# Mie Scattering Calculations: Advances in Technique and Fast, Vector-Speed Computer Codes 

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## ABSTRACT

Dave published the first widely-used Mie scattering codes in 1968. Even on the fastest computers, these codes and their descendants often took a great deal of computer time for problems of practical interest. In the intervening years, there have been a number of improvements in technique (some developed by this author and reported herein for the first time). At the same time, vector processing has increasingly become the wave of the future in scientific computing machines, and Mie computations can be effectively reorganized to take advantage of it.

The present document gathers these improvements in technique, together with the necessary reorganization to attain vector speed, to produce new Mie scattering codes suitable for modern computation.

Actually, two codes are presented. The first, MIEVO, attains as much vector speed as possible within the constraint of using the minimum possible memory. MIEVO is suitable for almost any computer, whether or not it has vector capabilities, and is generally faster and better designed than existing Mie codes.

The second code, MIEVI, attains maximum vector speed, at the expense of using more memory than MIEVO. It is most suitable for vector-processing computers. MIEV1 is anywhere from $10 \%$ to $300 \%$ faster on the CRAY-1 than MIEVO.

Detailed timing results are presented for both codes. The codes are thoroughly tested and documented and are exceptionally reliable and well-conditioned. Mie results up to size parameters of 20,000 have been generated without difficulty.

## PREFACE



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## 1. INTRODUCTION

Calculations of light scattering from particles are needed in the widest variety of research endeavors, ranging from astronomy (interstellar dust scattering) to zoology (bacterial scattering). The prototypical such calculation assumes that the particle is a homogeneous sphere, and the incident light a monochromatic plane wave. Clebsch worked out the mathematical machinery for this problem in 1861; in 1890 Lorenz gave a full solution for transparent spheres; in 1908 Mie, and in 1909 Debye, published completely general solutions. These references, and many others up through 1945, may be found in the excellent historical survey by Logan (1965). By an odd twist of fate, Mie's name has come to be exclusively associated with the problem; we shall adhere to this convention, but with full awareness that a misnomer is involved. Excellent accounts of Mie theory may be found in the books by Shifrin (1951), Van de Hulst (1957), Kerker (1969) and Born and Wolf (1975).

While the vast majority of scattering particles are not spherical, so that the Mie solution does not strictly apply to them, both intuition and experimental evidence (e.g., Zerull, 1976) indicate that, with averaging over orientation and/or size, mildly nonspherical particles scatter very much like 'equivalent' spheres. This, of course, vastly enhances the utility of the Mie solution. Van de Hulst (1957) and Kerker (1969) indicate some of the wide-ranging applications which are then possible.

The computational history of Mie scattering is quite different and much more recent than the theoretical history; Van de Hulst's
and Kerker's books both contain accounts of it. Van de Hulst notes that, while there have been some ambitious tabulations of various Mie quantities, these are useful mostly for checking computer codes. The reason is simply the rapid oscillation of most Mie quantities; these oscillations would be impossible to resolve in a comprehensive table, and they make tabular interpolation risky. Furthermore, there are resonances (sharp spikes) within Mie quantities whose scale is much finer even than the oscillations (Rosasco and Bennett, 1978; Chýlek et al., 1978). Hence Mie scattering is a field which, unlike some, absolutely demands computer calculations. (Analytic approximations to Mie's solution are usually very limited in their range of application and, even when available, have an unfortunate tendency to be at least as complicated as the Mie solution itself.) The number of Mie scattering calculations performed prior to the mid-1950s was expectably small. Things picked up rapidly thereafter, but until the late 1960 s Mie calculations were done without much understanding of computational error, particularly ill-conditioning from subtraction of nearly equal numbers, and instability in recursion relations. Defining the size parameter

$$
x=\frac{\text { circumference of sphere }}{\text { wavelength }}
$$

we may easily find cases where a straightforward programming of Mie's solution would incur serious computational error for x as small as 20-30. Thus, while many of the pre-1970 Mie results are undoubtedly correct, it would be foolish to place blind faith in them.

Because the Mie solution is a series with approximately $x$ terms, because early computers were slow, and because $\mathrm{x}>1$.was virtual terra Incognita, early computer calculations were generally restricted to $1<x<100$. Irvine's 1965 paper is an excellent and frequently cited example from this period. But the explosive growth of computer technology soon permitted calculations for much larger size parameters; Dave's 1968b paper, which considers up to $x=785$ is a good example.

A further development was Kattawar and Plass' (1967) paper pointing out the potential instability in the upward-recursive calculation of a Bessel function ratio in Mie theory (cf. Eq. 20). (Rayleigh actually discovered this around the turn of the century (Logan, 1965), but his observations had long been forgotten.) Their resolution of the difficulty, which has become standard, was to use downward recursion. Deirmendjian's -(1969) book describes the same instability problem but offers no solution to it.

Dave's (1968a, 1969a) IBM reports were important landmarks. They set forth an algorithm and a brace of computer codes for performing Mie calculations. While the number of different Mie codes in use today is undoubtedly large, most of them can trace their lineage back to Dave's subroutines.

With powerful subroutines like Dave's in hand, the 1970s saw an explosive growth in applications. My own experience may be illustrative. In 1971 I began investigating solar and longwave radiation transfer in an atmosphere containing clouds. The presence of clouds required Mie scattering calculations for a size distribution of water droplets for 100 or more wavelengths from $0.3 \mu \mathrm{~m}$ to $500 \mu \mathrm{~m}$. Consider a wavelength of $0.5 \mu \mathrm{~m}$ and a cloud with drop sizes ranging from $0.1 \mu \mathrm{~m}$ to $50 \mu \mathrm{~m}$ 。

The Mie calculation for this case proceeds from $x=1$ to $x=628$, in steps $\Delta x=0.1$ (Dave, 1969b); for each value of $x$ there are roughly $x$ terms to be summed, at each of say 100 angles, so the total number of terms to be summed is about 200 million. And each term by itself requires considerable computation to generate! Now imagine this calculation repeated for 100 wavelengths (it is less onerous for longer wavelengths) and it will become clear why 'staggering' is not an exaggerated description of the task. Yet, as the decade wore on, applications-oriented Mie calculations of this magnitude became increasingly commonplace.

In spite of this pressure of applications, the decade has so far brought forward no great changes in the algorithmic structure of Mie computations, save for Palmer's (1977) work suggesting that replacing series by continued fractions may be faster and more accurate. There have, however, been a few minor improvements. One is a new way to initialize the downward Bessel function ratio recursion (Lentz, 1976). Others are in the nature of more efficient ways to organize the computation, devised by the present author in response to the problem outlined in the previous paragraph and published here for the first time.

The present document has, as its overall purpose, the incorporation of these advances in technique, made in the decade since Dave (1968a, 1969a), Into a new set of Mie scattering codes. The specific goals of this effort are laid out in the following section, and the analytical and computational details are worked out in the remainder of the document.

To the uninitiated reader, the codes may appear as if they could have been written straightaway, without all the apparent niggling over small points. But their simplicity is deceptive; it conceals a multitude of blind alleys, pitfalls, instabilities, inefficiencies and inelegancies to which the "straightaway" approach would fall victim. A variety of decisions has to be made, often requiring considerable background study and some sophistication in numerical analysis. Further advances will undoubtedly be forthcoming; but these algorithms already represent quite an advanced stage.

## 2. SPECIFIC GOALS OF ALGORITHMS

The specific goals that guided the formulation of the algorithms and codes herein were:

- maximum speed (including vector processing wherever possible)
- generality (furnishing all Mie quantities necessary for full polarization-dependent studies)
- reliability over broad ranges of refractive index and size parameter
- avoidance of all numerical instability
- portability (immediate executability on computers having single precision of at least 14 significant digits, like CDC and CRAY; executability with minor alterations on computers having significantly lower single precision)
- accuracy: at least 5-6 significant digits
- as simple and straightforward as possible within the constraints imposed by the previous goals.

Another goal, the use of minimum computer memory, proved incompatible in part with the main goal of maximum speed. This is because vector processing requires quantities, which could otherwise be scalars, to be stored in arrays. Therefore two separate codes were devised which have much in common but which either (a) have maximum speed, using as much memory as needed to achieve it (MIEV1); or (b) use minimum memory, attaining as much speed as possible within that constraint (MIEVO).

## 3. MIE SCATTERING FORMULAE--GENERAL CASE

The Mie scattering formulae are given in several books (Van de Hulst, 1957; Kerker, 1969; Deirmendjian, 1969) and by Dave (1968a, 1969a), although not always in the forms most suited to computation. We merely transcribe most of the relevant formulae below and give a reference; for those which are new, short derivations are provided. The five formulae (6-9) give the quantities actually calculated and returned by the codes MIEVO and MIEV1.

The two important independent variables in Mie theory are the size parameter

$$
\begin{equation*}
x=\frac{2 \pi r}{\lambda} \tag{1}
\end{equation*}
$$

and

$$
\begin{equation*}
z=m \times \tag{2}
\end{equation*}
$$

where

$$
\begin{align*}
& r= \text { radius of scattering sphere } \\
& \lambda= \text { wavelength of incident plane wave } \\
& m= \text { complex refractive index of sphere relative } \\
& \text { to surrounding medium } \\
& m= m_{r e}-i_{i m}  \tag{3}\\
&|m|> 1  \tag{4}\\
& m_{i m}>0 \tag{5}
\end{align*}
$$

Restriction (4), which would, for example, exclude scattering from air bubbles in water, may not be necessary, but we have not tested the codes for such situations.

Extinction Efficiency Factor (Van de Hulst, Sec. 9.32)

$$
\begin{equation*}
Q_{e x t}=\frac{2}{x^{2}} \sum_{n=1}^{N}(2 n+1) \operatorname{Re}\left(a_{n}+b_{n}\right) \tag{6}
\end{equation*}
$$

Scattering Efficiency Factor (Van de Hulst, Sec. 9.32)

$$
\begin{equation*}
Q_{s c a}=\frac{2}{x^{2}} \sum_{n=1}^{N}(2 n+1)\left\{\left|a_{n}\right|^{2}+\left|b_{n}\right|^{2}\right\} \tag{7}
\end{equation*}
$$

Asymmetry Factor (Kerker, Eq. 3.11.6)

$$
\begin{align*}
g= & \frac{4}{x^{2} Q_{s c a}} \sum_{n=1}^{N}\left\{\frac{n(n+2)}{n+1} \operatorname{Re}\left(a_{n} a_{n+1}^{*}+b_{n} b_{n+1}^{*}\right)\right. \\
& \left.+\frac{2 n+1}{n(n+1)} \operatorname{Re}\left(a_{n} b_{n}^{*}\right)\right\} \tag{8}
\end{align*}
$$

Scattering Amplitudes (Van de Hulst, Sec. 9.31)

$$
\begin{align*}
& S_{1}(\mu)=\sum_{n=1}^{N} \frac{2 n+1}{n(n+1)}\left\{a_{n} \pi_{n}(\mu)+b_{n} \tau_{n}(\mu)\right\}  \tag{9a}\\
& S_{2}(\mu)=\sum_{n=1}^{N} \frac{2 n+1}{n(n+1)}\left\{a_{n} \tau_{n}(\mu)+b_{n} \pi_{n}(\mu)\right\} \tag{9b}
\end{align*}
$$

where $\mu=\cos \theta$ and $\theta$ is the angle of scattering.

The most efficient way to calculate the scattering amplitudes is in a loop over $n$, for suming, within which is a loop over $\theta$. (This will be explained when we discuss vectorization, Sec. 7.1.) Every extra operation in the $\theta$-loop can add significantly to the computation time. Each term of the sums (9a) and (9b) requires two multiplies and one add, if the factor $(2 n+1) / n(n+1)$ is incorporated into $a_{n}$ and $b_{n}$ outside the $\theta$-100p. We discovered that we could
eliminate one of the multiplies by calculating, not $S_{1}$ and $S_{2}$ but rather,

$$
\begin{align*}
& S^{+}(\mu)=S_{1}+S_{2}=\sum_{n=1}^{N} \frac{2 n+1}{n(n+1)}\left(a_{n}+b_{n}\right)\left\{\pi_{n}(\mu)+\tau_{n}(\mu)\right\} \\
& S^{-}(\mu)=S_{1}-S_{2}=\sum_{n=1}^{N} \frac{2 n+1}{n(n+1)}\left(a_{n}-b_{n}\right)\left\{\pi_{n}(\mu)-\tau_{n}(\mu)\right\} \tag{10a}
\end{align*}
$$

The factors multiplying $\left(\pi_{n} \pm \tau_{n}\right)$ are formed outside the $\theta$-loop. Then, when the $n$-loop is finished, $S_{1}$ and $S_{2}$ are easily recaptured:

$$
\begin{align*}
& S_{1}(\mu)=\frac{1}{2}\left[s^{+}(\mu)+s^{-}(\mu)\right]  \tag{11a}\\
& S_{2}(\mu)=\frac{1}{2}\left[s^{+}(\mu)-s^{-}(\mu)\right] \tag{11b}
\end{align*}
$$

If $\theta \in[0, \pi / 2]$, then its supplement $\pi-\theta$ has cosine $-\mu$. The angular functions of $\pi-\theta$ are then simply related to the angular functions of $\theta$ (Dave, 1969a):

$$
\begin{aligned}
& \pi_{n}(-\mu)=(-1)^{n+1} \tau_{n}(\mu) \\
& \tau_{n}(-\mu)=(-1)^{n} \tau_{n}(\mu)
\end{aligned}
$$

which leads to

$$
\begin{align*}
& S^{+}(-\mu)=\sum_{n=1}^{N}(-1)^{n+1} \frac{2 n+1}{n(n+1)}\left(a_{n}+b_{n}\right)\left\{\pi_{n}(\mu)-\tau_{n}(\mu)\right\} \\
& S^{-}(-\mu)=\sum_{n=1}^{N}(-1)^{n+1} \frac{2 n+1}{n(n+1)}\left(a_{n}-b_{n}\right)\left\{\pi_{n}(\mu)+\tau_{n}(\mu)\right\} \tag{12a}
\end{align*}
$$

Thus it requires only two extra multiplies in the $\theta$-loop to get $S^{+}(-\mu)$ and $S^{-}(-\mu)$, since the necessary quantities have already been formed in Eq. (10). For this reason, the codes are set up (as were Dave's, 1969a) to calculate the scattering amplitudes at an arbitrary set of
angles in $[0, \pi / 2]$, but only at the supplements of those angles in $[\pi / 2, \pi]$.

This is not as restrictive as it might seem. For example, in order to calculate the phase function moments, or other angular integrals over $[0, \pi]$, this is frequently the required structure of the angular quadrature point set. Also, when taking a dense mesh of angles near $\theta=0$ to resolve the forward diffraction peak, one automatically obtains good resolution of the structure In the glory region. Last, but not least, taking an arbitrary set of angles in $[\pi / 2, \pi]$ may significantly increase computation time, through the necessity of calculating $\pi_{n}(\mu)$ and $\tau_{n}(\mu)$ at those angles.

Note finally that, if one is only interested in the unpolarized approximation, as in many radiative transfer problems, the final step, Eq. (11), is unnecessary, for

$$
\left|s_{1}\right|^{2}+\left|s_{2}\right|^{2}=\left|s^{+}\right|^{2}+\left|s^{-}\right|^{2}
$$

However, the side-stepping of Eq. (11) is not explicitly provided for in the codes, since the savings in computer time would be relatively trivial,

Mie Coefficients (Dave, 1969a, Eqs. 2-3)

$$
\begin{equation*}
a_{n}=\frac{\left\{\frac{A_{n}(z)}{m}+\frac{n}{x}\right\} \psi_{n}(x)-\psi_{n-1}(x)}{\left\{\frac{A_{n}(z)}{m}+\frac{n}{x}\right\} \zeta_{n}(x)-\zeta_{n-1}(x)} \tag{16a}
\end{equation*}
$$

$$
\begin{equation*}
b_{n}=\frac{\left|m A_{n}(z)+\frac{n}{x}\right| \psi_{n}(x)-\psi_{n-1}(x)}{\left|\operatorname{mA}_{n}(z)+\frac{n}{x}\right| \zeta_{n}(x)-\zeta_{n-1}(x)} \tag{16b}
\end{equation*}
$$

Here we have used the Debye and Van de Hulst (1957, Sec. 9.22) notation for the Riccati-Bessel functions $\psi_{n}$ and $\zeta_{n}$, which are defined below along with the function $A_{n}$.

Ricatti-Bessel Functions (Abramowitz/Stegun, Sec. 10.3)

$$
\begin{aligned}
& \psi_{n}(x)=x j_{n}(x) \\
& \chi_{n}(x)=-x y_{n}(x) \\
& \zeta_{n}(x)=\psi_{n}(x)+i \chi_{n}(x)
\end{aligned}
$$

where $j_{n}, y_{n}$ are the familiar spherical Bessel functions. The RiccatiBessel functions satisfy the same recurrence relations as $j_{n}, y_{n}$ (Abramowitz/Stegun, Eq. 10.1.19), namely

$$
\begin{equation*}
\zeta_{n+1}(x)=\frac{2 n+1}{x} \zeta_{n}(x)-\zeta_{n-1}(x) \tag{17}
\end{equation*}
$$

Furthermore, by a simple modification of the cross-product relation for spherical Bessel functions (Abramowitz/Stegun, Eq. 10.1.31), we find

$$
\begin{equation*}
\psi_{n+1}(x)=\frac{\psi_{n}(x) \chi_{n+1}(x)-1}{\chi_{n}(x)} \tag{18}
\end{equation*}
$$

The initial values are (Abramowitz/Stegun, Eq. 10.3.2-3)

$$
\begin{align*}
& \psi_{0}(x)=\sin x  \tag{19a}\\
& x_{0}(x)=\cos x \tag{19b}
\end{align*}
$$

$$
\begin{align*}
& \psi_{1}(x)=\frac{1}{x} \psi_{0}(x)-\chi_{0}(x)  \tag{19c}\\
& \chi_{1}(x)=\frac{1}{x} \chi_{0}(x)+\psi_{0}(x) \tag{19d}
\end{align*}
$$

Careful attention to the accuracy of the $\psi_{n}, X_{n}$ calculation is necessary because: first, the $\psi_{\mathrm{n}}$ up-recurrence is numerically unstable (Abramowitz/Stegun, Introduction .7); second, the convergence of the Mie series hinges on the rapid decay of $\psi_{n}$ to zero when $n \gtrsim x$, with a concomitant blow-up of $X_{n}$, which forces $a_{n}$ and $b_{n}$ (Eq. 16) to zero; third, phenomena like the glory, surface waves, and resonances depend on Mie series terms with $n \gtrsim x$, and hence are particularly sensitive to errors in $\psi_{n}$ or $\chi_{n}$.

