 725 | 11.029 | 4.595 | 4.375 | 2.354 | 2.166 | 1.169 | 1.673 | . 950 |
| 3.8 | 3.787 | . 919 | . 492 | . 202 | 2.205 | . 694 | 10.412 | 3.900 | 4.160 | 2.229 | 2.046 | . 993 | 1.591 | . 900 |
| 3.9 | 3.382 | . 940 | . 481 | . 202 | 2.203 | . 661 | 9.794 | 3.133 | 3.945 | 2.103 | 1.926 | . 798 | 1.509 | . 850 |
| 4.0 | 2.978 | . 961 | . 470 | . 202 | 2.200 | . 623 | 9.201 | 2.366 | 3.731 | 1.978 | 1.811 | . 603 | 1.427 | . 800 |
| 5.0 | 1.663 | 1.076 | . 439 | . 202 | 2.213 | . 341 | 5.057 | 1.151 | 2.095 | 1.035 | . 999 | . 293 | . 801 | . 420 |
| 6.0 | 1.751 | 1.076 | . 439 | . 202 | 1.776 | . 186 | 2.980 | . 795 | 1.278 | . 580 | . 590 | . 202 | . 489 | . 233 |
| 7.0 | 1.751 | 1.076 | . 439 | . 202 | 1.325 | . 117 | 1.760 | . 582 | . 869 | . 300 | . 350 | . 148 | . 332 | . 120 |
| 8.0 | 1.751 | 1.076 | . 439 | . 202 | 1.325 | . 090 | 1.580 | . 368 | . 715 | . 255 | . 314 | . 094 | . 274 | . 105 |
| 9.0 | 1.817 | 1.076 | . 439 | . 202 | 1.325 | . 079 | 1.400 | . 155 | . 715 | . 210 | . 278 | . 039 | . 274 | . 090 |
| 10.0 | 2.531 | 1.076 | . 439 | . 202 | . 994 | . 072 | 1.265 | . 123 | . 673 | . 197 | . 251 | . 031 | . 258 | . 083 |
| 11.0 | 1.821 | 1.076 | . 439 | . 202 | . 663 | . 067 | 1.174 | . 117 | . 589 | . 183 | . 233 | . 030 | . 225 | . 077 |
| 12.0 | 1.552 | 1.076 | . 439 | . 202 | . 663 | . 063 | 1.083 | .111 | . 517 | . 170 | . 215 | . 028 | .198 | . 070 |
| 13.0 | 1.828 | 1.076 | . 439 | . 202 | . 663 | . 059 | 1.006 | . 105 | . 482 | . 162 | . 195 | . 027 | . 184 | . 066 |
| 14.0 | 1.754 | 1.076 | . 439 | . 202 | . 663 | . 055 | . 934 | . 099 | . 447 | . 154 | . 175 | . 025 | . 171 | . 062 |
| 15.0 | 1.754 | 1.076 | . 439 | . 202 | . 398 | . 052 | . 868 | . 094 | . 412 | . 146 | . 159 | . 024 | . 158 | . 058 |
| 16.0 | 1.764 | 1.076 | . 439 | . 202 | . 133 | . 051 | . 821 | . 088 | . 382 | . 138 | . 155 | . 022 | . 146 | . 054 |
| TIME | 25.494 | 13.799 | 5.894 | 2.668 | 15.825 | 2.602 | 39.007 | 9.298 | 16.421 | 9.376 | 7.667 | 2.366 | 6.281 | 2.779 |

TABLE VI. dt/dr (sec/Bohr), computer time for integrating a unit distance vs. $r$ for Test 2. E1 and E2 refer to first and second energy calculations, respectively. Time (at bottom of table) is the total time for integrating between the first and last values of $r$ in column 1.

