Interactive computations and display of characteristics of the radiation scattered by a sphere: A demonstration for PS/2 Model 80

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The Personal System/2® (PS/2®) Model 80 with its math coprocessor provides a considerable amount of computing power which can be used with advantage to solve technical problems interactively at a standalone workstation. To demonstrate this capability, a scientific program routinely used in diverse disciplines requiring significant computing power was modified to run on the PS/2 Model 80. It computes and displays variations of the specific intensity and degree of polarization of the electromagnetic radiation scattered by a sphere of given refractive index. For a sphere of size parameter of 100, about 475 000 double-precision floating-point calculations are performed and the results displayed in graphic format in less than ten seconds. The selected algorithm is routinely used in several different disciplines such as astronomy, atmospheric optics, chemical engineering, colloidal chemistry, and remote sensing. Because it requires the evaluation of spherical Bessel functions with complex arguments, and derivatives of the Legendre polynomials, it was selected as a representative problem of numerically intensive computing.

For increased productivity, scientists and engineers prefer to solve their technical problems interactively in a computing environment which is completely under their control. However, in order to solve problems of scientific and/or of economic importance, a very significant amount of computing power must be available in such an environment. Until now, although many useful functions can be performed at a standalone workstation such as the PC XT or PC AT®, numerically intensive computing has not been one of such functions. Hence, users have generally shied away from performing serious scientific/engineering applications on this class of computers.

To demonstrate that some of IBM's most recently announced products such as the PS/2® Model 80 and supporting software offer an acceptable approach to the aforementioned problem, a scientific program routinely used in diverse disciplines, and requiring significant and sophisticated computing power, was slightly modified to run on the PS/2 Model 80 with a math coprocessor. The physical problem selected was that of the radiation scattered by a spherical particle. The numerical solution to this problem is routinely required for several hundreds of parameters in such disciplines as astronomy, atmospheric optics, electrical engineering, chemical engineering, colloidal chemistry, and remote sensing. The particular calculation described is restricted to a single spherical particle whose size, scattering, and absorption characteristics can be selected by the user. However, a practical application requires the computation to be carried out for a cluster of particles having a specific size distribution. Typical of such applications is the correction of satellite observations for atmospheric effects. These calculations are also used for particle sizing in photographic emulsions, for mixing paint colors using polymer dispersions, and for detection of environmental pollution.

The calculation described is restricted to a single spherical particle.

Although the actual expressions for this problem were derived in the early part of this century, its numerical solution has posed problems for scientists and engineers until recently. This is because it requires interactive evaluation of spherical Bessel functions with complex arguments, leading to propagation of round-off errors and the need to develop alternative procedures and carry them out via double-precision arithmetic. In studying physical systems it is usually helpful to estimate the bounds of the problem or determine first-order solutions before attempting to obtain a complete or general solution. The interactive desktop approach using the PS/2 Model 80 allows the user to make calculations for various single particles which can be used to estimate the order of magnitude of the solution for a cluster of particles. Complete calculations can be carried out on a mainframe such as the IBM 3090.

The Mie computation,[1] which is of significant scientific interest, was used as a test bed for taking an existing FORTRAN program which had been designed and coded for batch processing on a host computer, and converting it for interactive execution on the PS/2 Model 80. To achieve this we made use of the TRYLON panel system.[2] However, any generally available PC panel system having a FORTRAN interface, such as EZ-VU,[3] could also have been used. The graphics processing was achieved using FORTRAN bindings of the Graphical Kernel System (GKS).

The program computes the characteristics of the electromagnetic radiation scattered by a spherical particle of given refractive index which has a real and an imaginary part. The basic formulas representing the solution of the well-known Maxwell's equations for the stated geometry were first derived in 1908 by Mie.[1] The number of minima and maxima in any of the four characteristics vs scattering angle curve is of the order of the size parameter, which is defined as the ratio of the circumference of the sphere to the wavelength of the incident radiation. The size parameter can assume any value in the range 0.001 (molecular scattering) to 5000 (scattering by raindrops leading to the formation of rainbows). Furthermore, reliable calculations demand that all computations be carried out using double-precision arithmetic procedures.