Dave (1968a, 1969a) used upward recurrence (Eq. 17) for $\zeta_{n}$, i.e., for both $\psi_{\mathrm{n}}$ and $X_{\mathrm{n}}$. He needed IBM double precision (equivalent to CDC or CRAY single precision) to minimize numerical instability, i.e., to minimize error growth relative to the magnitude of $\psi_{n}$ as the recurrence proceeded. In our own early experiments on a UNIVAC 1108, we also found that up-recurrence on $\psi_{\mathrm{n}}$ deteriorated much too catastrophically for $n>x$ when single precision ( 8 digits) was used, and it was necessary to go over to UNIVAC double precision (18 digits) to achieve satisfactory accuracy.

We tested three possible schemes for computing $\psi_{n} .\left(X_{n}\right.$ is always computed by upward recurrence, which is stable.) These were:
(a) upward recurrence (Eq. 17)
(b) cross product (Eq. 18)
(c) downward recurrence (Abramowitz/Stegun, Sec. 10.5)

All computations were carried out in CDC single precision (14 digits). Scheme (c), which is stable, was used for determining errors in the other two schemes. It was infialized, in the manner of Miller, by

$$
\begin{aligned}
& \psi_{N^{*}+1}=0 \\
& \psi_{N^{*}}=1
\end{aligned}
$$

where $N^{*}$ exceeds the largest index $N$ for which $\psi_{n}$ is needed. We tried both $\mathrm{N}^{*}=1.9 \mathrm{~N}$ and $\mathrm{N}^{*}=1.5 \mathrm{~N}$ and obtained identical values of $\psi_{n}(n=1$ to $N$ ) in either case, which satisfied us that the downrecurrence was an accurate and reliable benchmark.

Schemes (a) and (b) prove to be almost as accurate as downrecurrence for $n<x$ (except as noted below). Only when $n>x$ do they begin to deteriorate, and their errors grow monotonically as n continues to increase beyond $x$. Both schemes invariably have their largest error at $n=N$; these errors are shown in Table 1 for a wide range of $x$ 's. Up-recurrence is always more accurate than the crossproduct relation; typically, its error is two to four times smaller. This situation holds for $\mathrm{n}<\mathrm{N}$ as well.

Furthermore, up-recurrence has an acceptable error, as Table 1 witnesses (remember Table 1 shows worst errors; errors are much smaller for $n<N$ ). And since down-recurrence requires considerably more computation, more storage, and is also subject to overflow failure (because $\psi_{\mathrm{n}}$ grows when recursed downward), up-recurrence on $\psi_{\mathrm{n}}$ was the obvious choice for our algorithms. Thus, in the end, we made the same choice as Dave, but our confidence in that choice was considerably raised.

Table 1. Percent error in $\psi_{N}(x)$, as computed by two different methods, where $N$ is the largest index required in the Mie series. Exact values of $\psi_{N}$ were from downward recurrence. All computations done in CRAY-1 single precision.

| x | N | $\begin{aligned} & \text { \% error in } \psi \\ & \text { from up-recurrence } \end{aligned}$ | $\%$ error in $\psi_{N}$ from cross-product |
| :---: | :---: | :---: | :---: |
| 1 | 5 | $1.7 \times 10^{-5}$ | $2.5 \times 10^{-5}$ |
| 5 | 12 | $8.2 \times 10^{-5}$ | $17 \times 10^{-5}$ |
| 10 | 19 | $2.0 \times 10^{-4}$ | $-13 \times 10^{-4}$ |
| 20 | 31 | $2.7 \times 10^{-4}$ | $5.6 \times 10^{-4}$ |
| 40 | 54 | $7.2 \times 10^{-4}$ | $15 \times 10^{-4}$ |
| 80 | 98 | $1.9 \times 10^{-3}$ | $6.0 \times 10^{-3}$ |
| 200 | 224 | $1.4 \times 10^{-3}$ | $4.5 \times 10^{-3}$ |
| 400 | 430 | $2.4 \times 10^{-3}$ | $5.5 \times 10^{-3}$ |
| 600 | 634 | $5.6 \times 10^{-4}$ | $266 \times 10^{-4}$ |
| 800 | 837 | $2.6 \times 10^{-3}$ | $3.5 \times 10^{-3}$ |
| 1,000 | 1,040 | $3.6 \times 10^{-3}$ | $10 \times 10^{-3}$ |
| 2,000 | 2,050 | $5.5 \times 10^{-3}$ | $15 \times 10^{-3}$ |
| 4,000 | .4,063 | 0.010 | 0.047 |
| 8,000 | 8,080 | 0.026 | 0.090 |
| 12,000 | 12,091 | 0.060 | 0.095 |
| 16,000 | 16,100 | 0.041 | -0.17 |

There are also occasional values of $n<x$ at which the accuracy of both schemes (a) and (b) is reduced. These are invariably where $\psi_{\mathrm{n}}$ falls several orders of magnitude below its neighboring values $\psi_{n-1}$ and $\psi_{n+1}$. In all such cases, up-recurrence is still preferable to the cross-product relation and still has acceptable error.

Since the zero-subscript feature is not widely available in FORTRAN, the quantities actually calculated in the codes are $\hat{\psi}_{n}=\psi_{n-1}$ and $\hat{\zeta}_{\mathrm{n}}=\zeta_{\mathrm{n}-1}\left(X_{\mathrm{n}}\right.$ is never used explicitly).

An (Logarithmic Derivative of $\psi_{n}$ )

$$
A_{n}(z) \equiv \frac{\psi_{n}^{\prime}(z)}{\psi_{n}(z)}
$$

This can be calculated by up-recurrence (Dave, 1969a)

$$
\begin{equation*}
A_{n}(z)=-\frac{n}{z}+\frac{1}{\frac{n}{z}-A_{n-1}(z)} \quad(n=2, \ldots, N) \tag{20}
\end{equation*}
$$

with initial value

$$
\begin{equation*}
A_{1}(z)=-\frac{1}{z}+\frac{\tan z}{\frac{1}{z} \tan z-1} . \tag{21}
\end{equation*}
$$

Dave worried about two problem cases. First, $z=k \pi$ for any integer $k \neq 0$ leads to $A_{0}=\cot z=\infty$; but we never actually need $A_{0}$, and $A_{1}$, written as in Eq. (21), is perfectly well-conditioned at $z=k \pi$. Second, if $\tan z$ is written simplistically as $\sin z / \cos z, \exp (\operatorname{Im}(z))$ will occur in both numerator and denominator, causing overflow if $\operatorname{Im}(z)$ is large; but we circumvent this problem by writing $\tan z$ as

$$
\tan (x+i y)=\frac{2 e^{2 y} \sin 2 x+i\left(e^{4 y}-1\right)}{2 e^{2 y} \cos 2 x+1+e^{4 y}}
$$

which is calculated by the function CTAN listed in Appendix $I$. There remains the problem that $\tan z$ blows $u p$ when $z$ is an odd multiple of $\pi / 2$, but because of round-off in computing the denominator this never actually occurs.

Kattawar and Plass (1967) pointed out the instability in uprecurrence of $A_{n}$ when $\operatorname{Im}(z)$ is appreciable. They suggested down-recurrence

$$
\begin{equation*}
A_{n-1}(z)=\frac{n}{z}-\frac{1}{\frac{n}{z}+A_{n}(z)}\left(n=N^{\prime}, \ldots, N, \ldots, 2\right) \tag{22}
\end{equation*}
$$

as an alternative, and showed that it was stable. However, neither they nor subsequent investigators offered a clear-cut criterion as to when down-recurrence should be used. We have developed such a criterion, which is described in Sec. 5.

Kattawar and Plass, Dave (1969a), and many subsequent investigators initialized the down-recurrence by

$$
A_{N}(z)=0
$$

where, in principle, one must have $N^{\prime} \gg|z|$. Dave found that

$$
N^{\prime}=1.1|z|+1
$$

was sufficient. Of course, this causes more values of $A_{n}$ to be calculated than are actually needed in the Mie series, since $N^{\prime}>N$ and possibly $N^{\prime} \gg N$.

We found it preferable to initialize the down-recurrence by calculating $A_{N}(z)$ correctly to 5 or 6 significant digits, using the newly-developed method of Lentz (1976) discussed below. Besides being more aesthetic, this results in less computation and greater
code reliability, especially in difficult cases (e.g., $|m| \gg 1$ or $|m-1| \ll 1$ ) .

We note in passing that our early experiments on a UNIVAC 1108 showed that neither up- nor down-recurrence of $A_{n}$ was sufficiently accurate in its 8 -digit single precision. The down-recurrence sometimes deteriorated badly as $n \rightarrow 1$. UNIVAC double precision of 18 digits had to be employed.
$\mathrm{A}_{\mathrm{N}}$ from Lentz Method
The standard continued fraction representation of $A_{N}$, which follows directly from the down-recurrence (22), is

$$
\begin{equation*}
A_{N}(z)=\lim _{i \rightarrow \infty}\left[a_{1}, a_{2}, \ldots, a_{i}\right] \tag{23}
\end{equation*}
$$

where

$$
\begin{align*}
& {\left[a_{1}, a_{2}, \ldots, a_{i}\right]=a_{1}+\frac{1}{a_{2}}+\cdots+\frac{1}{a_{i}}}  \tag{24}\\
& a_{1}=(N+1) / z  \tag{25a}\\
& a_{k}=(-1)^{k+1}(2 N+2 k-1) / z \quad(k=2,3, \ldots) . \tag{25b}
\end{align*}
$$

But this is really no different from Dave's procedure; setting $A_{N^{\prime}}=0$ amounts to setting $A_{N}=\left[a_{1}, a_{2}, \ldots, a_{N^{\prime}-N}\right]$. Thus many terms are frequently required for convergence of the continued fraction (24), and recursive computation is impossible because $\left[a_{1}, \ldots, \dot{a}_{i+1}\right.$ ] is not simply related to a few prior values of $\left[a_{1}, \ldots, a_{1}\right]$ but must be computed completely anew.

Lentz has discovered a product representation of Eq. (24) which can be computed recursively, and which requires, in just those cases
where down-recurrence of $A_{n}$ is necessary, far fewer steps than Dave's method:

$$
\begin{equation*}
\left[a_{1}, \ldots, a_{1}\right]=\prod_{k=1}^{1} T_{k} \tag{26}
\end{equation*}
$$

where

$$
\begin{align*}
& T_{k}= \begin{cases}a_{1} & k=1 \\
N_{k} / D_{k} & k>1\end{cases}  \tag{27}\\
& N_{k}=\left[a_{k}, \ldots, a_{1}\right]  \tag{28a}\\
& D_{k}=\left[a_{k}, \ldots, a_{2}\right] \tag{28b}
\end{align*}
$$

and where, by definition,

$$
\left[a_{j}, a_{j}\right] \equiv a_{j}
$$

Unlike Eq. (24), Eq. (26) is well-suited to recursive computation in that

$$
\begin{equation*}
\left[a_{1}, \ldots, a_{i}\right]=\left[a_{1}, \ldots, a_{i-1}\right] T_{i} \tag{29}
\end{equation*}
$$

and both the numerator and denominator of $T_{1}$ follow immediately from the numerator and denominator, respectively, of $T_{1-1}$ :

$$
\begin{align*}
& N_{i}=a_{i}+\frac{1}{N_{i-1}}  \tag{30a}\\
& D_{i}=a_{i}+\frac{1}{D_{i-1}} \tag{30b}
\end{align*}
$$

We deem the iteration to have converged when $T_{i}=1$ to a certain degree of accuracy, 1.e., when

$$
\begin{equation*}
\left|\operatorname{Re}\left(T_{i}\right)-1\right|<\varepsilon_{2} \quad \text { and } \quad\left|I_{m}\left(T_{i}\right)\right|<\varepsilon_{2} \tag{31}
\end{equation*}
$$

where we generally take $\varepsilon_{2}=10^{-8}$ and, as a result, obtain at least 5 to 6 significant figures in $A_{N}$.

It may occur that

$$
\begin{equation*}
\left|\frac{N_{i}}{a_{i}}\right|<\varepsilon_{1} \quad \text { or } \quad\left|\frac{D_{i}}{a_{i}}\right|<\varepsilon_{1} \tag{32}
\end{equation*}
$$

where $\varepsilon_{1} \ll 1$ (we generally take $\varepsilon_{1}=10^{-2}$ ); this means that Eq. (30) has resulted in loss of significant digits in $N_{i}$ and/or $D_{i}$, which would be magnified in $N_{i+1}$ and/or $D_{i+1}$. In this case, we can sidestep the 111 -conditioning by skipping the convergence test (31) and striding two iterations instead of one; i.e., we go immediately to

$$
\begin{equation*}
\left[a_{1}, \ldots, a_{i+1}\right]=\left[a_{1}, \ldots, a_{i-1}\right] T_{i} T_{i+1} \tag{33}
\end{equation*}
$$

where

$$
\begin{align*}
& T_{i} T_{i+1}=\frac{\xi_{1}}{\xi_{2}}  \tag{34a}\\
& \xi_{1} \equiv 1+a_{i+1} N_{i}  \tag{34b}\\
& \xi_{2} \equiv 1+a_{i+1} D_{i} \tag{34c}
\end{align*}
$$

Unlike the ratios $T_{i}$ or $T_{i+1}$ individually, their product (34a) is well-conditioned. In order to re-start the iteration (30) without requiring the ill-conditioned results $N_{i+1}$ or $D_{i+1}$ we can use Eq. (30) twice to obtain

$$
\begin{align*}
& N_{i+2}=a_{i+2}+\frac{1}{a_{i+1}+\frac{1}{N_{i}}}=a_{i+2}+\frac{N_{i}}{\xi_{1}}  \tag{35a}\\
& D_{i+2}=a_{i+2}+\frac{D_{i}}{\xi_{2}} . \tag{35b}
\end{align*}
$$

In Table 2 is shown, for selected values of $m$ and $x$, the number of iterations of Lentz's method necessary to achieve convergence, i.e., the value of $i$ such that condition (31) is satisfied for either $\varepsilon_{2}=10^{-6}$ or $\varepsilon_{2}=10^{-8}$. Note that, for $\mathrm{x} \geq 100$ and $\operatorname{Im}(m)$ smal1 enough, the number of iterations is roughly $|m-I| x$. This is about the same number of iterations required by Dave's method $[(1.1|m|-1) x]$. But these cases of small $\operatorname{Im}(m)$ can be handled by up-recurrence (see Sec. 5). And for larger values of $\operatorname{Im}(m)$, Lentz's method requires far fewer iterations than Dave's.

## Angular Functions

$$
\begin{align*}
& \pi_{n}(\mu) \equiv P_{n}^{\prime}(\mu) \\
& \tau_{n}(\mu) \equiv \mu \pi_{n}(\mu)-\left(1-\mu^{2}\right) \pi_{n}^{\prime}(\mu) \tag{36}
\end{align*}
$$

(Dave, 1969a) where $P_{n}$ is a Legendre polynomial. These functions can most simply be calculated by upward recurrence, which is numerically stable (Abramowitz/Stegun, Introduction. 7). Since these recurrences are buried in the $\theta$-loop where $\mathrm{S}^{ \pm}$(Eq. 10) are calculated, formulating them more efficiently can lead to a substantial saving of computer time. Dave (1969a) gives particular forms for these recurrences; but we have discovered better ones which we derive below.