| $r$ | PC | DEVOG | MNN | LOGD | SAMS | INSCAT | GORDON El | VIVS E1 | $\begin{gathered} \text { RMAT } \\ \text { E1 } \end{gathered}$ | L2RMAT EI | $\begin{aligned} & \text { GORDON } \\ & \text { E2 } \end{aligned}$ | $\begin{gathered} \text { VIVS } \\ \text { E2 } \end{gathered}$ | $\begin{aligned} & \text { RMAT } \\ & \text { E2 } \end{aligned}$ | $\begin{gathered} \text { L2RMAT } \\ \text { E2 } \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3.5 | 14.089 | 2.521 | 3.710 | . 979 | 2.136 | 5.592 | 4.470 | 3.209 | 3.396 | 16.800 | . 610 | . 840 | 1.298 | . 790 |
| 3.6 | 12.262 | 2.157 | 3.143 | . 979 | 2.136 | 5.209 | 4.522 | 3.322 | 3.396 | 16.800 | . 633 | . 870 | 1.298 | . 790 |
| 3.7 | 10.435 | 1.793 | 2.576 | . 979 | 2.136 | 4.844 | 4.588 | 3.434 | 3.396 | 15.649 | . 661 | . 900 | 1.298 | 1.029 |
| 3.8 | 8.867 | 1.496 | 2.160 | . 979 | 2.136 | 4.494 | 4.653 | 6.519 | 3.396 | 14.499 | . 690 | 1.709 | 1.298 | 1.268 |
| 3.9 | 7.614 | 1.325 | 1.940 | . 979 | 2.136 | 4.160 | 4.718 | 9.033 | 3.396 | 13.348 | . 719 | 2.368 | 1.298 | 1.506 |
| 4.0 | 6.360 | 1.154 | 1.719 | . 979 | 2.136 | 3.840 | 4.783 | 8.812 | 3.396 | 12.198 | . 747 | 2.309 | 1.298 | 1.745 |
| 4.1 | 5.107 | . 983 | 1.499 | . 979 | 2.136 | 3.532 | 4.849 | 8.590 | 3.396 | 11.047 | . 776 | 2.251 | 1.298 | 1.984 |
| 4.2 | 3.853 | . 812 | 1.279 | . 979 | 2.136 | 3.235 | 4.914 | 4.727 | 3.396 | 9.896 | . 804 | 1.237 | 1.298 | 2.223 |
| 4.3 | 3.054 | . 708 | 1.147 | . 979 | 2.136 | 2.949 | 4.979 | 4.480 | 3.260 | 8.746 | . 833 | 1.173 | 1.246 | 2.462 |
| 4.4 | 2.940 | . 786 | 1.209 | . 979 | 2.136 | 2.669 | 5.045 | 4.660 | 2.989 | 7.595 | . 861 | 1.221 | 1.142 | 2.701 |
| 4.5 | 2.826 | . 865 | 1.271 | . 979 | 2.136 | 2.393 | 5.110 | 4.757 | 2.717 | 6.876 | . 890 | 1.248 | 1.038 | 2.762 |
| 4.6 | 2.712 | . 944 | 1.333 | . 979 | 2.136 | 2.113 | 4.895 | 3.835 | 2.445 | 6.588 | . 852 | 1.006 | . 934 | 2.647 |
| 4.7 | 2.598 | 1.023 | 1.394 | . 979 | 2.136 | 1.829 | 4.680 | 2.914 | 2.174 | 6.301 | . 814 | . 763 | . 831 | 2.531 |
| 4.8 | 2.508 | 1.089 | 1.444 | . 979 | 2.136 | 1.506 | 4.465 | 2.015 | 1.970 | 6.013 | . 776 | . 527 | . 753 | 2.416 |
| 4.9 | 2.463 | 1.091 | 1.444 | . 979 | 2.136 | 1.179 | 4.250 | 1.858 | 1.834 | 5.725 | . 738 | . 486 | . 701 | 2.300 |
| 5.0 | 2.418 | 1.093 | 1.444 | . 979 | 2.136 | 1.069 | 4.035 | 1.702 | 1.698 | 5.437 | . 700 | . 445 | . 649 | 2.184 |
| 6.0 | 2.248 | . 976 | 1.444 | . 979 | 2.136 | 1.565 | 2.960 | . 629 | 1.189 | 3.172 | . 510 | . 165 | . 454 | 1.276 |
| 7.0 | 1.667 | . 804 | 1.082 | . 979 | 1.897 | 1.314 | 2.620 | . 461 | 1.456 | 1.897 | . 454 | . 121 | . 556 | . 765 |