After providing some basic information about our standalone computing environment, we propose to outline the basic Mie scattering equations and then to describe some of the modifications necessary to download an earlier (publicly available) version developed to run in batch mode on the IBM System/360 Model 50. Finally, we provide information about the running of the demonstration program on a PS/2 Model 80.

Basic computing environment

The IBM PS/2 Model 80 workstation used to develop and run the Mie demonstration has the following features: An 80386 microprocessor supplemented with an 80387 math coprocessor, permanent memory (ROM) of 128 KB, 1 MB of random access memory (RAM), video graphics array (VGA) port to support a 640-by-480-pel display of 16 colors, one 1.44-MB 3.5-inch diskette drive, and one 44-MB fixed disk. The operating system running on this model is IBM PC DOS 3.3. The color display used was an IBM 8513.

The graphical representation of the output was created using the IBM release of GKS. This is the same level of release, Version 1.00, that was available for the IBM PC AT. GKS was selected as the graphics system because of its wide user acceptance as a standard for graphics on PC-class machines. The standard GKS defines an application-level programming interface to graphics systems. As such, it permits easy transportation of application programs between installations. The version of GKS used in this study is an implementation of basic functions described by the American National Standards for Information (ANSI).[4] To achieve device independence, GKS makes use of a device driver; this is software that is the device-dependent part of the graphics implementation which creates device-dependent output from device-dependent commands. The display devices which are part of the PS/2 family, such as the 8513 display used in this study, do require compatible device drivers. The application programmer accesses the GKS library of routines via several major high-level language bindings, including FORTRAN.

The Mie program requires the user to enter input parameters such as the size and refractive index of a particle. To make this parameter selection convenient, the user is provided a set of panels serving as an interface to the application. These panels and the linkages between them are decoupled from the Mie code, thereby reducing the programming effort. This was accomplished by using a set of programs called TRYLON.[2] TRYLON is a program for IBM internal use only which was developed to run on the PC and PS/2 family of computers that use the DOS operating system. The TRYLON software provides the capability to create full-screen panels during the code-development phase. At execution time, it supports the transfer of data from panels to the application. Panels were chosen for the user interface because they provide a suitable means of displaying input selections and also constitute a convenient way of packaging the application program when it is requested by colleagues.

Mie scattering

As mentioned earlier, expressions describing the radiation scattered by a sphere of known refractive index were first derived by Mie in 1908.[1] These expressions involve spherical Bessel functions with complex arguments, and the first and second derivatives of Legendre polynomials. Because of several complexities, investigators of the 1910–1960 period found it practically impossible to readily evaluate them despite the availability of various forms of automated computing help. It was only in the middle 1960s that research publications providing useful results began to appear on a regular basis. Many details concerning the formulation of the problem and the derivation of the Mie scattering equations can now be found routinely in several books.[5–7] We therefore restrict ourselves to a basic outline, and refer the interested reader to other publications.

A beam of electromagnetic radiation is vectoral in nature, requiring four parameters for its complete definition. A detailed discussion of these parameters is not given here. Reference 7 provides a thorough review of radiative transfer, including the description of the mathematical relationships among the parameters. Two of these physical quantities, the specific intensity, I, and the degree of polarization, P, are computed and discussed in the next section. The specific intensity is the energy contained per unit frequency interval which crosses a unit area per unit time. The degree of polarization is expressed as $P = (I_e - I_r)/(I_e + I_r)$, where $I = I_e + I_r$, and e and r are the two orthogonal directions in the plane normal to the directions of propagation. I_e and I_r respectively represent the intensity components along these directions. Since the four parameters, including these latter two, are of different dimensions, they are unsuitable for mathematical manipulation, and a transformation is made obtaining four related parameters which are used in the mathematical formula of a radiative transfer problem.[8]