The usual 3-term recurrence relation for Legendre polynomials is

$$
(n+1) P_{n+1}(\mu)=(2 n+1) \mu P_{n}(\mu)-n P_{n-1}(\mu)
$$

Differentiating this, and using the relation

$$
\pi_{n+1}(\mu)-\pi_{n-1}(\mu)=(2 n+1) p_{n}(\mu)
$$

Table 2. Number of Lentz method iterations (Eq. 29) necessary to converge to $A_{N}(m x)$ for a range of size parameters $x$ and refractive indices m. First figure refers to $\varepsilon_{2}=10^{-6}$, second (in parentheses) to $\varepsilon_{2}=10^{-8}$.

| x | N | m | number of Lentz method iterations to get $A$ (mx) |
| :---: | :---: | :---: | :---: |
| 1 | 5 | $\begin{aligned} & 1.05-\left\{10^{-6}-1\right\}_{i} \\ & 1.95-\left\{10^{-6}-1\right\} i \end{aligned}$ | $\begin{aligned} & 4(5) \\ & 5(6) \end{aligned}$ |
| 10 | 19 | $1.05-\left\{10^{-6}-1\right\}_{i}$ $1.95-\left\{10^{-6}-1\right\}{ }_{i}$ | $\begin{aligned} 7-8 & (8-10) \\ 11-12 & (14) \end{aligned}$ |
| 100 | 119 | $1.05-\left\{10^{-6}-1\right\}_{i}$ $1.50-\left\{10^{-6}-10^{-2}\right\}_{i}$ $1.50-0.1 i$ | $\begin{aligned} 13 & (16) \\ 51-52 & (55-57) \\ 40 & (46) \end{aligned}$ |
|  |  | $1.50-\mathrm{i}-6{ }^{-2}$ | 18 (22) |
|  |  | $1.95-\left\{10^{-6}-10^{-2}\right\}_{i}$ | 97-99 (102-103) |
|  |  | $1.95-0.1$ i | 79 (87) |
|  |  | 1.95 - i | 25 (31) |
| 1,000 | 1,040 | $1.05-\left\{10^{-6}-10^{-3}\right\}_{i}$ $1.05-10_{i}$ | $\begin{array}{r} 59-50(58) \\ 44(53) \end{array}$ |
|  |  | $1.05-0.1 \mathrm{i}$ | 25 (32) |
|  |  | 1.05-i ${ }^{\text {- }}$ - ${ }^{\text {c }}$ - | 15 (20) |
|  |  | $1.50-\left\{10^{-6}-10^{-3}\right\}_{i}$ | 500-502 (509-512) |
|  |  | $1.50-10^{-2} \mathrm{i}$ | 459 (479) |
|  |  | $1.50-0.1 \mathrm{i}$ | 104 (135) |
|  |  | $1.50-1$ | 22 (28) |
|  |  | $1.95-\left\{10_{-2}^{-6}-10^{-3}\right\}_{i}$ | 953-956 (964-967) |
|  |  | $1.95-10^{-2} \mathrm{i}$ | 880 (919) |
|  |  | $1.95-0.1$ i | 203 (254) |
|  |  | 1.95 - i | 33 (42) |
| 10,000 | 10,086 | $1.05-\left\{10_{-2}^{-6}-10^{-4}\right\}_{i}$ | 492-495 (510-513) |
|  |  | $1.05-10^{-2} \mathrm{i}$ | 183 (232) |
|  |  | 1.05-0.1 i | 31 (40) |
|  |  |  | 16 (20) |
|  |  | $1.50-\left\{10^{-6}-10^{-4}\right\}$ i | 4496-5001 (5017-5021) |
|  |  | $1.50-10^{-2} \mathrm{i}$ | 1092 (1384) |
|  |  | 1.50-0.1 i | 124 (161) |
|  |  |  | 23 (30) |
|  |  | $1.95-\left\{10^{-6}-10^{-4}\right\}_{i}$ | 9501-9510 (9525-9533) |
|  |  | $1.95-10^{-2} \mathrm{i}$ | 2055 (2599) |
|  |  | 1.95-0.1 i | 236 (309) |
|  |  | 1.95 - i | 34 (44) |

from Whittaker and Watson (1965, chapter 15) leads to

$$
n \pi_{n+1}(\mu)=(2 n+1) \mu \pi_{n}(\mu)-(n+1) \pi_{n-1}(\mu)
$$

which for our own purposes we write in the strung-out form

$$
\begin{align*}
s & \equiv \mu \pi_{n}(\mu)  \tag{37a}\\
t & \equiv s-\pi_{n-1}(\mu)  \tag{37b}\\
\pi_{n+1}(\mu) & =s+\left(\frac{n+1}{n}\right) t \tag{37c}
\end{align*}
$$

Written thus, only two multiplies and two adds are required, since the purely numerical factor $(n+1 / n)$ may be precalculated.

$$
\begin{aligned}
& \text { For } \tau_{n} \text {, differentiate the relation } \\
& \left(1-\mu^{2}\right) \pi_{n}(\mu)=n\left[P_{n-1}(\mu)-\mu P_{n}(\mu)\right]
\end{aligned}
$$

and use the relation

$$
n P_{n}(\mu)=\mu \pi_{n}(\mu)-\pi_{n-1}(\mu)
$$

(both from Whittaker/Watson, chapter 15) to obtain

$$
\left(1-\mu^{2}\right) \pi_{n}^{\prime}(\mu)=2 \mu \pi_{n}(\mu)-(n+1)\left[\mu \pi_{n}(\mu)-\pi_{n-1}(\mu)\right]
$$

Putting this into the definition (36) of $\tau_{n}$ leads to

$$
\begin{align*}
\tau_{n}(\mu) & =(n+1) t-s  \tag{38a}\\
& =n t-\pi_{n-1}(\mu) \tag{38b}
\end{align*}
$$

where $t$ and $s$ were defined in Eq. (37). This requires only one multiply and one add, for a total of three multiplies and three adds to calculate $\pi_{n+1}$ and $\tau_{n}$. This compares with six multiplies and four adds in Dave's (1969a) recurrences.

The recurrences are initialized by

$$
\begin{align*}
& \pi_{0}=0  \tag{39a}\\
& \pi_{1}=1 . \tag{39b}
\end{align*}
$$



Yet, in spite of this simple form, we were unable to come up with a recurrence directly for $\pi_{n} \pm \tau_{n}$, which avoided calculating $\pi_{n}$ and $\tau_{n}$ individually, and was at the same time more efficient than Eqs. (3738). This must remain a challenge for future investigators.

By using a fixed set of angles $\mu_{m}$, one could precalculate the angular functions once for all, as matrices $A_{n m} \equiv \pi_{n}\left(\mu_{m}\right)$ and $B_{n m} \equiv \tau_{n}\left(\mu_{m}\right)$. This might offer advantages if one were to restrict oneself to Mie series no longer than $\sim 1000$ terms and to no more than 50-100 angles. But outside these limits the computer storage requirements would be prohibitive; and even with only 100 terms and 50 angles, $A_{n m}$ and $B_{n m}$ would take up a total of 10,000 words of storage, which might well strain a smaller computer. Furthermore, a fixed set of angles would be too inflexible for many applications. Thus, in the interests of a general purpose code, we have rejected this approach.
4. MIE SCATTERING FORMULAE-SMALL PARTICLE LIMIT

It is necessary to compute the small-particle (Rayleigh) case, $x \rightarrow 0$, separately, not only because $1 / x$ occurs in several places in the Mie formulae, but because:
(a) the calculation of $A_{n}$ is numerically ill-conditioned as $x \rightarrow 0 ; e . g .$,
$\mathrm{A}_{1}(z)=-\frac{1}{z}+\frac{1}{\frac{1}{z}-\frac{1}{\tan z}}=\frac{2}{z}+0(z)$
and the subtraction of $1 / \tan z$ from $1 / z$ causes significant digits to be lost; similarly,

$$
A_{2}(z)=-\frac{2}{z}+\frac{1}{\frac{2}{z}-A_{1}(z)}
$$

and the subtraction of $A_{1}(z)$ from $2 / z$ further compounds the ill-conditioning.
(b) The subtraction in the upward recurrence for $\psi_{\mathrm{n}}$ loses significant digits, and the ill-conditioning rapidly compounds; e.g.,

$$
\begin{aligned}
\psi_{1}(x) & =\frac{1}{x} \sin x-\cos x=\left(1-\frac{x^{2}}{6}+\ldots\right)-\left(1+\frac{x^{2}}{2}+\ldots\right) \\
& =\frac{x^{2}}{3}+\ldots \\
\psi_{2}(x) & =\frac{3}{x} \psi_{1}(x)-\psi_{0}(x)=\frac{3}{x}\left(\frac{x^{2}}{3}+\ldots\right)-\sin x \\
& =(x+\ldots)-(x+\ldots) .
\end{aligned}
$$

(c) The subtraction in the numerator of $b_{n}$ becomes ill-conditioned.

The $\mathrm{x} \rightarrow 0$ formulae are also computationally faster, which would make them desirable even were they unnecessary. We should bear in mind Van de Hulst's (1957, Sec. 10.3) warning, however:
"Aside from their simplicity, they (the small-x formulae) have little advantage. They describe the very first deviations from Rayleigh scattering, but further deviations appear very soon after the first have become prominent, so that the full Mie formulae have to be used."

In view of this warning, we set ourselves the modest goal of applying the $\mathrm{x} \rightarrow 0$ formulae only over a range of x sufficient to avoid serious ill-conditioning and to give six significant digits in all Mie quantities. The $x \rightarrow 0$ formulae which we found most suitable, and the range over which they are to be applied, are given below.

The obvious approach is to expand the Mie coefficients (Eq. 16) in powers of the size parameter $x$. It is necessary to expand the dominant coefficient $a_{1}$ at least out to $O\left(x^{6}\right)$, or else the extinction efficiency (Eq: 6) for $\operatorname{Im}(m) \ll 1$ will be vanishingly small; for the first nonnegligible contribution to $Q_{\text {ext }}$ is $O\left(x^{6}\right)$ in such cases. But by carrying $a_{1}$ out to $O\left(x^{6}\right)$, one must for consistency keep $a_{2}$ and $b_{1}$ also, for they are both $O\left(x^{5}\right)$. The remaining values of $a_{n}$ and $b_{n}$ are $O\left(x^{7}\right)$ or higher. ${ }^{\dagger}$

Some authors insert the expansions for $a_{1}, a_{2}$ and $b_{1}$ into Eqs. (6-9) and continue expanding and truncating those series. This is useful for
$\dagger$ The asymptotic forms as $\mathrm{x} \rightarrow 0$ are:

$$
\begin{aligned}
& a_{n} \sim i \frac{n+1}{(2 n-1)!!(2 n+1)!!} \frac{m^{2}-1}{n^{2}+n+1} x^{2 n+1} \\
& b_{n} \sim i \frac{m^{2}-1}{(2 n+3)[(2 n+1)!!]^{2}} x^{2 n+3} .
\end{aligned}
$$

seeing the leading terms, but every additional step of expansion/ truncation must cause additional error, so we have chosen instead to use Eqs. (6-9) as is, namely:

$$
\begin{align*}
& Q_{\text {ext }}=6 x\left\{\operatorname{Re}\left(\hat{a}_{1}+\hat{b}_{1}\right)+\frac{5}{3} \operatorname{Re}\left(\hat{a}_{2}\right)\right\}  \tag{40a}\\
& Q_{\text {sca }}=6 x^{4} T  \tag{40b}\\
& g=\operatorname{Re}\left[\hat{a}_{1}\left(\hat{a}_{2}+\hat{b}_{1}\right) *\right] / T  \tag{40c}\\
& S_{1}(\mu)=\frac{3}{2} x^{3}\left[\hat{a}_{1}+\left(\hat{b}_{1}+\frac{5}{3} \hat{a}_{2}\right) \mu\right]  \tag{40d}\\
& S_{2}(\mu)=\frac{3}{2} x^{3}\left[\hat{b}_{1}+\hat{a}_{1} \mu+\frac{5}{3} \hat{a}_{2}\left(2 \mu^{2}-1\right)\right] \tag{40e}
\end{align*}
$$

where

$$
\begin{equation*}
T \equiv\left|\hat{a}_{1}\right|^{2}+\left|\hat{b}_{1}\right|^{2}+\frac{5}{3}\left|\hat{a}_{2}\right|^{2} \tag{40f}
\end{equation*}
$$

and where a factor of $x^{3}$ has been taken out of each coefficient,

$$
\hat{a}_{1} \equiv \frac{a_{1}}{x^{3}}, \quad \text { etc. }
$$

in order to avoid $\frac{0}{0}$ singularities as $x \rightarrow 0$.
An additional advantage of Eqs. (40) is that, unlike many of the expansions one finds in the literature, they are internally consistent, being simply special cases of the Mie formulae with $a_{3}=a_{4}=\ldots=b_{2}=b_{3}=\ldots=0$. For example, Eqs. (40a-c) can be derived directly from Eqs. (40d,e).

Comparisons were made between the exact Mie results and Eqs. (40), using two different approximations for $\hat{a}_{1}, \hat{a}_{2}$ and $\hat{b}_{1}$, for a wide range of values of $x$ and $m$. First, we tried the 3 -term expansion of $a_{1}$ and the 1 -term expansions of $a_{2}$ and $b_{1}$, as given by Van de Hulst (1957, Sec. 10.3), to wit,

$$
\begin{align*}
& \hat{a}_{1}=i \frac{2}{3} \frac{m^{2}-1}{m^{2}+2}\left[1+\frac{3}{5} \frac{m^{2}-2}{m^{2}+2} x^{2}-i \frac{2}{3} \frac{m^{2}-1}{m^{2}+2} x^{3}+0\left(x^{4}\right)\right] \\
& \hat{b}_{1}=i \frac{m^{2}-1}{45} x^{2}+0\left(x^{4}\right)  \tag{41a}\\
& \hat{a}_{2}=\frac{i}{15} \frac{m^{2}-1}{2 m^{2}+3} x^{2}+0\left(x^{4}\right) \tag{41c}
\end{align*}
$$

(Errors may still be found in such results; e.g., Kerker (1969, Sec. 3.9) has the wrong sign for $b_{1}$.) These were found to give our desired 6-digit accuracy for all Mie quantities, provided $\operatorname{Im}(\mathrm{m})$ was large enough. But when $\operatorname{Im}(\mathbb{m}) \ll 1$, the accuracy of $Q_{\text {ext }}, \operatorname{Re}\left(S_{1}\right)$ and $\operatorname{Re}\left(S_{2}\right)$ deteriorated to as little as 3 digits even for very small values of $x$. Examples of such errors are shown, for $Q_{\text {ext }}$, in Table 3. The remaining quantities, like $Q_{s c a}$ or $\operatorname{Im}\left(S_{1}\right)$, retained 6-digit accuracy out to $x \sim 0.08$.

We diagnosed the problem to be that $Q_{\text {ext }}, \operatorname{Re}\left(S_{1}\right)$ and $\operatorname{Re}\left(S_{2}\right)$ all depend only on the real parts of $\hat{a}_{1}, \hat{a}_{2}$ and $\hat{b}_{1}$. For Eqs. (41), with $\operatorname{Im}(m) \ll 1$, only the smallest-order term in $\hat{a}_{1}$ contributes to $\operatorname{Re}\left(\hat{a}_{1}\right)$, and both $\operatorname{Re}\left(\hat{a}_{2}\right)$ and $\operatorname{Re}\left(\hat{b}_{1}\right)$ are nearly zero. Clearly a correction term would be desirable in $\operatorname{Re}\left(\hat{a}_{1}\right)$, and presumably in $\hat{a}_{2}$ and $\hat{b}_{1}$ as well. Such a correction term can only be obtained by continuing the expansion of $\hat{a}_{1}$ out to $0\left(x^{5}\right)$. We also realized that it would be preferable to leave $\hat{a}_{1}$ in quotient form, that is, to just expand its numerator and denominator in Eq. (16). The further expansion of the quotient as a polynomial is just an extra and unnecessary step of approximation. Hence we used the following formulation:

Table 3. Values of $Q_{\text {ext }}$ in the small-particle limit, as given by Mie theory and by Eq. (40) with two approximations for $a_{1}$, $a_{2}$ and $b_{1}$. The digits in error are underscared for each approximation.

| x | m | Eqs. $(40,41)$ | Eqs. $(40,42)$ | Exact |
| :---: | :---: | :---: | :---: | :---: |
| 0.02 | $\begin{aligned} & 1.5-10^{-6} \mathrm{i} \\ & 1.95-10^{-6} \mathrm{i} \\ & 1.95-10^{-5}{ }_{i} \end{aligned}$ | $\begin{aligned} & 7.677 \underline{94} \times 10^{-8} \\ & 1.27341 \times 10^{-7} \\ & 3.77644 \times 10^{-7} \end{aligned}$ | $\begin{aligned} & 7.67805 \times 10^{-8} \\ & 1.27355 \times 10^{-7} \\ & 3.77659 \times 10^{-7} \end{aligned}$ | $\begin{aligned} & 7.67805 \times 10^{-8} \\ & 1.27355 \times 10^{-7} \\ & 3.77659 \times 10^{-7} \end{aligned}$ |
| 0.04 | $\begin{aligned} & 1.05-10^{-6} i \\ & 1.5-10^{-6} i \\ & 1.5-10^{-4} i \\ & 1.95-10^{-4} i \end{aligned}$ | $\begin{aligned} & 1.12183 \times 10^{-7} \\ & 6.7 \underline{337} \times 10^{-7} \\ & 8.57 \underline{01} \times 10^{-6} \\ & 7.16 \underline{164} \times 10^{-6} \end{aligned}$ | $\begin{aligned} & 1.12179 \times 10^{-7} \\ & 6.70403 \times 10^{-7} \\ & 8.57007 \times 10^{-6} \\ & 7.16259 \times 10^{-6} \end{aligned}$ | $\begin{aligned} & 1.12179 \times 10^{-7} \\ & 6.70403 \times 10^{-7} \\ & 8.57008 \times 10^{-6} \\ & 7.16259 \times 10^{-6} \end{aligned}$ |
| 0.08 | $\begin{aligned} & 1.05-10^{-6} i \\ & 1.5-10^{-6} i \\ & 1.5-10^{-4} i \\ & 1.95-10^{-4} i \end{aligned}$ | $\begin{aligned} & 3.28743 \times 10^{-7} \\ & 9.60869 \times 10^{-6} \\ & 2.54 \underline{505} \times 10^{-5} \\ & 3.66727 \times 10^{-5} \end{aligned}$ | $\begin{aligned} & 3.28478 \times 10^{-7} \\ & 9.61291 \times 10^{-6} \\ & 2.54547 \times 10^{-5} \\ & 3.67335 \times 10^{-5} \end{aligned}$ | $\begin{aligned} & 3.28478 \times 10^{-7} \\ & 9.61292 \times 10^{-6} \\ & 2.54547 \times 10^{-5} \\ & 3.67336 \times 10^{-5} \end{aligned}$ |
| 0.20 | $\begin{aligned} & 1.05-0.01 i \\ & 1.05-i \\ & 1.95-0.01 i \\ & 1.95-i \end{aligned}$ | $\begin{aligned} & 5.25292 \times 10^{-3} \\ & 5.79 \underline{042} \times 10^{-1} \\ & 3.8 \underline{8981} \times 10^{-3} \\ & 2.5854 \times 10^{-1} \end{aligned}$ | $\begin{aligned} & 5.25256 \times 10^{-3} \\ & 5.78532 \times 10^{-1} \\ & 3.905 \underline{26} \times 10^{-3} \\ & 2.586 \underline{26} \times 10^{-1} \end{aligned}$ | $\begin{aligned} & 5.25263 \times 10^{-3} \\ & 5.78539 \times 10^{-1} \\ & 3.90548 \times 10^{-3} \\ & 2.58637 \times 10^{-1} \end{aligned}$ |

$$
\begin{align*}
\hat{a}_{1}= & 2 i \frac{m^{2}-1}{3} \frac{N_{1}}{D_{1}}  \tag{42a}\\
N_{1} \equiv & 1-\frac{1}{10} x^{2}+\frac{4 m^{2}+5}{1400} x^{4}+0\left(x^{6}\right) \\
D_{1} \equiv & m^{2}+2+\left(1-\frac{7 m^{2}}{10}\right) x^{2}-\frac{8 m^{4}-385 m^{2}+350}{1400} x^{4} \\
& +2 i \frac{m^{2}-1}{3} x^{3}\left(1-\frac{1}{10} x^{2}\right)+0\left(x^{6}\right) \\
\hat{b}_{1}= & i \frac{m^{2}-1}{45} x^{2} \frac{1+\frac{2 m^{2}-5}{70} x^{2}+0\left(x^{4}\right)}{1-\frac{2 m^{2}-5}{30} x^{2}+0\left(x^{4}\right)}  \tag{42b}\\
\hat{a}_{2}= & i \frac{m^{2}-1}{15} x^{2} \frac{1-\frac{1}{14} x^{2}+0\left(x^{4}\right)}{2 m^{2}+3-\frac{2 m^{2}-7}{14} x^{2}+0\left(x^{4}\right)} \tag{42c}
\end{align*}
$$

To be consistent, and because the amount of extra computation is trivial, we have expanded $\hat{b}_{1}$ and $\hat{a}_{2}$ to the same order as $\hat{a}_{1}$, even though nefther one acquires thereby a significant real part when $\operatorname{Im}(\mathrm{m}) \ll 1$, and therefore neither one significantly improves the approximation to $Q_{\text {ext }}$ in such cases. But we have ignored $\hat{b}_{2}$ and $\hat{a}_{3}$, the leading terms of whose expansions contribute at the $O\left(x^{4}\right)$ level; these leading terms are purely imaginary when $\operatorname{Im}(\mathbb{m})=0$, and therefore do not improve the approximation to $Q_{\text {ext }}$. Carrying $\hat{b}_{2}$ and $\hat{a}_{3}$ only extends the range of the approximation slightly (cf. the Van de Hulst quote earlier in this section) and simply would not be worthwhile.