| 8.0 | 1.401 | . 691 | . 722 | . 979 | 1.658 | 1.046 | 2.020 | . 372 | 1.844 | 1.615 | . 354 | . 098 | . 704 | . 651 |
| 9.0 | 1.107 | . 624 | . 722 | . 538 | 1.418 | . 830 | 1.660 | . 328 | 1.916 | 1.411 | . 289 | . 086 | . 732 | . 568 |
| 10.0 | . 954 | . 587 | . 722 | . 538 | 1.179 | . 665 | 1.357 | . 285 | 1.673 | 1.515 | . 234 | . 075 | . 639 | . 610 |
| 11.0 | . 937 | . 565 | . 722 | . 538 | . 940 | . 537 | 1.223 | . 254 | 1.430 | 1.619 | . 212 | . 067 | . 547 | . 652 |
| 12.0 | . 756 | . 553 | . 722 | . 538 | . 837 | . 435 | 1.090 | . 223 | 1.187 | 1.615 | . 190 | . 058 | . 454 | . 649 |
| 13.0 | . 784 | . 545 | . 722 | . 538 | . 735 | . 351 | . 957 | . 192 | . 944 | 1.584 | . 168 | . 050 | . 361 | . 636 |
| 14.0 | . 639 | . 541 | . 722 | . 538 | . 632 | . 280 | . 823 | .162 | . 701 | 1.540 | . 146 | . 042 | . 268 | . 619 |
| 15.0 | . 847 | . 538 | . 722 | . 430 | . 530 | . 213 | . 754 | . 142 | . 458 | 1.486 | . 133 | . 037 | . 175 | . 598 |
| 16.0 | . 550 | . 537 | . 722 | . 430 | . 427 | . 170 | . 705 | .134 | .440 | 1.414 | . 124 | . 035 | . 168 | . 570 |
| 17.0 | . 612 | . 535 | . 722 | . 430 | . 427 | .130 | . 657 | . 125 | . 421 | 1.241 | . 115 | . 033 | .161 | . 501 |
| 18.0 | . 651 | . 535 | . 722 | . 430 | . 427 | .141 | . 608 | .117 | . 402 | 1.068 | . 105 | . 031 | . 153 | . 432 |
| 19.0 | . 788 | . 535 | . 722 | . 430 | . 427 | . 164 | . 560 | .109 | . 383 | . 895 | . 096 | . 028 | . 146 | . 364 |
| 20.0 | . 707 | . 535 | . 722 | . 430 | . 427 | . 174 | . 512 | . 100 | . 364 | . 807 | . 087 | . 026 | .139 | .328 |
| 25.0 | . 871 | . 535 | . 722 | . 074 | . 427 | . 168 | . 318 | . 065 | . 269 | . 476 | . 050 | . 017 | .103 | . 194 |
| 30.0 | . 649 | . 535 | . 722 | . 061 | . 427 | . 149 | . 272 | . 056 | . 174 | . 257 | . 043 | . 015 | . 067 | . 105 |
| 35.0 | . 555 | . 535 | . 722 | . 052 | . 427 | .131 | . 226 | . 048 | . 079 | . 224 | . 036 | . 012 | . 030 | . 091 |
| 40.0 | . 716 | . 535 | . 722 | . 046 | . 248 | .117 | . 179 | . 039 | . 075 | .191 | . 029 | . 010 | . 029 | . 078 |
| 45.0 | . 658 | . 537 | . 722 | . 041 | . 126 | . 105 | .133 | . 030 | . 071 | .158 | . 021 | . 008 | . 027 | . 064 |
| 50.0 | . 658 | . 537 | . 722 | . 036 | .107 | . 095 | . 086 | . 025 | . 067 | . 125 | . 014 | . 007 | . 026 | . 050 |
| 100. | . 658 | . 537 | . 722 | . 018 | . 107 | . 048 | . 020 | . 013 | . 040 | . 059 | . 003 | . 003 | . 015 | . 023 |
| 150. | . 658 | . 537 | . 722 | . 012 | . 107 | . 032 | . 013 | . 007 | . 025 | . 046 | . 003 | . 002 | . 010 | . 019 |
| TIME | 110.176 | 81.001 | 108.733 | 15.137 | 38.449 | 22.754 | 37.945 | 14.529 | 28.598 | 56.514 | 6.407 | 3.805 | 10.927 | 19.634 |