The radiation beam incident on a sphere, and that scattered by it, along a direction making an angle θ with the direction of the incident radiation, can be polarized. Hence, a four-by-four matrix is required for computing the derived parameters of the scattered radiation from those of the incident radiation. The nonvanishing elements of this matrix can be obtained from the complex amplitudes $S_1(x, m, \theta)$ and $S_2(x, m, \theta)$ given by

$$S_1(x, m, \theta) = \sum_{n=1}^{\infty} \frac{(2n+1)}{n(n+1)} \{a_n(x, m)\pi_n(\mu) + b_n(x, m)\tau_n(\mu)\} \tag{1}$$

and

$$S_2(x, m, \theta) = \sum_{n=1}^{\infty} \frac{(2n+1)}{n(n+1)} \{b_n(x, m)\pi_n(\mu) + a_n(x, m)\tau_n(\mu)\}. \tag{2}$$

The quantity x appearing in these equations represents the size parameter of the sphere given by $2\pi r/\lambda$, where r is the radius of the sphere and λ is the wavelength of the incident radiation. The quantity m, given by $m = n_1 - in_2$, is the refractive index of the material of the sphere with respect to its surroundings. Finally, $\mu = \cos\theta$. The complex character of the refractive index is required to accommodate absorption by the sphere. The complex functions $a_n(x, m)$ and $b_n(x, m)$, and the phase functions $\pi_n(\mu)$ and $\tau_n(\mu)$ are readily computed according to the algorithms given below.

The complex functions $a_n(x, m)$ and $b_n(x, m)$ are expressible in terms of the spherical Bessel functions of the first and second kind. Because of the large exponent range, it is advantageous to use a logarithmic derivative form. Here we give only the latter version; the reader interested in reviewing the spherical Bessel functions is referred to Reference 8. Accordingly,

$$a_n(x, m) = \frac{\left\{\frac{A_n(mx)}{m} + \frac{n}{x}\right\} \mathrm{Re}[W_n(x)] - \mathrm{Re}[W_{n-1}(x)]}{\left\{\frac{A_n(mx)}{m} + \frac{n}{x}\right\} W_n(x) - W_{n-1}(x)} \tag{3}$$

and

$$b_n(x, m) = \frac{\left\{mA_n(mx) + \frac{n}{x}\right\} \mathrm{Re}[W_n(x)] - \mathrm{Re}[W_{n-1}(x)]}{\left\{mA_n(mx) + \frac{n}{x}\right\} W_n(x) - W_{n-1}(x)}. \tag{4}$$

A recursive definition of the complex function $A_n(mx)$ and $W_n(x)$ appearing in Equations (3) and (4) is as follows:

$$A_n(mx) = -\frac{n}{mx} + \frac{1}{\frac{n}{mx} - A_{n-1}(mx)}, \tag{5}$$

with

$$A_0(mx) = \cot(mx); \tag{6}$$

$$W_n(x) = \frac{2n-1}{x} W_{n-1}(x) - W_{n-2}(x), \tag{7}$$

with

$$W_{-1}(x) = \cos x - i \sin x, \tag{8}$$

and

$$W_0(x) = \sin x + i \cos x. \tag{9}$$

The phase functions $\pi_n(\mu)$ and $\tau_n(\mu)$, which are the first derivatives of the Legendre polynomials appearing in Equations 1 and 2, can be computed using the following recurrence relationships:

$$\pi_n(\mu) = \frac{2n-1}{n-1} \mu\pi_{n-1}(\mu) - \frac{n}{n-1} \pi_{n-2}(\mu), \tag{10}$$

and

$$\tau_n(\mu) = \mu[\pi_n(\mu) - \pi_{n-2}(\mu)] - (2n-1)(1-\mu^2)\pi_{n-1}(\mu) + \tau_{n-2}(\mu), \tag{11}$$