Even though the neglect of $\hat{b}_{2}$ and $\hat{a}_{3}$ is a technical inconsistency, the practical effect is nil. As Table 3 indicates, Eqs. (42) lead to a dramatic improvement in accuracy over Eqs. (41) in both problem $(\operatorname{Im}(m) \ll 1)$ and normal cases. The more accurate formulation retains

4-5 significant digits at $x=0.2$, and $2-3$ signiffcant digits even at $x=0.5$. In order to retain 6 significant digits, we selected the rather conservative criterion that the small-particle formulae (Eqs. 40 and 42) are to be used whenever

$$
\begin{equation*}
|m| x \leq 0.1 \tag{43}
\end{equation*}
$$

where the factor $|m|$ was included based on the well-known fact (cf. Kerker et al., 1978), which is also apparent in Eqs. (42), that the approximation breaks down as $|m|$ increases.
5. $A_{n}$ UP-RECURRENCE CRITERION

Kattawar and Plass (1967), Dave (1969a) and subsequent investigators were aware that up-recurrence for $A_{n}$ may fall, but were unclear as to exactly when this would occur, except that $\operatorname{Im}(m)$ had to be significant and $x \gg 1$ (the latter condition ensures sufficiently many iterations for the instability to develop).

To determine the precise regions of size parameter $x$ and refractive index $m$ wherein up-recurrence is satisfactory, an extensive comparison was made between exact Mie results and results obtained using uprecurrence for $A_{n}$. Exact Mie results were generated using downrecurrence for $A_{n}$, which is always stable, and a stringent convergence criterion of $\varepsilon_{2}=10^{-10}$ for the Lentz method calculation of $A_{N}$. Uprecurrence was regarded as failing whenever its concomitant values of $Q_{\text {ext }}, Q_{\text {sca }}$ or $g$ (Eqs. 6-8) had relative errors exceeding $10^{-6}$, or its scattered intensity or degree of polarization

$$
\begin{align*}
& i_{1}+i_{2}=\left|s_{1}\right|^{2}+\left|s_{2}\right|^{2}  \tag{44}\\
& d_{p o l}=\frac{\left|s_{2}\right|^{2}-\left|s_{1}\right|^{2}}{\left|s_{2}\right|^{2}+\left|s_{1}\right|^{2}} \tag{45}
\end{align*}
$$

had relative errors exceeding $10^{-5}$ at any of 61 Lobatto quadrature angles. (These angles are such that they cluster in the forward peak $\left(\theta \gtrsim 0^{\circ}\right)$ and glory ( $\theta \lesssim 180^{\circ}$ ) regions and are relatively more sparse around $\theta=90^{\circ}$.)

In practice, it was always these angular functions which first heralded failure; the relative errors in $Q_{\text {ext }}, Q_{s c a}$ and $g$ were always between $10^{-12}$ and $10^{-8}$ when some angular function error reached $10^{-5}$.

This is because there is no cancellation in the $Q_{\text {ext }}, Q_{\text {sca }}, g$ series, whereas at some angles the $n<x$ terms in the $S_{1}, S_{2}$ series almost cancel, leaving only the $n>x$ terms, which are most affected by $A_{n}$ up-recurrence instability.

The calculation was structured in the form of an upward search on $m_{i m}$, for fixed $m_{r e}$ and $x$, to determine the smallest value, $m_{i m}^{c r i t}$, such that up-recurrence on $A_{n}$ failed. (Preliminary study showed that, when failure occurs for $m_{i m}=m_{i m}^{c r i t}$, it continues to occur for all $m_{i m}>m_{i m}^{c r i t}$.) The search for $m_{i m}^{c r i t}$ was successively refined to pinpoint it to 3 significant digits. Size parameter was varied in the range $1 \leq x \leq 10,000$ and $m_{r e}$ was varied from 1.05 to 2.50 in steps of 0.05.

It very quickly became evident that, for fixed $m_{r e}$, as $x$ increased the product $\mathrm{xm}_{\mathrm{im}}^{\text {crit }}$ rapidly approached, from above, an asymptote. Thus there was a function $f\left(\mathrm{~m}_{\mathrm{re}}\right)$ such that

$$
\begin{equation*}
x_{\operatorname{im}}^{\text {crit }} \geq \min _{\mathrm{X}}\left(\mathrm{xm}_{\mathrm{im}}^{\mathrm{crit}}\right) \equiv \mathrm{f}\left(\mathrm{~m}_{r e}\right) \tag{46}
\end{equation*}
$$

and such that the inequality was, in fact, roughly an equality over almost the entire range of $x$. The data for $\min _{\mathrm{x}}\left(\mathrm{xm}_{\mathrm{im}}^{\mathrm{crit}}\right)$ as a function of $m_{r e}$ are given in Table 4 and plotted in Fig. 1.

It is plain from Fig. 1 that $f\left(\mathrm{~m}_{r e}\right)$ has an upward curvature. A straight line would not give a very good fit. Therefore, we fitted a quadratic to the data and then subtracted 1.0 from the constant term of the quadratic in order that the fit might lie slightly under all the data points (except for two which are obviously out-of-line).
The function so obtained is:


Figure 1

Table 4. The smallest value of the product $\mathrm{xm}_{\mathrm{im}}^{\mathrm{crit}}$ at each value of $m_{r e}$, where $\mathbb{m}_{i m}^{c r i t}$ is the value of $m_{i m}$ above which up-recurrence on $A_{n}$ fails ( $x \leq 10,000$ for this study).

| ${ }^{\mathrm{m}_{\mathrm{re}}}$ | $\min _{\mathrm{X}}\left(\mathrm{xm}_{\mathrm{im}}^{\mathrm{crit}}\right)$ | $\mathrm{m}_{\text {re }}$ | $\underbrace{\left.\min ^{(x m i t}\right)}_{\underline{i m}}$ |
| :---: | :---: | :---: | :---: |
| 1.05 | 12.2 | 1.80 | 53.0 |
| 1.10 | 14.9 | 1.85 | 57.8 |
| 1.15 | 16.9 | 1.90 | 60.7 |
| 1.20 | 19.6 | 1.95 | 65.2 |
| 1.25 | 22.2 | 2.00 | 67.5 |
| 1.30 | 24.7 | 2.05 | 72.1 |
| 1.35 | 27.0 | 2.10 | 75.5 |
| 1.40 | 30.3 | 2.15 | 80.0 |
| 1.45 | 33.2 | 2.20 | 81.9 |
| 1.50 | 36.0 | 2.25 | 88.6 |
| 1.55 | 39.5 | 2.30 | 91.2 |
| 1.60 | 40.7 | 2.35 | 97.2 |
| 1.65 | 44.5 | 2.40 | 99.0 |
| 1.70 | 47.4 | 2.45 | 104.8 |
| 1.75 | 50.6 | 2.50 | 110.4 |

$f\left(m_{r e}\right)=16.35 m_{r e}^{2}+8.42 \mathrm{~m}_{r e}-15.04$
and it is plotted in Fig. 1 as a solid line.
From Eq. (46) we deduce that up-recurrence may be used for $A_{n}$ if

$$
\begin{equation*}
m_{i m}<\frac{f\left(m_{r e}\right)}{x} \tag{48}
\end{equation*}
$$

but that, otherwise, down-recurrence should be used. This criterion, since it concerns the onset of numerical instability, is obviously precision-dependent, although probably not sensitively so. Also, being only empirical, it may break down for values of mare which are much larger than 2.50 , as may occur for water in the microwave region for example.

## 6. NUMBER OF TERMS IN MIE SERIES

Dave (1969a) stopped suming the Mie series at the first value of $n$ for which

$$
\begin{equation*}
\left|a_{n}\right|^{2}+\left|b_{n}\right|^{2}<10^{-14} \tag{49}
\end{equation*}
$$

(cf. Eq. 16). He was confident that this led to 6 significant digits in the results. We used this criterion for several years, but were forced to abandon it in order to attain vector speed in our Mie codes.

The reason is simply that vector processing is not possible for a loop containing a test like (49). Calculation of the entire vectors $\left\{a_{1}, \ldots\right\}$ and $\left\{b_{1}, \ldots\right\}$ at one stroke cannot occur if the value of each $a_{n}, b_{n}$ decides whether or not to calculate $a_{n+1}, b_{n+1}$.

We were just as glad to abandon Dave's criterion for two other reasons as well. First, the figure $10^{-14}$ may not be applicable to computers of differing precision. Related to this is the fact that the upward recurrence on $\psi_{n}$, whose fall to zero for $n \gtrsim x$ is the primary cause of Mie series convergence, rapidly becomes unstable near the very point where (49) must be satisfied. Eq. (49), in effect, is asked to "head off" the mushrooming instability in the $\psi_{n}$ calculation, and this seems too heavy a burden to lay upon it.

Second, even though our codes always carried the same precision (14 digits) as Dave's, the test (49) would sporadically fail in the middle of lengthy calculations, typically for $x>800$ or so. Examination of every such case revealed that failure was caused by $\left|a_{n}\right|^{2}+\left|b_{n}\right|^{2}$ falling to, but not below, some low level (e.g., $5 \times 10^{-14}$ ). Further examination showed that convergence was nevertheless
satisfactory in such cases, and the test (49) merely failed to recognize it.

For these reasons, the test (49) was replaced by an a priori estimate of $N$, the number of terms in the various Mie series ( $6-10$ ). We first determined $N$ for a wide range of size parameters ( $0.1 \leq x$ $\leq 20,000$ ) and refractive indices $\left(1.05 \leq m_{r e} \leq 2.50 ; 0 \leq m_{\mathrm{im}} \leq 1\right.$ ) using criterion (49) with $5 \times 10^{-14}$ replacing $10^{-14}$. Table 5 shows selected results for the range $\left[N_{\min }, N_{\max }\right]$ of values of $N$ at each size parameter.

It is immediately apparent that $N$ exhibits only a slight dependence on refractive index. This bears out what we said earlier about $\psi_{n}$ and $X_{n}$, which are functions of $x$ alone, being the prime controllers of convergence. And since $\psi_{n}$ decreases rapidly for $n \gtrsim x$, it is clear why $N \sim x$ is a good first approximation.

Several authors (e.g., Khare, 1976) have suggested, on theoretical grounds, the following functional form for $N$ :

$$
N=x+c x^{1 / 3}
$$

We have found that the following modification of this formula fits our data for $N_{\max }$ exceptionally well:

$$
N_{\max }=\left\{\begin{array}{ll}
x+4 x^{1 / 3}+1 & 0.02 \leq x \leq 8  \tag{50}\\
x+4.05 x^{1 / 3}+2 & 8<x<4200 \\
x+4 x^{1 / 3}+2 & 4200 \leq x \leq 20,000
\end{array}\right\}
$$

This gives an almost perfect fit to $135 \mathrm{~N}_{\max }$ values which we generated. It is low by 1 at 8 of these data points, and high by 1 or (rarely) 2 at 35 of them; at the remainder, it is exact. We set $N=N_{\text {max }}$.

Table 5. The range $\left[N_{\min }, N_{\max }\right.$ ] of the number of terms in the Mie series, as a function of size parameter $x$. The range was determined by varying $\operatorname{Re}(\mathrm{m})$ from 1.05 to 2.50 and $\operatorname{Im}(m)$ from 0 to 1 in small steps.

| x | $N_{\text {min }}-N_{\text {max }}$ | $x$ | $\stackrel{N}{\text { min }}-\mathrm{N}_{\text {max }}$ |
| :---: | :---: | :---: | :---: |
| 0.1 | 2-3 | 3,000 | 3,052-3,058 |
| 0.3 | 3-3 | 6,000 | 6,068-6,074 |
| 1 | 5-5 | 8,000 | 8,076-8,080 |
| 3 | 8-9 | 10,000 | 10,081-10,087 |
| 10 | 18-20 | 12,000 | 12,086-12,092 |
| 33 | 44-47 | 14,000 | 14,090-14,097 |
| 100 | 117-120 | 16,000 | 16,087-16,101 |
| 333 | 357-362 | 18,000 | 18,094-18,105 |
| 1,000 | 1,038-1,041 | 20,000 | 20,102-20,108 |

## 7. MIE SCATTERING SUBROUTINES

The present section describes the two Mie scattering subroutines MIEVO (Sec. 7.2) and MIEV1 (Sec. 7.3), which are based on the techniques and equations given in Secs. 3-6. Why two subroutines are necessary was explained in Sec. 2. These subroutines are listed and flowcharted in Appendices $I$ and II. Detailed timing studies are presented in Sec. 7.5 and a description of testing procedures in Sec. 7.4. Sample results from the subroutines are given in Appendix IIT.

An important a priori decision was whether or not to take advantage of FORTRAN complex arithmetic. In my earlier Mie routines, I avoided complex arithmetic entirely because it tended to be considerably slower than real arithmetic (for example, multiplying a real by a complex variable would compile as four floating point multiplies, instead of two). But the loss of code readability and simplicity from separating every expression into real and imaginary parts was drastic. In recent years, the dramatic rise in use of complex arithmetic, primarily because of the invention of the Fast Fourier Transform, has forced compiler-writers to do a much better job with it. It is, therefore, increasingly possible to write dramatically simpler Mie codes Without loss of speed, using complex arithmetic; that is the path chosen here.

Double precision arithmetic is not used anywhere in the subroutines, but users whose machines carry less than roughly 11 digits in single precision should carry out the $\sigma_{n}$ and $A_{n}$ recurrences in double precision and truncate the results back so single precision.

The two subroutines share a substantial amount of coding, in particular: the small-x limit; the $N$ formula; the $A_{n}$ computation; and the $\theta$-loops where $S^{ \pm}, S_{1}$ and $S_{2}$ are calculated. They both rely on compiler recognition of repeated subexpressions (an increasingly common capability).

The input and output variables used by MIEVO and MIEVI are in a common block (an argument list would be computationally slower) and are thoroughly described in comment cards. The only question which might arise is: How would one go about picking a value of the input variable N2CUT? (The code assumes $\operatorname{Im}(m)=0$, and takes faster branches, when $|\operatorname{Im}(m)| \leq N 2 C U T$.$) There is no easy answer.$ It depends on the largest size of particle being considered; the largest optical depth being considered (individual sphere absorptions may be very small and yet add up to a substantial value in an optically thick medium); and how small absorption must be before one is willing to neglect it. The user must either experiment a little with N2CUT--or set it to zero and forget about it.

### 7.1 VECTORIZATION

A few preliminary comments on vector processing are in order (Johnson, 1978, gives a good introduction to the subject in relation to the CRAY-1 computer). It should be emphasized at the outset that the Mie codes are designed to execute perfectly well, albeit more slowly, on ordinary "scalar" computers; but they have been written specifically to take advantage of vector processing when it is available.

Vector processing is applicable to loops of a very special form, in which entire arrays can be operated on as if they were scalars. Any so-called "vector denenmencies" (e.g., in the recurrences for $\left\{\zeta_{0}, \ldots, \zeta_{N}\right\}$ or $\left\{A_{1}, \ldots, A_{N}\right\}$, where one array element depends on one or two previous array elements, prevents "vectorization" of the associated loop. Such recurrences are unvectorizable in principle.

Other constructs, such as scalar temporary variables, user-defined function or subroutine references, and certain IF statements, may superficially prevent vectorization of a loop in which they occur; but a redesign of the loop coding often allows vectorization. Loops in which only some parts are unvectorizable can often be split into two loops, the first of which isolates the unvectorizable parts and the second of which is tully vectorizable. Some operations, like summing the elements of. an aridy, which at first glance seem unvectorizable, can be "partially vectorized"; this is exactly what is done in MIEV1 to sum the series fur " ext, 'sca and g. These tricks, and others, are discussed at more length by Higbie (1978). All this, of course, leads to code which seems, in some sense, "unnatural," but one is quickly reconciled to such unnatural code when one sees the dramatic speed increases it pioduces.

In Mie calculations there are two types of loops: over number $N$ of terms in the Mie series and over number $N$ ang of angles. A third type of lonp, uver size parameter $x$, is often used, for example, when integrating Mie पuantities over a size distribution. This loop is normally outside the $H i \in$ subroutine. Some advantage could be reaped by having this loup inside the Mie subroutine. In particular,
unvectorizable elements in MIEVO and MIEVI, like the $A_{n}$ and $\zeta_{n}$ recurrences, could be vectorized by making the $x$-loop the innermost one and adding an extra $x$-dimension to $A_{n}, \zeta_{n}$, etc. However, two disadvantages also accrue: the Mie subroutine would be much less general-purpose, and the memory requirements could become prohibitive. Users who wish to try this route should be warned that: (a) if $N$ ang is, say, 30 or more, little speed-up will be realized, because the $N_{\text {ang }}-$ loop dominates the execution time; (b) $N$ depends on $x$, and with $x$-loops innermost and $N$-loops outside, this dependence cannot be accounted for (taking $N$ sufficient for the largest $x$ could cause the $A_{n}$ and $\zeta_{n}$ up-recurrences for smaller $x$ 's to go wildly unstable). Calculating $S_{1}$ and $S_{2}$ involves one $N-100 p$ and one $N_{a n g}-100 p$, nested. But only inner loops are vectorizable. In the $N-100 p, S_{1}$ and $S_{2}$ are computed by suming, which is only a partially vectorizable operation; hence, the natural choice was to make the $N_{\text {ang }}-100 p$ the inner one (it is completely vectorizable, provided several arrays are furnished to contain temporary variables). The $\mathrm{N}_{\text {ang }}$-loop-innermost structure is found in both MIEVO and MIEV1.