TABLE VII. dt/dr (sec/Bohr), computer time for integrating a unit distance vs. $r$ for Test 3. E1 and E2 refer to first and second energy calculations, respectively. Time (at bottom of table) is the total time for integrating between the first and last values of $r$ in column 1.

| $r$ | PC | DEVOG | MNN | LOGD | SAMS | INSCAT | $\begin{gathered} \text { GORDON } \\ \text { EI } \end{gathered}$ | $\begin{gathered} \text { VIVS } \\ \text { EI } \end{gathered}$ | RMAT EI | $\underset{E 1}{\text { L2RMAT }}$ | $\begin{gathered} \text { GORDON } \\ \text { E2 } \end{gathered}$ | vivs E2 | $\begin{aligned} & \text { RMAT } \\ & \text { E2 } \end{aligned}$ | $\begin{gathered} \text { L2RMAT } \\ \text { E2 } \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| . 2 | 13.599 | 3.601 | 7.160 | . 216 | . 229 | 4.254 | 14.943 | 1.560 | 2.677 | 5.910 | 2.900 | . 380 | 1.025 | . 326 |
| . 4 | 10.695 | 2.809 | 5.371 | . 216 | . 229 | 4.316 | 7.043 | 1.560 | 2.677 | 5.910 | 1.364 | . 380 | 1.025 | . 358 |
| . 6 | 6.313 | 1.662 | 2.921 | . 216 | . 229 | 2.868 | 6.088 | 2.086 | 2.590 | 5.910 | 1.179 | . 508 | . 991 | . 390 |
| . 8 | 2.222 | . 555 | . 800 | . 216 | . 229 | 2.213 | 5.132 | 2.663 | 2.244 | 4.952 | . 994 | . 649 | . 859 | . 408 |
| 1.0 | 1.641 | . 453 | . 650 | . 216 | . 229 | 1.776 | 4.443 | 3.373 | 1.898 | 3.994 | . 860 | . 822 | . 726 | . 426 |
| 1.2 | 1.060 | . 351 | . 500 | . 215 | . 229 | 1.401 | 3.931 | 3.240 | 1.552 | 3.036 | . 761 | . 789 | . 594 | . 444 |
| 1.4 | . 852 | . 275 | . 409 | . 213 | . 229 | 1.224 | 3.419 | 2.262 | 1.205 | 2.078 | . 662 | . 550 | . 461 | . 462 |
| 1.6 | 1.174 | . 240 | . 385 | . 212 | . 229 | 1.073 | 2.907 | 1.855 | . 981 | 1.120 | . 563 | . 452 | . 375 | . 480 |
| 1.8 | 1.497 | . 205 | . 361 | . 210 | . 229 | . 951 | 2.395 | 1.449 | . 878 | 1.013 | . 464 | . 353 | . 336 | . 431 |
| 2.0 | 1.281 | . 181 | . 321 | . 208 | . 2229 | . 868 | 1.883 | 1.144 | . 774 | . 907 | . 364 | . 280 | . 296 | . 382 |
| 3.0 | . 199 | . 089 | . 178 | . 102 | . 229 | . 582 | 1.267 | . 764 | . 430 | . 552 | . 245 | . 186 | . 165 | . 222 |
| 4.0 | . 103 | . 048 | . 169 | . 102 | . 223 | . 442 | . 942 | . 509 | . 344 | . 397 | . 182 | . 124 | . 132 | . 156 |
| 5.0 | . 103 | . 081 | . 089 | . 102 | . 130 | . 352 | . 739 | . 387 | . 258 | . 334 | .142 | . 094 | . 099 | . 135 |
| 6.0 | . 875 | . 095 | . 089 | . 102 | . 023 | . 293 | . 657 | . 316 | . 258 | . 279 | .127 | . 077 | . 099 | . 128 |