### 7.2 MIEVO

MIEVO aims at minimum storage. The only significant dimensioned array is for $A_{n}$. (Arrays dimensioned only by the number of angles are usually short and rarely contribute significantly to the storage burden.) It requires a storage allocation because it may have to be precomputed by down-recurrence. The rest of the computation unfolds naturally as an up-recurrence requiring no storage of intermediate
results. Because of this, MIEVO appears simple and straightforward, especially by comparison to MIEVI.

The only significant vectorization in MIEVO is of the $N_{\text {ang }}-$ loops necessary in the $S_{1}, S_{2}$ computation, as described in Sec. 7.1. But, as the timing studies will show (Sec. 7.5), these are by far the most important loops to vectorize if $S_{1}$ and $S_{2}$ are computed at any reasonable number of angles.

By setting $N_{\text {ang }}=0$ in MIEVO, one can calculate $Q_{\text {ext }}, Q_{\text {sca }}$ and $g$ only, which is all one needs for simple radiative transfer approximations 1ike delta-Eddington (Wiscombe, 1977). But MIEVO is two to three times slower than MIEV1 in this mode, so MIEV1 should be used for such applications whenever possible.

The numerical coefficients needed in the various Mie series are formed in MIEVO by the following efficient procedure:

$$
\begin{align*}
& 2 n+1=n+(n+1)  \tag{51a}\\
& \frac{(n+1)(n-1)}{n}=n-\frac{1}{n}  \tag{51b}\\
& \frac{n+1}{n}=1+\frac{1}{n}  \tag{51c}\\
& \frac{2 n+1}{n(n+1)}=\frac{1}{n}+\frac{1}{n+1} . \tag{51d}
\end{align*}
$$

Only one division is actually done ( $1 / n+1$ ) because the value of $1 / n$ is saved from the previous pass through the n-loop. The coefficient $(-1)^{\mathrm{n}+1}$ is contained in an integer variable which is initialized to 1 and then has its sign flipped each time through the n-loop.

### 7.3 MIEV1

MIEV1 aims for the maximum amount of vectorization. It vectorizes all those $N_{\text {ang }}$-loops which are vectorized in MEVO and, in addition, it vectorizes several N -loops. To do so it divides computations into separate loops which were combined into a single loop in MIEVO. Also, MIEV1 requires 11 arrays of length $N$, rather than 2 as in MIEVO (a complex array counting as 2), even though every effort has been made to minimize storage.

Four of the 11 N-arrays in MIEVI contain the numerical coefficients
$n, 2 n+1, \frac{2 n+1}{n(n+1)}$, and $\frac{n(n+2)}{n+1}$

It is necessary to store these in arrays in order for certain $N$-loops to vectorize. Vectorization is inhibited unless all operands in an arithmetic expression are either constants or vectors; functions of the loop index like (52) are, as they stand, neither.

Summing of the series for $Q_{\text {ext, }}, Q_{\text {sca }}$ and $g$ (Eqs. 6-8) is done in MIEV1 using a partially-vectorized subroutine. It is based on the following conceptual rearrangement into matrix form of the linear array being summed:

$$
\begin{aligned}
& \left\{\begin{array}{l}
x_{1} \\
\cdot \\
\cdot \\
\cdot \\
x_{64}
\end{array}\right\} \longrightarrow \begin{array}{lll}
x_{1} & y_{1} & \\
\bullet & \cdot & \\
\cdot & \cdot & \\
x_{64} & y_{64} &
\end{array} \\
& \left\{\begin{array}{l}
y_{1} \\
\cdot \\
\cdot \\
y_{64}
\end{array}\right\} \longrightarrow
\end{aligned}
$$

Each successive group of 64 elements in the array is regarded as a column of the matrix. Matrix row sums are then formed in a loop which vectorizes:

$$
\begin{equation*}
S_{i}=x_{i}+y_{i}+\ldots \quad(i=1 \text { to } 64) \tag{53}
\end{equation*}
$$

Then these row sums are added in an unvectorizable loop to give the desired sum:

$$
\begin{equation*}
s=s_{1}+\ldots+s_{64} . \tag{54}
\end{equation*}
$$

It is because this last loop is unvectorizable that we call the procedure only "partially vectorized."

The above procedure has been coded into the FORTRAN subroutine TOTAL, listed along with MIEV1 in Appendix II. Obviously, TOTAL offers no speed advantage when less than 65 elements are to be summed; in that case TOTAL branches to a simple scalar loop

TOTAL $=\mathrm{A}(1)$
$\mathrm{DO} 1 \mathrm{I}=2, \mathrm{~N}$
1 TOTAL $=$ TOTAL $+A(I)$.

According to Johnson (1978), summing may be speeded up even more on the CRAY-1 by doing a vector add between steps (53) and (54). This extra step is vectorizable and results in having to sum only 8 elements, instead of 64 , in the final unvectorizable step (54). Unfortunately, it is necessary to use assembly language coding to reap this extra speed and this would make MIEVI nonportable. But those who use MIEV1 on the CRAY-1 may want to avail themselves of this fast sum routine.

Timing comparisons for sums of various lengths are presented in Table 6 for the three summing methods: standard (Eq. 55), TOTAL, and assembly language. For sums of more than 40 terms, assembly language summing takes only one-third to one-sixth the time of TOTAL. Note also that TOTAL is actually slower than the standard method for sums of less than about 100 terms; the overhead associated with calling a subroutine outweighs the benefits of vectorization up to this point. But beyond 100 terms, TOTAL quickly shows its advantage on just those sums which take the most computer time. For sums of 1000 terms and more, it takes only one-fourth to one-fifth the computer time of the standard method, albeit a factor of 3 to 4 more time than the assembly language method.

### 7.4 TESTING

The following parts of the basic routine MIEVO were tested extensively by themselves:

- the recurrences for $\psi_{n}, \chi_{n}$ and $A_{n}$, particularly their possible instability (Sec. 3)
- the Lentz method (Sec. 3)
- the recurrences for $\pi_{n}, \tau_{n}$ (Sec. 3)
- the small-x limit (Sec. 4)
- the empirical function $N(x)$ (Sec. 6)
- the $A_{n}$ up-recurrence criterion (Sec. 5) .

MIEVO was then tested as a whole for internal consistency, for stability and for well-conditioning; its results were compared to a considerable variety of published Mie scattering data, and to the author's previous Mie code.

Table 6. Timing comparisons between various summing methods: standard (Eq. 55), partially-vectorized FORTRAN (TOTAL), and assembly language (Johnson, 1978).

Ratio of TOTAL
 Standard method time (millisec)

$$
2.1 \times 10^{-3}
$$

$$
3.7 \times 10^{-3}
$$

$$
7.0 \times 10^{-3}
$$

$$
1.3 \times 10^{-2}
$$

$$
2.0 \times 10^{-2}
$$

$$
3.3 \times 10^{-2}
$$

$$
4.9 \times 10^{-2}
$$

$$
6.6 \times 10^{-2}
$$

$$
9.8 \times 10^{-2}
$$

$$
0.16
$$

$$
0.33
$$

$$
0.65
$$

6.5

20,000
to standard
method time

Ratio of assembly language
to standard method time
0.77
0.45
0.27
0.21
0.15
0.12

0,10
0.084
0.071
0.061
0.057
0.052

The internal consistency checks consisted in ascertaining, in numerous test cases, that the code results were the same to at least 6 significant digits when (a) various formulas were restructured, (b) varying levels of precision were used, and (c) convergence flags were varied within reasonable limits.

The stability and well-conditioning tests consisted in exercising the code over broad ranges of $x$ (up to 20,000) and $m$ (real part from 1.05 to 2.50 ; fmaginary part from $10^{-7}$ to 1 ) and seeing if any overflows or unreasonble results turned up. No published data exist over most of these ranges, but there are a number of checks which one can make; e.g., that $Q_{\text {ext }} \rightarrow 2$ and $Q_{\text {sca }}$ and $g$ approach well-known asymptotes as $x \rightarrow \infty$; that these approaches should be more rapid--the larger $\operatorname{Im}(m)$ is; that increasing $\operatorname{Im}(\mathbb{m})$ damps out the ripple structure--the more so the larger x is; that rainbows and glories should occur; and so on. Numerous graphs were made of the results and, after considerable experience with Mie scattering data, I have found that calculational errors are relatively easy to spot on such graphs since they cause deviations from what is usually a fairly regular pattern. The final form of MIEVO in Appendix I has passed all such tests.

The published data against which MIEVO was tested included both graphs and tables in Van de Hulst (1957), Irvine (1965), Kerker (1969), Dave (1968b), and Deirmendjian (1969); and tables in Deirmendjian (1963), Denman et al. (1966), and Dave (1968a). Such data are restricted to $x \leq 1000$ and, while being able to reproduce them gave considerable confidence in the codes, the sorts of tests described in the last paragraph are equally as important; for extrapolating the code to $\mathrm{x} \leq 20,000$ might overwhelm numerical techniques which are perfectly adequate for $\mathrm{x} \leq 1000$.

Of course the Mie codes were modified and improved several times after their initial testing. Rather than rerun the tests, comparisons were made for wide ranges of $x$ and $m$ between all output quantities of the new and old versions. This enabled errors to be quickly detected and ensured that the final versions presented here passed all the tests that their predecessors did. It also was the method used to test MIEV1 (against MIEVO).

Sample results from MIEVI, rounded to 6 significant digits, are presented in Appendix III. Users should reproduce these results before attempting to apply MIEVO or MIEVI. There are 8 cases: $x=10,100$, 1000, and 5000; for each $x, m=1.5$ and $m=1.5-0.1$ i. $Q_{\text {ext }}, Q_{\text {Sca }}$, $Q_{a b s}=Q_{e x t}-Q_{s c a}, G$, and the time to execute each case are shown, as well as $\mathrm{S}_{1}$ and $\mathrm{S}_{2}$ for $\theta=0^{\circ}\left(5^{\circ}\right) 180^{\circ}$. The intensity and degree of polarization (Eqs. 44-45) are also shown; these were tabulated by Dave (1968a) for our-two $x=1000$ cases, and the Appendix III results agree with his to all digits which he tabulates, except that the sign of our degree of polarization is opposite to his (we believe his is wrong in this respect).

Note that Dave gives execution times of 50.36 sec ( $m=1.5$ ) and $52.32 \mathrm{sec} .(m=1.5-0.1$ i) for his test cases. The MIEV1 times are 3300 and 2900 times faster, respectively.

### 7.5 TIMING

Claims of computer code timing superiority turn up frequently, although rarely are they backed up by the sort of thorough, quantitative study presented below for MIEVO and MIEV1. Therefore, I would like to begin with a few general comments on the meaning and utility (or lack thereof) of timing comparisons.

My main observation-mand this has been seasoned by years of experience with a variety of codes and computing systems--is that many claims of timing superiority are meaningless. They are simply down in the noise level. I base this incredulity on several elements of experience.

First, the comparisons are almost never thorough or comprehensive, but rather are based on a tiny sample of cases which may not be representative or even important.

Second, timing on a computer is inherently a noisy operation, and the results may not be exactly reproducible. It depends on the workload, the $I / O$ burden, and many other unreckonable factors. It may vary even among computers of the same kind, depending on the sophistication of their operating systems and compilers (which are often a local product or an extensively modified company product). The 'perfect' timiñg study would be a pure CPU job, involving no I/O other than printing the times at the end, and executing with no other jobs present. These conditions are rarely met.

Third, the putatively slower code is not usually optimized. I have seen professional 'code speeder-uppers' reorganize a code, put the slowest or most frequently executed parts in assembly language, etc., and improve the timing by several factors. Indeed, after such optimization, the slower code might become the faster one.

- As a result, I have come to regard, as a rough rule-of-thumb, that only a timing factor of 4 or more between two entirely different codes is significant. (Of course, timing improvements from modifying similar codes on the same computer are significant at a much lower level, possibly as low as $5-10 \%$.)

Another point to bear in mind is what benefit will accrue from a timing improvement. A code executing in 1 microsecond will not benefit from a speed-up unless it is called many millions of times. At the other end of the scale, a code requiring 100,000 hours will not become any more feasible with a factor of 10 speed-up. It is usually only calculations requiring times in the mid-range (seconds to hours) which will benefit from a speed-up. Mie calculations are of such a type.

By way of an example of a useful timing comparison, Table 7 shows flmes for Dave's (1969a) Mie code, for 182 angles and $\mathrm{x}=1,10,100$, 1000 and 5000; and corresponding times for vectorized MIEV1. MIEV1 is 3000-4000 times faster, which divides up as follows. Our scalar-mode CRAY-1 is roughly 100 times faster than Dave's IBM 360/50. Another factor of roughly 5 is due to our improvements in numerical technique and a final factor of about 7 can be ascribed to our partiallyvectorized code design.

Palmer (1977), using the same kind of computer as Dave, reported a new numerical technique (continued fractions instead of series) which gave factors of 9-15 improvement over Dave's times in Table 7 for $\mathrm{x}=1,10$ and 100. The fact that both Palmer and I obtained such large improvements from entirely different directions suggests that, from the timing standpoint, Dave's codes were far from ideal.

We now examine the times required by three versions of our codes: unvectorized MIEVO, vectorized MIEVO, and vectorized MIEV1. These times, in CRAY-1 milliseconds, are presented in Tables $8-10$, respectively, for size parameters from 1 to 5000 , for numbers of angles from 0 to 255, and for two imaginary refractive indices--0 and 0.1. Each

Table 7. Execution times for Dave (1969a) Mie code compared to vectorized MIEV1 time. 182 angles were used for both codes. Dave used an IBM 360/50, which is roughly 100 times slower than the CRAY-1 in its normal scalar mode.

| x | Dave (1969a) <br> code time (sec) | vectorized MIEV1 <br> code time (sec) | ratio <br> of times |
| :---: | :---: | :---: | :---: |
| 1 | 0.7 | $1.8 \times 10^{-4}$ | 3900 |
| 10 | 3.7 | $3.6 \times 10^{-4}$ | 3100 |
| 100 | 22 | $9.8 \times 10^{-4}$ | 3800 |
| 1000 | 194 | $5.4 \times 10^{-3}$ | 4100 |
| 5000 | 945 | $4.56 \times 10^{-2}$ | 4300 |
| 1 |  | 0.222 | 4300 |

Table 8. CRAY times in milliseconds to execute the unvectorized MIEVO code for various combinations of size parameter and number of angles. Each time represents an average over $\operatorname{Re}(\mathrm{m})=1.1(0.2) 2.5$.

$$
\operatorname{Im}(m)=0
$$

| No. of Angles | Mie Size Parameter |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 3.3 | 10 | 33 | 100 | 333 | 1000 | 5000 |
| 0 | 0.081 | 0.11 | 0.19 | 0.41 | 1.0 | 3.0 | 8.4 | 41 |
| 3 | 0.13 | 0.18 | 0.33 | 0.72 | 1.8 | 5.3 | 15 | 74 |
| 7 | 0.16 | 0.24 | 0.44 | 0.98 | 2.4 | 7.3 | 21 | 101 |
| 15 | 0.23 | 0.35 | 0.66 | 1.5 | 3.7 | 11 | 32 | 155 |
| 31 | 0.38 | 0.58 | 1.1 | 2.5 | 6.3 | 19 | 54 | 262 |
| 63 | 0.66 | 1.0 | 2.0 | 4.5 | 11 | 34 | 98 | 476 |
| 127 | 1.2 | 2.0 | 3.7 | 8.6 | 22 | 65 | 186 | 905 |
| 255 | 2.4 | 3.8 | 7.3 | 17 | 42 | 127 | 363 | 1760 |

$\underline{I m}(\mathbf{m})=0.1$

| 0 | 0.099 | 0.14 | 0.24 | 0.50 | 1.2 | 3.7 | 12 | 53 |
| ---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 3 | 0.14 | 0.21 | 0.37 | 0.82 | 2.0 | 6.1 | 19 | 86 |
| 7 | 0.18 | 0.27 | 0.48 | 1.1 | 2.7 | 8.0 | 25 | 113 |
| 15 | 0.25 | 0.38 | 0.70 | 1.6 | 3.9 | 12 | 36 | 167 |
| 31 | 0.39 | 0.61 | 1.1 | 2.6 | 6.5 | 20 | 58 | 274 |
| 63 | 0.68 | 1.1 | 2.0 | 4.6 | 12 | 35 | 102 | 488 |
| 127 | 1.3 | 2.0 | 3.8 | 8.7 | 22 | 66 | 190 | 918 |
| 255 | 2.4 | 3.8 | 7.3 | 17 | 42 | 127 | 367 | 1780 |

Table 9. CRAY times in milliseconds to execute the vectorized MIEVO code for various combinations of size parameter and number of angles. Each time represents an average over $\operatorname{Re}(m)=$ 1.1 (0.2) 2.5.

$$
\operatorname{Im}(m)=0
$$

| No. of Angles | Mie Size Parameter |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 3.3 | 10 | 33 | 100 | 333 | 1000 | 5000 |
| 0 | 0.081 | 0.11 | 0.19 | 0.41 | 1.0 | 3.0 | 8.4 | 41 |
| 3 | 0.12 | 0.18 | 0.32 | 0.70 | 1.7 | 5.1 | 15 | 71 |
| 7 | 0.13 | 0.18 | 0.32 | 0.71 | 1.7 | 5.2 | 15 | 72 |
| 15 | 0.14 | 0.20 | 0.35 | 0.78 | 1.9 | 5.7 | 16 | 79 |
| 31 | 0.16 | 0.23 | 0.41 | 0.92 | 2.3 | 6.8 | 19 | 94 |
| 63 | 0.20 | 0.30 | 0.54 | 1.2 | 3.0 | 8.9 | 25 | 123 |
| 127 | 0.28 | 0.43 | 0.80 | 1.8 | 4.4 | 13 | 38 | 182 |
| 255 | 0.46 | 0.72 | 1.4 | 3.0 | 7.6 | 23 | 66 | 315 |

$$
\operatorname{Im}(m)=0.1
$$

| 0 | 0.099 | 0.14 | 0.24 | 0.50 | 1.2 | 3.8 | 12 | 53 |
| ---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 3 | 0.14 | 0.20 | 0.36 | 0.78 | 1.9 | 5.9 | 18 | 83 |
| 7 | 0.14 | 0.21 | 0.37 | 0.80 | 2.0 | 6.0 | 19 | 84 |
| 15 | 0.15 | 0.22 | 0.40 | 0.87 | 2.1 | 6.5 | 20 | 91 |
| 31 | 0.17 | 0.25 | 0.46 | 1.0 | 2.5 | 7.5 | 23 | 106 |
| 63 | 0.21 | 0.32 | 0.58 | 1.3 | 3.2 | 9.6 | 29 | 135 |
| 127 | 0.30 | 0.45 | 0.82 | 1.8 | 4.6 | 14 | 41 | 194 |
| 255 | 0.48 | 0.74 | 1.4 | 3.1 | 7.8 | 23 | 69 | 327 |

Table 10. CRAY times in milliseconds to execute the vectorized MIEVI code (the fastest one) for various combinations of size parameter and number of angles. Each time represents an average over $\operatorname{Re}(m)=1.1(0.2) 2.5$.

$$
\operatorname{Im}(m)=0
$$

| No. of Angles | Mie Size Parameter |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 3.3 | 10 | 33 | 100 | 333 | 1000 | 5000 |
| 0 | 0.062 | 0.074 | 0.11 | 0.19 | 0.38 | 0.99 | 2.7 | 13 |
| 3 | 0.11 | 0.15 | 0.24 | 0.50 | 1.2 | 3.3 | 9.4 | 45 |
| 7 | 0.11 | 0.15 | 0.25 | 0.51 | 1.2 | 3.5 | 9.7 | 47 |
| 15 | 0.12 | 0.17 | 0.28 | 0.58 | 1.4 | 4.0 | 11 | 54 |
| 31 | 0.14 | 0.20 | 0.34 | 0.72 | 1.7 | 5.0 | 14 | 69 |
| 63 | 0.18 | 0.26 | 0.46 | 1.0 | 2.4 | 7.1 | 20 | 99 |
| 127 | 0.27 | 0.39 | 0.71 | 1.6 | 3.8 | 11 | 32 | 157 |
| 255 | 0.45 | 0.68 | 1.3 | 2.8 | 7.0 | 21 | 60 | 290 |

$\underline{I m}(m)=0.1$

| 0 | 0.083 | 0.10 | 0.14 | 0.25 | 0.53 | 1.5 | 5.6 | 21 |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 3 | 0.13 | 0.18 | 0.28 | 0.57 | 1.3 | 3.8 | 12 | 53 |
| 7 | 0.13 | 0.18 | 0.29 | 0.59 | 1.4 | 4.0 | 13 | 55 |
| 15 | 0.14 | 0.20 | 0.32 | 0.66 | 1.5 | 4.5 | 14 | 62 |
| 31 | 0.16 | 0.23 | 0.39 | 0.80 | 1.9 | 5.5 | 17 | 77 |
| 63 | 0.20 | 0.29 | 0.51 | 1.1 | 2.6 | 7.7 | 23 | 106 |
| 127 | 0.29 | 0.42 | 0.75 | 1.6 | 4.0 | 12 | 35 | 165 |
| 255 | 0.47 | 0.73 | 1.3 | 2.9 | 7.2 | 22 | 63 | 298 |

time represents an average over eight real refractive indices from 1.1 to 2.5 in steps of 0.2 .

For $\operatorname{Im}(m)=0$, up-recurrence is always used for $A_{n}$, as well as faster code branches for calculating $a_{n}, b_{n}$, so these times are invariably less (typically by $5-30 \%$ ) than the corresponding ones for $\operatorname{Im}(m)$ $=0.1$. For $\operatorname{Im}(m)=0.1$, up-recurrence for $A_{n}$ may or may not be used; depending on Eq. (48); for $\operatorname{Re}(m)=1.1$, for example, it is used only for the $x \leq 100$ cases, while for $\operatorname{Re}(m)=2.5$ it is used for all except the $x=5000$ case. The sudden switch to down-recurrence on $A_{n}$ thus occurs somewhere between the $x=100$ and $x=5000$ columns of the tables, but the elevating effect of this on the quoted times is diminished somewhat by averaging over the eight values of $\operatorname{Re}(m)$.

The patterns in Table 8 are typical of what one may expect on computers without vector capabilities. For fixed $x$, the $N_{a n g}$-loop embedded in the $N-100 p$ increasingly dominates the computation time, until, for $N_{a n g} \geq 31$, the time is almost linear in $N_{\text {ang }}$. For fixed $N_{\text {ang }}$, the time rises a bit less than linearly with $N$ or, equivalently, with $x+4 x^{1 / 3}$ (cf. Eq. 50).

For vectorized MIEVO, Table 9, the times for 0 and 3 angles are almost identical to those for unvectorized MIEVO, Table 8; this is to be expected, since only $\mathrm{N}_{\text {ang }}$-loops have been vectorized. But for $N_{\text {ang }}>3$, the times in Table 9 increase much more slowly with rising $N_{\text {ang }}$ than they did in Table 8. For 15 angles, there is an advantage of 1.8-1.9 over unvectorized MIEVO for all $x$; for 31 angles, 2.4-2.8; for 63 angles, 3.5-3.9; up to 5.2-5.7 for 255 angles. This advantage factor rises roughly logarithmically in $N_{\text {ang }}$, increasing by about unity
every time $N_{\text {ang }}$ doubles. As $x$ increases for fixed $N_{\text {ang }}$, the times in Table 9 rise in almost the exact same way they did in Table 8 (Inearly in $N$ ) ; again, this is not surprising since no $N$-loops are vectorized.

The fastest code times are those for vectorized MIEVI, in
Table 10. Compared to Table 9, improvement over MIEVO is greatest for 0 angles-as large as a factor of 3 and at least a factor of 2 whenever $x^{2} 33$. This shows the advantage from vectorizing $N$-loops in its best light. For $N_{\text {ang }} \geq 3$, on the other hand, vectorized MIEVO never takes over $60 \%$ more time than vectorized MIEVI; vectorized MIEVI offers the most advantage for $3 \leq N_{\text {ang }} \leq 63$ and $x \leq 100$, in which regime vectorized MIEVO takes $25-60 \%$ more time. (Of course, it is just this large-x regime which requires the most computer time.) But for 255 angles, Table 9 times are never more than $10 \%$ above those in Table 10 , reflecting the almost total dominance of the $N_{\text {ang }}-$ loops at that point.

There is a big rise, by a factor of $2-3$, between the times for $N_{\text {ang }}=0$ and those for $N_{a n g}=3$ in Table 10. But after this initial jump, the further rise as $N_{\text {ang }}$ increases is slow; it is necessary to go all the way to 63 angles to double the $N_{\text {ang }}=3$ time. Beyond 63 angles, the rise in execution time is more rapid, approaching linearity in $\mathrm{N}_{\text {ang }}$; this reflects the vector length of 64 on the CRAY-1. For $x \leq 33$, the Table 10 times rise considerably more slowly than linearly in $N$, reflecting the vectorization of $N$-loops. For $x \geq 100$, the times go up more nearly linearly in $N$, again due to the CRAY-1 vector length.

Using the assembly language sum routine (Sec. 7.3) can speed-up vectorized MIEV1 by anywhere from $1 \%$ to $20 \%$. Unfortunately, the larger
speed gains are associated with the smaller values of $x$ and $N$ ang' which take less computer time anyway. For example, for $\mathrm{x}=33$, the gain ranges from 15-18\% for 0 angles to $0-2 \%$ for 255 angles; while for $x=333$ it never exceeds $7 \%$. For maximum speed the fast sum routine can certainly be recommended, especially for $N_{\text {ang }}=0$ cases, but no dramatic improvements in timing result therefrom.

These timing studies furnish a more solid basis than has heretofore existed for (a) estimating how much time a particular Mie computation will require and. (b) establishing by how much, and in what cases, future Mie codes improve on these times.
8. SUMMARY

This document describes a number of improvements in numerical technique for Mie scattering calculations, and incorporates them into two well-documented and tested computer codes. These improvements are as follows:

1. Design for vector processing (Sec. 7.1)
2. Lentz method for starting the downward recurrence of $A_{n}$ (Eqs. 23-35)
3. New criterion for down-recurrence of $A_{n}$ (Sec. 5)
4. Better treatment of small-particle limit (Sec. 4)
5. A priori formulas for number of series terms (Sec. 6)
6. Simpler $\pi_{n}(\mu), \tau_{n}(\mu)$ recurrences (Eqs. 37, 38)
7. Faster branches for no-absorption cases (Sec. 7.5)
8. $S^{ \pm}$, rather than $S_{1}, S_{2}$, calculated internally, for greater speed (Eqs. 9-12)
9. Complex arithmetic, no double precision (Secs. 3, 7).

The codes execute some 30 to 40 times faster than those of Dave (1968a, 1969a) even after differences in machine speed are factored out. While this may seem a bit like flogging a dead horse, considering that Dave's codes may have been very inefficient to begin with (see Sec. 7.5), the statistic is important because many people are still using Dave's codes or slight variations thereof.

With codes such as those presented herein, Mie calculations which were literally unthinkable only 5 to 10 years ago may now be done routinely.

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## APPENDIX 1. MIEVO FLOW CHART AND LISTING






```
C PINHI(J)"-----IITILE:PI-SUZ-(\ddot{*-1)}
C IMP(J) IEMPORARY ARRAY USED IN COYPUTING PIN,IAUN
C SP(J) S* SIOSZ FOR JTH ANGLE
C SH(J) S- SI-ST FOR JIMANGLE
C SPS(J) S* - SI+S2 TOR (NN2-J)TH ANGLE
C SMS(J) S-E SI-S2 FDR (NN2-JITH AMGIE
C
CUSE COMIO
ANGULAR OIMENSIONS
    Parameter (NANGLE255)
    COMPLEX IOR, S1, S2
    REAL HZCUT
    GOMMON/INOUT/XX,IOR,NZCUT, NUMANG, XMU(MANGL), QEXT, QSCA,GFAC,
    - SI(MANGL),S2(NANEL)
CENO
    PARAMETER (NANGLZ=(MANGL+1)/2)...
    PARAMETER (MTI=20150)
    REAL MPIDN
    LOEICAL NOIMAF. MOANGS
    COMP:EX CTAN
    COMPLEX A1,A2,B1,IORS2,RAT
    COMPLEX ZINY,FF,AK, DEN,NUN,NTN,OTD,TT, OIGA,IORINV,AK,BN,ANKL,BMM1,
        ANP,BMP,ANPK,GNPM, ZET, ZETN, ZETNP1,SSP,SN,SPS,SNS
    DIMENSION SP(MAKOLZ2I,SN(NANGL2),SPS(MANELZ2), SMS(MANGLZ),
    - PIN(NANGL2), PINHL(MANGL2), TAUN(NAMGL2), TMP(NANGL2),日IGA(MTI),
        EQ日IGA(MT1)
    EQUIVALENCE (8IGA(8), EQBIGA(1))
    EQUI YALENCE (S1(1),PIN(1)),(S1(MANGL2);PINMI(1)),
                            (S2(1),TAUN(1)),(S2(NANGL2),TMP(1))
        F(REN)=-15.14* REN*(8.42+16.35*REN)
        OATA EPSI/1.E-2/1, EPS2/1.E-B/
        DATA MAXIT/10000/
C
    IFINUMANG.GT.NANGL .OR. NUMANG.LT.OS STOP }200
    HNZ = NNMANG*&
    MM = WN2/2
    MOANGS = MUMAMG.EQ.E
    AIMIOR = ABS(AIMAG(IOR))
    REIOR = REAI.(IOR)
    NOIMAG E AIMIOR.LE.MZGUT
    IF(CABS(IOR)=XX.67.S.1) 60 10 7
            SMALL-PARTICLE LIMIT
        IORSQ = IOR**2
        RAT = (0.00.666666666666667)0(IORSO-1.0)
        11. RAT*(1.0-0.1*XK*=2*:6.FIOR5Q+5.1/1408.*(xX**4))
    - /(IORSO+2.1-(1.0-0.7*IORSOI*(XX**2)-(8.010RSQ**2-305."IORSO
```



```
    B1=(xX**2/38.)-RAT*(1.1+(2.*IORSQ-5.)/70.*(xX**2)).
    - /(1.8-(2.*1ORSQ-5.)/38.0(xX**2))
    A2 = (0.1*x'*-2)*RAT*(1.8-xX0*2/16.)
    * /(2.*IORSQ+3.-(2.*IORSR-7.)/14.*(XX*-2))
```



```
    QSCA = 6.*(xX*-b)*TEM
    GFAC= REAL(A1*CONJG(AZ+B1))/TEN
    QEXT = QSCA
    IF(AIMIOR.GT.1.E-12) QEXT = b.*XX*REAL(A1+81*(5.13.1:AZ)
    C
        TEN=1.5* XX0.3
        A2=(5.13.)*A2
    C **** VECTORIZABLE LDOP OF##*
    OO 5 J = 1.NN
    S1(J)= IEN*(A1*(B1*A2)*XMU(J))
```



```
            00 6 J = 1.NM
            SI(MNz-J) = TEMP(A1-(B1+AZ)*XRU(J)
            6 S2(MN2-J)= rEn+(B1-AI*XRU(J)*AZ*(2."XHU(J)**2-1.))
    C
    C CALCULATE mUNBER OF TERHS IN MIE SERIES (A LEAST UPPER BOUNOS
        USING EMPIRIGAL FORMULAS WHICN VERE FIITED FOR SIIE PARAMETERS
        UP TO 20,000
```



```
        IFIXX.GT.B.C .ANO. XX.Lf.42gi.) NY = XX+4.050xX=0(1./3.) +2.
```



```
        WTP\ = NT+1
                            MAKE SURE ARRAY IIEA MILL BE GARGE EMOUGH
        IFINTPI.LE.NTIS SO TO &:
        MRITE(G,&JOC) NT, XX
    0000 FORHATH/1: ESTIMATED LENGTH OF MIE SERIES MI=EIG,
        * FOR SI2E PARANE"FIZ.2/O ENCEEOS IIOA OIMENSIONSO)
    C
            COMPUTE ALGA
        10 XINY = 1.0/xX
        ZINY = XINYIIOR
            OEGIOE WHETHER BIEA-N CBN BE CALCULATED IT UP-RECURREMCE
        IFIAIMIOR .LT. FIREIORI/XX: :O TO 200
            PREPARE FOR DOKN-RECURIEENEE---
            CORMJIE INITIAL HIGH-ORDES IIGAM USIMG LENTI NETHOO
        FF = MTPIO2INV
        MM = -1
        KK=2*NTAS
        AK= (MN*KK)•ZINV
        DEN = AX
        MUN = OEN & 1.BIFF
        KOUNT = 1
    C
        20 KOUNT = ROUNT*1
            IF(XCUNP.GT.MAXITI :0 T0 to
    IF(GAES(MUM/AK) EIT.EPSS .ANO. CABS(DEM/AK).GT.EPSS) GO TO 3A
                            ILL-COMDITIONE'J CASE--STRIDE TWO TERMS INSTEAD OF ONE
    PM = -MM
    RK = KK+2
    AKE (m-KK)PIINV
    MTN - AK@NUN: 1.0
    OTO AKPOEN - 2.0
    FF E (MTM/OTD) * FF
    MN - -mN
    KK=KX+2
    AK = (NMEKKI PIINV
    mUM - AK - MUAINTN
    DEN = AK - ORM/OIO
    KOUNT = KOUNP+1
    60 10 20
        C
        30 TT = NUM/DEN
    FF = iT*FF
            CHECK FJR COMVEROENCE
        SF(AOS(REAL(TT)-1.8).LT.EPSS .AMO. ABS(AIMAG(TI)).LT.EPSZ) SOTO 50
    AN = -MM
    xK = xk+2
```

```
AK = (mm0nkIPIING
        NUM = AK 1.I/NUN
        OEN = AK 1.0/OEN
        60 10 20
    C
    4" WRITE(G,0001) NT, XX, IOR, AK,NUN,DEN,TT,FF
    COO& FORMATI/ING CONTINUEO FRACIIION FOR A-SUGONT FAILEO TO CONYERGE&/
        * NTEOIG/O X=OEZJ.O/P REFR INOEXEF2E2O.8/O AK=42E2O.8/
        STOP 1002
    C
    5& aIGA(MT) : FF
    C
    C DOWMAARO RECURRENGE FOR BIGA-M
        DO 7e M=MT,2,-1
        70 116A(M-1)=(NO2IKV)-1.0/(INO2INV)08IGA(N))
    C
180 IF(m0\mug) 60 10 140
            general case
        FF = CTAN(IOR"XX)
        3IGA(1)=-2INY FF/(21NYPFF-1.0)
        00120 N = 2,KT
        120 !1GA(N)=-(N-ZIMV)+1.0/((N*2INV)-0IGA(N-1))
    60 ro 200
C
102.
103.
104.
105.
166.
10%.
C
10%.
119.
128.
C
111.
112.
113.
114.
115.
116.
117.
118.
119.
    C
128.
121.
    COMNI = INAB,0.OJ
C QEXIMITIALIZE SUNS FOR EFFICIENCIES ANO ASYMMETEV FACTOR
122.
123.
124.
200 cON7IMUE
    IORINV = 1.0/10R
    RIORIV = 1.0/REIOR
            IMIIIALIZE QUAMTITIES USED FOR EFFICIENT CALCULATION OF
            MUNERICAL COEFFICIENTS IN MIE SERIES
    FN = }8.
    RN = 1.0
    mn=1
            IMITIALIZE RIEATII-BESSEL FUNCTION ZETA FOR UPMARD RECURRENCE
    PSIN = SIN(xX)
    CHIM = COS(xx)
    PSIMPI = XINY*PSIN-CHIN
    CHINPI = XIMVOCHINOPSIN
    ZETM = CMPLX(PSIN,CHIN)
    ZETMPI - ENPLX(PSINPI,CHINPI)
            INITIALIZE PREVIOUS COEFFICIENTS (A-SUB-N-I, B-SUB-N-1)
            FOR USE IN ASYMAETRT FACTOR SERIES
    anns = (0.0.0.0)
    QEXT =0.0
    osca - 0.0
    GFAC = 0.0
```



```
125. 00250 J=1,IN
126. SP(J)= (0.6.0.0)
    SN(J)= (0.J.0.0)
    SPS(J)=(0.0.0.0)
    SMS(J)=(0.0,0.0)
    PINMI(J)=C.O
    250 PIN(J)=1.0
    C
    C
        OO 500 M= 1,MT
        COMPUTE THE VARIOUS MUMERICAC' COEFFICIEMTS NEEDEO
        FNP1 E FM+1.0
        TMONPI = FM&FMPI
        RNP1 = 1.0/FMP1
        CJEFF =RN+RNPI
        MPION=1.O&RN
            CALCULATE THE MIE SERIES COEFFICIENTS LITTLE-A ANO LITTLE-B
        IF(NOINAG) 60 TO 300
            GENERAL CASE
        AM=(GIORINV*BIGA(M)O(FM*XINV))*PSIMPI-FSINI/
            ((IORINV*BIGA(N)+(FM*XINV))* ZETNPI-ZETM)
        BN:(\ IOR'日IGA(M)* (FN*XIWV))*PSIMPI-PSINI/
                IOR*BIGA(Y)*(FM*XIMV)) [ETNPI-2ETM)
            IMCREMENT SERIES FOR SCAYTERING EFFIEIENCY
```



```
        -
        60 TU 350
    C
    300 CONTINUE
        MO-ABSORPTION CASE
        AN = ((RIORIVEEQ3IGA(M)+(FWNIMVI)OPSIMPI-PSIN)/
            ((RIOPIV*EQEIGA(M)+(FN*XINVI)*ZETMPI-ZETN)
        BN: (I REIOR+EQSIGI(M) +(FNEXINV))&PSIMPI-PSIM)/
            (( REIOR*EQSIGA(M)*(FN*XIMVI)* ZETidPI-ZETN)
    C
    350 CONIINUE
        INCREMENT SERIES FOR ASYMMETRY FACTOR ANO EXTIMCTION EFFIGIEMCY
        GFAC = GFAC +(FN-RN)*REAL(ANMI*CONJG(AN) BNM& CONJG(BN))
        * COEFF=REAL(AN*COMJG(BN))
        QEXT - QEXT TMONPI*REAL (AMFBN)
        IF(MOANGS) 6O TO 45j
            PUT MIE SERIES COEFFICIENTS IM FORM MEEDEO FOR COMPUTING S+: S-
        ANP = COEFF*(AMOBN)
        BMP = COEFF=(AN-BM)
        AMPM = MM*ANP
        8MPM = MH* GNP
        *OE* VECTORIZABLE LDOP E*E**
        00 400 J = 1,MH
        IOO UP SUNS HHILE UPMARD RECURSIMG AMEULAR FUNCTIONS LITTLE PI
            ANO LITTLETIU
        TMP(J) = (XNU(J)0P[M(J)) - FINM1(J)
        TAL\(J) = FNETMP(J) - PINMI(J)
        SP(J) a SP(J) * AMPF(PIN(J)\bulletTAUN(J):
        SNS(J)= SHS(J) ENPM*(PIN(J)&TEUN(J))
        SH(J) = SM(J) - 3NP*(PIN(J)-TMUN(J))
        SPS(J)= SPS(J)* AMPM*(PIN(J)-TMUN(J):
        PIMML(J) = PIN(J)
        PIN(J) = (XMU(J)*PIM(J)) - MPIOM*TMP(J)
        4O CONTINUE
    C
            UPOATE RELEVANT QUANTITIES FOR MEXT PASS THROUGH LDOP
        MM = - MM
```

```
    165. 450 FN=FNP1
    168. BHNL = BN
                            CALCULATE RICATTI-BESSEL FUNCTIONS ET UPWARO RECURRENCE
    169.
    170.
    171.
    172.
    173.
    174.
    C
    c
    C MULTIPLY SUNS OT APPROPRIAYE FACTORS TO GET QEXT, QSCA, GFAC
    175.
    176. QSCA =2.O(XINVOE2)OQSCA
    177. IF(MOIMAG) QSEA - QEXI
    178. GFAC=4.0(XINY**2)-5FAC/OSCA
    179. IF(MOAMGS) RETURN
    C
    C RECOYER SI ANO S2 FROM SA; S-
    180.
    101.
    182.
    C
    C *OEO VECTORIZABLE LOOP ***O*
            DO 900 J = 1,NN
            S1(MM2-J)-(.5*(SPS(J)*SMS(J))
        988 S2(MN2-J)=8.5*(SPS(d)-S.4S(d))
            C
            RETURN
..186.
.. 187.
HIEvO
MIEVO
MIEvo
MIEVO
MIEVO
MIEVO
```

```
    CRAT FORTRAN CUSPILER VERSION 1.05 05/O4/T9
    COMPIDAJION CATE NNO IINE -...07/C9/7Y -.-. 1111P139
    1. COMPLES FUNCTION CTAN(2)
        COMPLEX TAMGENT OF 2
    COMPLEX Z
        C
    3. TmOX = 2.*REAL(Z)
```



```
    5. EGY=E2YO&2
    b. LEN = d./((z.0E2T)*CCS(TMOX)+EGrOd.)
        CTAN = CMPLX( (Z.0EZY)-SIN(TMCX)OCEN, (E&Y-1.).JEN)
        RFTURM
        ENE
```