| 7.0 | . 330 | . 104 | . 089 | . 102 | . 023 | . 250 | . 574 | . 251 | . 258 | . 243 | . 111 | . 061 | . 099 | . 153 |
| 8.0 | . 120 | . 108 | . 089 | . 102 | . 023 | . 221 | . 492 | . 224 | . 172 | . 206 | . 096 | . 055 | . 066 | . 179 |
| 9.0 | . 273 | .111 | . 089 | . 102 | . 023 | . 193 | . 410 | . 198 | . 172 | . 182 | . 080 | . 048 | . 066 | . 171 |
| 10.0 | . 244 | .114 | . 089 | . 102 | . 023 | . 177 | . 390 | . 171 | . 166 | .167 | . 076 | . 042 | . 064 | . 138 |
| 11.0 | .163 | .115 | . 089 | . 102 | . 023 | . 162. | . 370 | . 144 | .155 | . 153 | . 071 | . 035 | . 059 | . 104 |
| 12.0 | .123 | .116 | . 089 | . 102 | . 023 | . 146 | . 350 | .118 | . 143 | .138 | . 067 | . 029 | . 055 | . 071 |
| 13.0 | . 123 | .117 | . 089 | . 102 | . 023 | .135 | . 330 | . 101 | .131 | . 127 | . 063 | . 025 | . 050 | . 051 |
| 14.0 | . 104 | .118 | . 089 | . 102 | . 023 | .127 | . 310 | . 098 | .117 | . 120 | . 058 | . 024 | . 045 | . 048 |
| 15.0 | . 078 | .119 | . 089 | . 102 | . 023 | .119 | . 290 | . 094 | . 103 | .113 | . 054 | . 023 | . 040 | . 045 |
| 16.0 | . 087 | .119 | . 089 | . 102 | . 023 | .110 | . 270 | . 090 | . 089 | . 106 | . 050 | . 022 | . 034 | . 042 |
| 17.0 | . 089 | .119 | . 089 | . 102 | . 023 | . 102 | . 250 | . 087 | . 076 | . 099 | . 045 | . 021 | . 029 | . 039 |
| 18.0 | . 097 | . 120 | . 089 | . 102 | . 023 | . 097 | . 230 | . 083 | . 069 | . 092 | . 041 | . 020 | . 026 | . 037 |
| 19.0 | . 212 | . 120 | . 089 | . 102 | . 023 | . 093 | . 217 | . 079 | . 069 | . 087 | . 039 | . 019 | . 026 | . 035 |
| 20.0 | . 096 | . 120 | . 089 | . 102 | . 023 | . 089 | . 211 | . 076 | . 069 | . 084 | . 038 | . 018 | . 026 | . 033 |
| 25.0 | .112 | .121 | . 089 | . 102 | . 023 | . 070 | . 182 | . 057 | . 063 | . 068 | . 033. | . 014 | . 024 | . 027 |
| 30.0 | . 151 | . 122 | . 089 | . 102 | . 023 | . 059 | . 153 | . 039 | . 052 | . 057 | . 028 | . 009 | . 020 | . 023 |
| 35.0 | . 120 | . 122 | . 089 | .102 | . 023 | . 050 | . 124 | . 024 | . 040 | . 050 | . 023 | . 006 | . 015 | . 020 |
| 40.0 | . 134 | . 122 | . 089 | . 102 | . 023 | . 044 | . 110 | . 023 | . 034 | . 043 | . 021 | . 005 | . 013 | . 017 |
| 45.0 | . 134 | . 122 | . 089 | . 102 | . 023 | . 038 | .110 | . 021 | . 032 | . 041 | . 021 | . 005 | . 012 | . 016 |
| 50.0 | . 134 | . 122 | . 089 | . 102 | . 024 | . 035 | .110 | . 020 | . 031 | . 041 | . 021 | . 005 | . 012 | . 016 |
| TIME | 14.422 | 7.298 | 7.592 | 5.321 | 2.128 | 9.375 | 22.095 | 9.352 | 7.937 | 11.778 | 4.222 | 2.280 | 3.038 | 3.345 |