## APPENDIX II: MIEVI FLOW CHART AND CODE LISTING






```
    C SH(J)
C SHS(J) S-a SL-S2 FOR (NN2-J)TH ANGLE
cuse conio
angular oinensions
    2.
    3.
    4.
    CEND
    PARAMETER (NANGL2=(NANGL+1)/2)
    PARAMETER (NT1=5100)
    PARAMETER (NTI2=2*NTI)
```



```
    REAL NPION
    LOGICAL NOIMAG
    COMPLEX CTAN
    COMPLEX A1,A2,G1,IORSO,RAT
    COHPLEX SP,SN,SPS,SMS,ANPM,BMPN,AN,BN,BIGA,ZETA,
    * IORINV,AK,NUM, DEN,FF, ZINV,NIN,OTD,TT
    OIHENSION SP(NANGL2), SH(MANGL2),SPS(MANGL2),SHS(MANGL2),
    * PIN(NANGL2), PINML(MANGL2), TAUN(NANGL2), THP(MANGLL), AM(NT1),
    - BN(MT1), छIGA(NT1),EQBIGA(MT12),PSI(NT1)
        EQUIVALENCE (BIGA,EQBIGA)
    EQUIVALENCE (SI(1),PIN(1)),(SI (NANGL2),PINM1(1)),
    *
                            (S2(1), TAUN(1)),(S2(NANGL2), TMP(1))
    F(REM) = -15.14 + REM*(0.42+16.35*REM)
    DATA EPS1/1.E-2/, EPS2/1.E-8/
    DATA HAXIT/10800/
    DATA IPASS/C/
    C
    IF(IPASS.NE.8! 60 TO 2
    IPASS = 1
        CAlCulate mecessary mumerical coefficients for mie series
    001 N=1,NT1
    FM(N)=N
    TMONP1(N) = M*(N+1)
    COEFF(N) = THONP1(N);(N*(N+1))
    GCOEF(N)=(N+1)-1.0 %(N+1)
    1 CONTINUE
    C
    2 IFSNUMANG.GT.NANGL .OR. MURANG.LT.0) STOP 10BO
    NN2 = NUNANG+1
    MN = NN2/2
    AIMIOR = ABS(AIMAG(IOR))
    REIOR = REAL(IOR)
    MOINAG = AIMIOR.LE.MZCUT
    C
    C
    C
        SMALL-PARTICLE LIHIT
    IORSO = IOR**2
    RAT = (0.,0.66666666666667)*(IORSQ-1.0)
    A1.. RAT*(1.8-0.1*xXF*2+(4.FIORSO+5.)/1400.*(xX**4))
    * . (IIORSO*2.0+(1.0-0.7*IORSQ)*(XX**2)-(8."IORSQ**2-385.*IORSQ
    * +350.)/2400.*(xx-*4)+(xx**3)*RAT*(1.0-0.1*xx**2))
    B1 = (xX**2/30.)*RAT*(1.0+(2.*IORSQ-5.)/70.*(xX**2))
    /(1.0-(2.FIORSQ-5.)/30."(xx+*2))
    A2 = (A.14*X*F2)*RAT*(1.0-XX=* 2/14.)
    * /(2:-IORSO+3.-(2.-1ORSQ-7.)/14.*(xX-C21)
    TEM = CABS(A1)+*2+CABS(B1)*E2+(5.13.)*CABS(A2)**2
```

```
IF(CABS(NUM/AK).GT.EPSI..ANO. CABS(OEN/AK).GT.EPSI) GOTO 30
                        ILL-CONIITIONED CASE--STRIDE THO TERKS INSTEAD Of ONE
    NM = -MH
    KK=KK+2
    AK = (MA*KK)-ZINY
    NTN = AK*NUM + 1.0
    DTO = AK+DEN + 1.0
    FF= (NTN/OTJ): FF
    NM=-NM
    KK=KK+2
    AK = (MH+KK)*ZINV
    NUH = AK + NUH/NTN
    DEN = AK * DEN/OTO
    KOUNT = KOUNT+1
    60 10 20
    C
        30 TT = NUM/DEN.
        FF = TT*FF
            ChECK FOR CONVERJENCE
        IF(ABS(REAL(TT)-1.0)..LT.EPSZ .AND. ABS(AIMAG(TT).).LT.ESPSZ GOTO 50
        MH = -MM
        KK = KK+2
        AK = (NH*KK)"ZINV
        NUM = AK + 1.0/NUN
        DEN = AK + 1.0/DEN
        60 TO 20
    C
    108.
    109.
110.
111.
112.
113.
114.
115.
-116.
    117.
118.
1 1 9 .
120.
121.
122.
123.
124.
125.
126.
40 WRITE(6,8001) NT, XX, IOR, AK,NUM,DEN,TT,FF
8001 FORHATI/I/* CONTINUED FRACTION FOR A-SUG-NT FAILED TO CONYERGE*/
    * * NT=416/* XI*E20.8/E REFR INDEX=F2E20.8/* AK=*2E20.8/
```



```
        STOP 1002
    C
    50 gIGA(NT) = FF
C
DOMNHARO RECURRENCE FOR BIGA-N
        DO 70 N = NT,2,-1
    70 BIGA(N-1) = (FN(N)* LINV) - 1.0/((FN(N)*ZINV)*BIGA(N))
        60 10 180
    C
C
C
        genERAL case
        FF= CTAN(IOR*XX)
        BIGA(I) = -ZINV.FF/(ZINVFFF-1.0)
        DO 120 N = 2,MT
    120 BIGA(N)=-(N*ZINV)+1.8/((*N+IINV)-BIGA(N-1))
    60%0180
C
C NO-ABSORPIION CASE
140 REZ * REIOR'XX
        REZINV = 1.0/REZ
        TEM = TAN(REZ)
        EQ日IGA(1) = -RELINV + TEN/(REZINY*TEM-1.0)
        OO160N = 2,NT
        160EQBIGA(N)= - (FN(N)*REZINV) & 1.O/((FN(N)*REZINY)-EQBIGA(N-1))
            calculate the mie series coefficients little-a and little-b
            fOR THE NO-ABSORPTION CASE
```

```
127. RIORIV = 1.C/REIOR
C **** VECTORIZABLE LOOP *****
            DO 170 M = 1,NT
            AN(N)=((RIORIV*EQRIGA(N) +(XINV*FN(N)))*PSI(N+I) - PSI(N))
                        /((RIORIY*EQEIGA(N)+(XINV*FN(N)))* BN(N+1) - BN(N))
            BN(N)=({ REIOR*EQBIGA(N) +(XINV*FN(N))):PSI(N+1) - PSI(N))
            * ((C REIOR*EQBIGA(N)* (XINV*FN(N))) BN(N+1) - BN(N))
            170 CONTINUE
            60 TO 200
C
C CALCULATE THE MIE SERIES SOEFFICIENTS LITTLE-A AND LITTLE-B
            FOR THE GENERAL CASE
    180 CONIINUE
            IORINV = 1.0/IOR
    C F*FF% VECTORIZASLE LOOP *****
        DO 190 N = 1,NT
        AN(N)=((IORINV*GIGA(N)*(XINY*FN(N)))*PSI (N+1) -PSI(N))
            * /((IORINV*BIGA(N) +(XINV*FN(N)))* EN(N+1) - 3N(N))
            GN(N)=(( IORFBIGA(N)+(XINV*FN(N)))*PSI(N+1)-PSI(N))
                            /((IOR*EIGA(N)*(XINY*FN(N)))* BN(N+1)-BN(N))
    190 CONTINUE
                    CALCULATE TERNS OF SERIES FOR SCATTERING EFFIEIENCYM AND SUM
    *F#** VECTORIZABLE LOOP.. *****-
            DO 195N = 1,NT
    195 EQEIGA(N) = TWONPI (M)* (REAL(AN(N))*F2*AIMAG(AN(N))**2
                                    *REAL(AN(N))* * 2+AIMAG(BN(N))**2)
                            C
                            C
                            C
142.
    200 CONTINUE
        *****.VECFORIZABLE LOOP ******
            00 3GON = 1,MT
    300 EQEIGA(N)_E.TMONPI (N) FREAL(AM(NL&BN(M&)S
            QEXT = 2.F(XINY**2)*TOTAL(MT, EQBIGA)
            IF(MOIMAG). QSCA = QEXT
            CALCULATE TERNS OF SERIES FOR ASTMNETRY FACTOR AND SUM THEN
                    GSET FOLLOWINS COEFFICIENTS TO ZERO BECAUSE THEY OCCUR IN
                    LAST TERH OF SERIES FOR ASYMMETRY FACTORI
            AN(MTP1) = (0.0.0.0)
            3N(NTP1) = (0.0,0.0)
            ** VECTORIZABLE LDOF
            00 400 N = 1,NY
        400 EOZIGA(N) = COEFF(N)FREAL(AN(N)#CONJG(BN(N)))
                        * GCOEF(N) FREAL(AN(N) PCONJG(AN(N+1)) +BN(N)GCONjG(8N(N+1)))
            GFAC = 4.*(XINV**2)*TOTAL(NT,EOECIGA)/OSCA
            IF(NUNANG.EQ.B) RETURN
            COMPUTE S*,S - OVER ANGULAR MESH
            PUT MIE COEFFICIENTS IN FORM NEEDEO
    se*e& VECTORIZABLE LOOP -S***
    DO 450N=1,NT
    BIGA(N) = AN(N)
    AN(N)=COEFF(N)* (AM(N)*BN(N))
    450 BN(N) = COEFF(N)*(BIGA(N)-BN(N))
```

```
    C INITIALIZE SUMS (S*,S-) AND ANGULAR FUNCTIONS (LITTLE PI)
    C ***** VECTORIZABLE LOOP *****
    157.
    158.
    159.
    160.
    161.
    162.
    163.
%}\begin{array}{r}{C}\\{C}\\{C}
C
    500 PIN(J) = 1.0
C AOD UP SUMS KHILE UPWARD RECURSING ANSULAR FUNCTIONS LITTLE PI
                    AND LITTLE TAU
            MM =1
    165. DOTOON: 1.NT
    166. NP1ON=(N+1)/FLOAT(M)
    167. ANPM = MN*AN(N)
    168. BNPM = MM*BN(N)
    MM = - MM
C F**** VECTORIZABLE LOOP ******
    00600 J = 1,NN
    TMP(d)=(XMU(J)EPIM(j)) - PIMMI(J)
    TAUN(J)=FN(M)*TMP(J) - PINMI(J)
    SP(J) = SP(J) & AN(N)= (PIN(J)+TAUN(J))
    SMS(J) = SMS(J) + BNPN*(PIN(J) +TAUN(J))
    SN(J)=SM(J) + BN(N)*(PIN(J)-TAUN(J))
    SPS(J) = SPS(J) & ANPN*(PIN(J)-TAUN(J))
    PINMI(J) = PIN(J)
    PIN(J) = (XMU(J)*PIM(J)) + NP\ION=TMP(J)
        600 CONTINUE
        700 CONTINUE
            C
C
C RECOYER S1 AND SZ FROM St, S-
    181.
    182.
    183.
        800 S2(J)=0.5*(SP(J)-SM(J))
            C
        ***** VECTORIZABLE LOOP *E***
            00900 J = 1,NN
            S1(MN2-J) = .5*(SPS(J)+SMS(yj)
        900 S2(MN2-J)=0.5*(SPS(J)-SMS(J))
    C
    187
. 188.
MIEV2
MIEVI
MIEV1
MEVI
MIEY1
MLEV1
HIEVI
MIEV1
HLEVI
VECTOR GLOCK BEGINS AT SEQ. NO. 153, P= 1113250
HIEV1 VECTOR BLOCK GEGINS AT SEQ. NO. 15%, P= 1113351C
MIEV1 VECTOR BLOCK BEGINS AT SEQ. NO. 1. 165, PE 18, 1114070
MIEV1 VECTOR BLOCK BEGINS AT SEQ. MO. 181, PE 1114450
HIEVI VECTOR BLOCK BEGINS AT SEQ. NO. 184, Pe 1115200
```

```
CRAY FORTRAN COMPILER VERSION 1.C4 12/27/78
    COMPILATION DATE AND TIME 02!C9/79 - 221:4132
    1.
    FUNCTION TOTALILENGTH,ARRAY)
        C
        C PARTIALLY-VECTORIZED SUM ROUIINE
        C I NPUT
        C ARRAY VECTOR OF TERMS IO BE SUMMED
        LENGTH. NUHBER OF TERHS IN GRRAY* TO BE SUMMED
        OUTPUT
            TOTAL = SUM(ARRAY(I)), I = 1 TO LENETH
            NOTE--RELIES ON THE ZERO TRIP COUNT FEATURE, WHEREBY IF A
                OO-LOOP IS ALREADY SATISFIED AB INITIO, IT IS SKIPPED
                RATHER THAN BEING EXECUTEO ONCE
            DIMENSION ARRAY(1), HELPER(64)
            IF(LENGTH.GT.G4) 50 TO 5
            TOTAL = ARRAY(1)
            001 N = 2,LENGTH
            2 TOTAL = TOTAL + ARRAY{N}
            RETURN
            C
            5 \text { CONTINUE}
            C ***** VECTORIZABLE LOOP *****
            00 10N=1,64
        10 HELPER(N) = GRRAY(N)
    C
            XOUNT = (LENGTH-64)/64.
            JS =63
            DO 30 J = 1, KOUNT
    C F*** VECTORIZABLE LOOP *****
            DO 20 N = 1,64
        20 HELPER(N) = HELPER(N) * ARRAY(N&JS+1)
        30 JS = JS+64
    C
            LAST = (LENGTH-64) -64*KOUNT
    C W*** VECTORIZABLE LOOP WHEBE
            00 40 N = 1,LAST
        tO HELPER(N) = HELPER(N) + ARRAY(LENGGTH*I-N)
            TOTAL = HELPER(1)
            00 50 N=2,64
        50 TOTAL = TOTAL + MELPER(N)
            RETURN
            END
OTAL VECTOR ELOCK BEGINS AT SEQ. NO. B, P= 143C
DTAL VECTOR BLOCK BEGINS AT SEQ. NO. 13; Pa 166A
OTAL VECTOR BLOCX BEGINS AT SEQ. NO. 17, Pa 2070
```


## APPENDIX III: SAMPLE CODE RESULTS

```
prograh main
    C RUN TEST GASES
    CuSE COMIO
    C angular oimensioms
2. PARAMETER (NANGL=255)
    COMPLEX IOR, S1, S2
    REAL NZCUT
    COMMON/INOUT/XX,IOR,NZCUT, NUMANG,XHU(NANGL),QEXT,QSCA,GFAC,
        - SI(NANGL),SZ(NANSL)
    CEND
        REAL I1,I2,INTEN
    C
        N2CUT = 1.E-T
        PI = 2.*ASIN(1.0)
        MUMANG = 37
        OO 1 I = 1,NUNANG
        1 XMU(I) = Cos((I-1)*PI/36.)
    C
    DO 100 MIOR = 1,2
        IF(MIOR.EQ.1) IOR = (1.5,0.0)
        IF(NIOR.EQ.2) IOR = (1.5,-0.1)
        OO 100 NXX = 1,4
        IF(NXX.EQ.1) XX=10.
        IF(NXX.EQ.2) XX = 100.
        IF(NXX.EQ.3) XX=1000.
        IF(NXX.EQ.4) XX = 5000.
        I1 = SECONO(DUN)
        CALL MIEVI
        T2 = SECONO(DUN)
        DT = T2-T1
        QAES = QEXT-QSCA
        MRITE(6,100G) XX,IOR
        DO IO I = 1,NUMANG
        ANGLE = 100./PIFACOS(XAU(I))
        I1=(REAL(SI(I)))**2+(AINAG(SI(I)))=E2
        I2=(REAL(S2(I)))**2+(AIMAG(S2(I)))**2
        INTEN = 0.5*(II+I2)
        OEGPOL = (I2-II)/(I2+I1)
        10 WRITE(6,1001) ANSLE,S1(I),S2(I),INTEN,OESPOL
            WRITE(6,1002) QEXT,QSCA,QABS,GFAC,OT
        1%0 CONTINUE
    C
        CALL EXIT
        1000 FORMAT(1H1, 5X,*HIE SIZE PARAMETER =*FA.2,15X,*REFRAGTIVE INDEX =*
    * FT.3,E12.3//* ANSLE*,11X,*S-SUB-1*,21X,*S-SUB-2*,15X,
        -INTENSITY*, 2X,*DEG OF POLZN*I
    1001 FORNAT(F7.2,5E24.6,F10.4)
    1002 FORMATI/29X,"EXTINGTION SCATTERING ABSORPIION*/
        * 7X,*EFFICIENCY FACTDRS*,3F14.6/ 7X,*ASYNMETRT FACTOR **F9.6/
        - 7X,*TIME FOR THIS CASE IN SECONOS -*E12.3)
39.
        ENO
```



HIE SIZE PARAMETER $=100.00$ REFRACTIVE INOE'X $=1.520$ 0.000E400



MIE SIZE PARAMETER $=5000.00$
REFRACTIVE INDEX = 1.500 0.000E+30



| ANGLE | S-SUB-1 |  | S-SU3-2 |  | INTENSITY | DEG CF POLZ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0.00 | $0.522455 E+04$ | -0.261694E+03 | $0.522455 E+04$ | -0.261694E+03 | $0.273645 E+00$ | -0.0000 |
| 5.00 | $0.305086 E+03$ | N. $161883 \mathrm{E}+02$ | $0.298131 E+C 3$ | 0.49119JE*01 | $0.911574 E+05$ | -0.0247 |
| 10.00 | -0.116407E+03 | $0.238768 E+02$ | -0.107378E+03 | $0.195041 E+02$ | $0.130172 E+05$ | -0.0.048 |
| 15.00 | 0.44TT29E+02 | -0.434139E+02 | $0.392926 E+02$ | -0.292025E+02 | $0.314304 E+04$ | -0.2375 |
| 20.00 | 0.228785E+01 | 0.4 $23966 \mathrm{E}+02$ | -0.130945E+01 | $0.251409 E+02$ | $0.121824 E+04$ | -0.4798 |
| 25.00 | -0.310537E 02 | -0.211364E+02 | -0.173787E+C2 | -0.104328E+02 | $0.911319 E+03$ | -0.5484 |
| 30.00 | $0.336796 \mathrm{E}+02$ | -0.105491E+02 | $0.177529 E+02$ | -0.652844E+01 | $0.801673 E+03$ | -0.5537 |
| 35.00 | -0.909879E*01 | $0.336759 E+02$ | -0.5105'82E*01 | $0.144508 E+02$ | $0.629347 E+03$ | -0.6268 |
| 40.00 | -0.213207E 02 | -0.189676E+02 | -0.713673E+01 | -0.812180E*O1 | $0.465786 E+03$ | -0.7490 |
| 45.00 | $0.220539 \mathrm{E}+02$ | -0.160293E+J2 | $0.681356 E+01$ | -0.350405E+01 | $0.370932 E+03$ | -0.0418 |
| 50.00 | 0.101882E*02 | $0.222762 E+12$ | $0.196302 E+01$ | $0.555678 E+01$ | $0.317391 E+03$ | -0.8905 |
| 55.00 | -0.206372E+02 | $0.987364 E+01$ | -0.392682E+01 | $0.947194 E+00$ | $0.269848 \mathrm{E}+03$ | -0.9395 |
| 60.00 | -0.129074E+02 | -0.170105E+02 | -0.61276CE+00 | $-0.207280 E+01$ | $0.230451 E+03$ | -0.9797 |
| 65.00 | $0.101149 E+02$ | -0.173895E+02 | $0.876630 E+00$ | -0.208839E+00 | $0.202758 E+03$ | -0.9960 |
| 70.00 | $0.189202 E+02$ | -0.134859E+01 | -0.669262E+00 | 0.749534E+00 | $0.1804015+03$ | -0.9944 |
| 75.00 | $0.139393 E+02$ | $0.112006 E+52$ | -0.187769E*01 | -0.736574E+00 | $0.162813 E+03$ | -0.9750 |
| 00.00 | $0.615211 E+01$ | $0.158596 E+32$ | -0.161371E+01 | -0.253497E+01 | $0.149203 E+03$ | -0.9395 |
| 85.00 | 0.153726E+01 | $0.160982 E+02$ | -0.893979E+00 | -0.382594E+01 | $0.138475 E+03$ | -0.8885 |
| 90.00 | $0.119224 E+01$ | $0.153732 E+02$ | -0.850854E+00 | -0.466332E+01 | $0.130113 E+03$ | -0.8273 |
| 95.00 | $0.476301 E+01$ | $0.139482 \mathrm{E}+02$ | -0.217232E+01 | -0.502404E+01 | $0.123599 E+03$ | -0.7576 |
| 100.00 | $0.107160 E+02$ | $0.920299 E+01$ | -0.489459E+01 | -0.368998E+01 | $0.110559 E+03$ | -0.6831 |
| 105.00 | $0.134863 E+02$ | -0.154765E+01 | -0.661969E+01 | $0.110542 E+01$ | $0.114659 E+03$ | -0.6072 |
| 110.00 | $0.424798 \mathrm{E}+01$ | -0.123699E+02 | -0.206t43E+01 | $0.593202 E+01$ | $0.111687 E+03$ | -0.5316 |
| 115.00 | -0.112976E+02 | -0.565574E+01 | $0.699496 E+01$ | $0.321258 E+11$ | $0.109437 E+03$ | -0.4586 |
| 120.00 | -0.334094E*01 | 0.117717 E 02 | 0.204077 CHO | -0.785874E+01 | $0.107749 E+03$ | -0.3897 |
| 125.00 | $0.115402 E+02$ | - J.c83158E+01 | -0.818386E+01 | $0.219927 E+01$ | $0.106503 E+03$ | -0.3257 |
| 130.00 | -0.102052E+02 | -0.529585E+01 | $0.788721 E+01$ | $0.308961 E+01$ | $0.105600 E+03$ | -0.2673 |
| 135.00 | $0.74803 C E+01$ | $0.845910 E+01$ | -0.6106C5E+01 | -0.671763E+01 | $0.104961 E+03$ | -0.2148 |
| 140.00 | -0.715616E+01 | -0.842059E+01 | 0.61119CE* 01 | $0.704053 E+01$ | 0.104521E+03 | -0.1684 |
| 145.00 | $0.936308 E+01$ | $0.566682 E+01$ | -0.027119E+01 | -0.474255E+81 | $0.104229 E+03$ | -0.1278 |
| 150.00 | - $0.105309 E+02$ | $0.102926 E+01$ | 0.955976E+01 | -0.172014E+01 | $0.104044 E+03$ | -0.0932 |
| 155.00 | $0.340006 E+01$ | -0.994907E 01 | -0.315956E+01 | 0.934199E+01 | $0.103935 E+03$ | -0.0643 |
| 160.00 | $0.931348 E+01$ | $0.462414 E+01$ | -0.895099E+01 | -0.441695E+01 | $0.103877 E+03$ | -0.0409 |
| 165.00 | -0.221822E+01 | $0.100651 E+J 2$ | $0.215464 E+01$ | -0.984025E+01 | $0.103850 E+03$ | -0.0229 |
| 170.00 | -0.941598E+01 | $0.402882 E+01$ | $0.931863 E+C 1$ | -8.399378E+01 | $0.103840 E+03$ | -0.0101 |
| 175.00 | -0.100624E402 | -0.168764E+01 | 0.100372E+02 | $0.168188 E+1$ | $0.103837 E+03$ | -0.0025 |
| 180.00 | -0.954952E+01 | -0.355581E*1 | $0.954952 E+01$ | 0.355561E+01 | $0.103837 E+03$ | -0.0000 |
|  |  | EXIINCT | TION SCATTER | RING ABSORPI |  |  |
|  | EFFICIENCY FACI | IORS 2.089 | 822 1.132 | 1340.957 | 88 |  |
|  | ASYMAETRY FACTOR | OR = 0.950392 |  |  |  |  |
|  | TIME FOR THIS C | Case in seconos | S 0.200E-02 |  |  |  |



REFRACIIVE IVDEX $=1.500-0.100 E+00$

| angle | S-SUB-1 |  | S-SUB-2 |  | INTENSITY | DEG OF POLZN |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0.00 | 0.125423E+08 | -0.666472E+J5 | $0.125423 E+08$ | $-0.6664725+05$ | $0.157315 E+15$ | -0.0000 |
| 5.00 | $0.222714 E+04$ | 0.190241E+04 | $0.200270 E+04$ | $0.169246 E+04$ | 0.772728E+07 | -0.1103 |
| 10.00 | - v. $208972 \mathrm{E}+04$ | 0.798514E+J3 | -0.17229LE+04 | $0.620805 E+03$ | $0.417917 E+07$ | -0.1975 |
| 15.00 | -0.198699E+04 | $0.275570 E+03$ | -0.14759EE+04 | $0.152643 E+03$ | J. $311291 E+07$ | -0.2927 |
| 20.00 | $0.141605 E+64$ | $0.118670 \mathrm{E}+34$ | $0.899033 \mathrm{E}+03$ | $0.930170 E+03$ | $0.245545 E+07$ | -0.3902 |
| 25.00 | $0.365848 E+03$ | $0.167373 E+04$ | $0.153163 E+03$ | $0.996380 E+03$ | $0.197572 E+07$ | -0.4856 |
| 30.00 | -0.818828E+03 | -0.136541E+J4 | -0.365770E+03 | -0.736552E+03 | $0.160555 E+07$ | -0.5788 |
| 35.00 | $-0.695859 E+03$ | 0.130789E+J4 | -0.366383E+03 | $0.549989 E+J 3$ | $0.131668 \mathrm{E}+07$ | -0.6680 |
| 40.00 | $0.120796 \mathrm{E}+04$ | $0.670896 E+03$ | $0.420519 E+03$ | $0.306897 E+J 3$ | $0.109011 E+07$ | -0.7513 |
| 45.00 | $0.377639 E+03$ | -0.123406E+04 | $0.174189 E+03$ | -0.357729E+03 | $0.911909 E+06$ | -0.8264 |
| 50.00 | -0.737055E+03 | $0.956727 E+03$ | -0.223330E+03 | $0.189279 E+03$ | $0.771474 E+06$ | -0.8906 |
| 55.00 | -0.760225E+03 | $-0.832129 E+03$ | -0.871019E+02 | -0.176458E+03 | $0.660667 \mathrm{E}+06$ | -0.9414 |
| 60.00 | -0.106248E+04 | -0.625555E+J2 | -0.101042E*03 | -0.581135E+02 | $0.573177 E+06$ | -0.9763 |
| 65.00 | $0.698164 \mathrm{E}+03$ | -0.719402E+03 | $0.552444 E+02$ | $0.124093 E+02$ | $0.504609 E+06$ | -0.9936 |
| 70.00 | -0.736341E+03 | -0.594638E+03 | $0.564372 E+02$ | -0.115428E+02 | $0.449555 E+06$ | -0.9926 |
| 75.00 | -0.704422E+03 | -0.553289E+03 | $0.10015 C E+03$ | $0.270281 \mathrm{E}+02$ | $0.436550 E+06$ | -0.9735 |
| 00.00 | $0.510198 E+02$ | -0. $048290 E+03$ | $0.279151 E+02$ | $0.149684 E+03$ | 0.372691E+06 | -0.9378 |
| 85.00 | $0.789722 E+03$ | -0.172201E+03 | -0.182738E+03 | $0.738612 \mathrm{E}+02$ | 0.346095E+06 | -0.8878 |
| 90.00 | 0. $54381 \mathrm{CEF}+03$ | 0.546205E+03 | - $0.187405 E+03$ | $-0.146093 E+03$ | $0.325266 E+06$ | -0.0264 |
| 95.00 | $0.460068 \mathrm{E}+03$ | $0.575586 E+13$ | -0.190918E+03 | $-0.196543 E+03$ | $0.309020 E+06$ | -0.7570 |
| 100.00 | $0.632089 E+03$ | -0.315106E+33 | -0.26319EE+03 | $0.157238 \mathrm{E}+03$ | 0.296412E+06 | -0.6829 |
| 105.00 | -0.521195E+03 | $0.434773 E+03$ | $0.244271 E+03$ | -0.230296E+03 | $0.286689 E+06$ | -0.6069 |
| 110.00 | -0.620403E+03 | $0.206778 E+03$ | $0.337167 E+03$ | -0.130982E+03 | $0.279248 E+06$ | -0.5315 |
| 115.00 | $0.622942 E+03$ | 0.105012E*O3 | -0.381748E+03 | -0.490048E+02 | 0.273608E+D6 | -0.4586 |
| 120.00 | $0.582781 \mathrm{E}+03$ | $0.186360 E+03$ | -0.389915E+03 | -0.111223E+03 | 0. $269384 \mathrm{E}+06$ | -0.3897 |
| 125.00 | $-0.563023 E+03$ | $0.109764 E+03$ | $0.397962 E+03$ | -0.145440E*03 | 0.266266E+06 | -0.3258 |
| 130.00 | $0.309726 E+03$ | $0.488408 E+03$ | -0.243028E+03 | -0.366541E+03 | 0.264005E+06 | -0.2674 |
| 135.00 | $0.396647 E+03$ | $0.401624 E+03$ | -0.323875E+03 | -0.317995E+03 | $0.262403 E+06$ | -0.2149 |
| 140.00 | -0.14781uE+03 | $0.532403 E+33$ | $0.119311 E+03$ | -0.450626E+03 | $0.261300 E+06$ | -0.1684 |
| 145.00 | -0.410444E+03 | -0.354151E+03 | $0.363689 E+03$ | $0.308185 E+03$ | $0.260568 E+06$ | -0.1279 |
| 150.00 | $0.51206[E+03$ | $0.146039 E+33$ | -0.467928E+03 | $-0.130004 E+03$ | $0.260105 E+06$ | -0.0932 |
| 155.00 | $-0.501483 E+03$ | -0.158270E+03 | $0.470863 \mathrm{E}+03$ | $0.146344 E+03$ | 0.259832E+06 | -0.0643 |
| 160.00 | $0.429276 E+03$ | $0.293303 E+33$ | -0.412840E+03 | -0.280406E+03 | $0.259684 E+06$ | -0.0409 |
| 165.00 | -0.279973E+03 | -0.432636E* 03 | $0.274284 E+03$ | $0.422422 E+03$ | $0.259616 E+06$ | -0.0229 |
| 170.00 | $0.101686 E+03$ | $0.511835 E+03$ | -0.101195E+03 | -0.496708E+03 | 0.259591E+06 | -0.0101 |
| 175.00 | $0.307655 E+02$ | -0.5U9210E+03 | -0.306023E+02 | $0.507929 E+03$ | $0.259585 E+06$ | -0.0025 |
| 180.00 | $-0.777833 \mathrm{E}+02$ | $0.503522 E+03$ | $0.777333 \mathrm{E}+02$ | $-0.503522 E+03$ | $0.259585 E+06$ | -0.0000 |
|  |  | EXTINC | ON SCATTER | ING ABSORP | ON |  |
|  | EFFICIENCY FACT | TORS 2.00 | 751.099 | 91930.937 | 58 |  |
|  | ASYMMETRY FACTOR | OR $=3.953650$ |  |  |  |  |
|  | TIME FOR IHIS CA | Case In SECONOS | $=0.8 C 6 E-01$ |  |  |  |