TABLE VIII. Integrated total times from Tables V-VII arranged in ascending order on the time. The HYBRID times are the sum of the times for LOGD integrated from $r_{\text {min }}$ to $r_{0}$ and for VIVS integrated from $r_{0}$ to $r_{\text {max }}$. $r_{0}$ is $8.0,6.0$, and 4.0 for Test 1, Test 2, and Test 3, respectively.

| Method | Test 1 |  |  | Test 2 |  | Test 3 |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Energy | Time (sec) | Method | Energy | Time (sec) | Method | Energy | Time (sec) |
| VIVAS | 2nd | 1.03 | VIVAS | 2nd | 2.2 | VIVAS | 2nd | 1.10 |
| HYBRID | 2nd | 1.31 | HYBRID | 2nd | 3.3 | HYBRID | 2nd | 1.56 |
| VIVAS | 1st | 1.65 | VIVS | 2nd | 3.8 | SAMS |  | 2.13 |
| HYBRID | 1st | 2.08 | VIVAS | 1st | 5.9 | VIVS | 2nd | 2.28 |
| VIVS | 2nd | 2.37 | GORDON | 2nd | 6.4 | VIVAS | 1st | 2.89 |
| INSCAT |  | 2.60 | HYBRID | 1st | 9.5 | L2RMAT | 2nd | 3.34 |
| LOGD |  | 2.67 | RMAT | 2nd | 3.04 | GORDON | 2nd | 4.22 |
| L2RMAT | 2nd | 2.78 | RMAT | 2nd | 10.9 | HYBRID | 1st | 4.43 |
| MNN |  | 5.87 | VIVS | 1st | 14.5 | LOGD |  | 5.32 |
| RMAT | 2nd | 6.28 | LOGD |  | 15.1 | DEVOG |  | 7.30 |
| GORDON | 2nd | 7.67 | L2RMAT | 2nd | 19.6 | MNN |  | 7.59 |
| VIVS | 1st | 9.30 | INSCAT |  | 22.8 | RMAT | 1st | 7.94 |
| L2RMAT | 1st | 9.38 | RMAT | 1st | 28.6 | VIVS | 1st | 9.35 |
| DEVOG |  | 13.80 | GORDON | 1st | 37.9 | INSCAT |  | 9.37 |
| SAMS |  | 15.82 | SAMS |  | 38.4 | L2RMAT | 1st | 11.73 |
| RMAT | 1st | 16.42 | L2RMAT | 1st | 56.5 | PC |  | 14.42 |
| PC |  | 25.49 | DEVOG |  | 81.0 | GORDON | 1st | 22.09 |
| GORDON | 1st | 39.01 | MNN <br> PC |  | $\begin{aligned} & 108.7 \\ & 110.2 \end{aligned}$ |  |  |  |



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Fig. 1. Test 1. Comparison of $\mathrm{dt} / \mathrm{dr}$ for the LOGD, VIVS, and INSCAT programs. El and E2 indicate first and second energy calculations respectively.


Fig. 2. Test 2. Same as Fig. 1.


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Fig. 3. Test 3. Comparison of $\mathrm{dt} / \mathrm{dr}$ for the LOGD, VIVS, and SAMS programs. E1 and E2 indicate first and second energy calculations respectively.

This report was done with support from the United States Energy Research and Development Administration. Any conclusions or opinions expressed in this report represent solely those of the authors) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the United States Energy Research and Development Administration.


[^0]:    a The channel numbers i and j correspond to those in Table II.
    $b$ - indicates the power of 10 .