where

$$\pi_0(\mu) = 0, \tag{12}$$

$$\pi_1(\mu) = 1, \tag{13}$$

$$\tau_0(\mu) = 0, \tag{14}$$

and

$$\tau_1(\mu) = \mu. \tag{15}$$

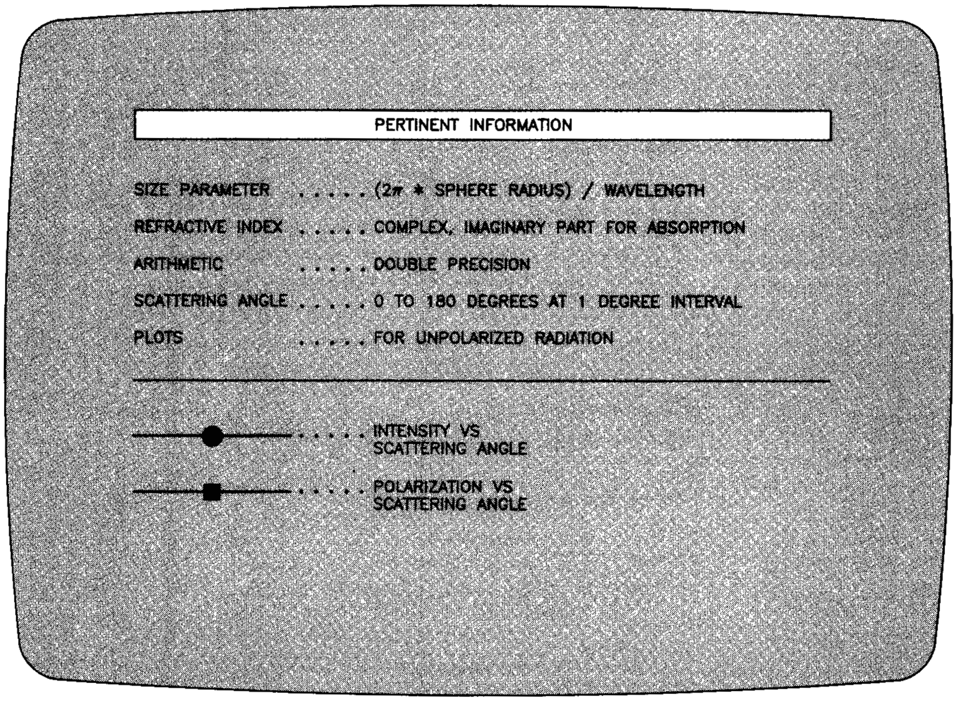
Downloading the earlier (publicly available) version

The Mie scattering equations given in the last section were programmed in 1967 for an IBM System/360 Model 50 in the form of a FORTRAN subroutine using double-precision complex arithmetic. Two versions were developed, and the subroutines were named DAMIE and DBMIE. These routines respectively use an upward and a downward recurrence procedure for computation of the complex function $A_n(mx)$. The downward recurrence, DBMIE, provides reliable results for all possible values of the size parameter and for the refractive index. The findings and listings of these subroutines are well documented[8] in a 1968 report which has been reprinted several times due to continuing demand and is still available on request.

Both subroutines were written to return results for user-provided values of the size parameter and the refractive index, and for up to one hundred values of the scattering angle. After all calculations are completed, values of various optical cross sections of the sphere and of the four nonvanishing elements of the four-by-four scattering matrix are returned to the calling program. Because of the special relationships between the phase functions for a given scattering angle and the supplement of this angle, values of the nonvanishing elements are also returned for the supplements of the scattering angles supplied by the user.

Because of its greater usefulness in comparison with DAMIE, the DBMIE subroutine was downloaded to the PS/2 Model 80. The routine, originally written in FORTRAN IV, was recompiled using the IBM Profes-

Figure 1 Panel defining input parameters and nature of outputs to be displayed



sional FORTRAN compiler. This release of FORTRAN is designed according to the specifications of the American National Standard Programming Language, FORTRAN/77 (ANSI X3.124),[9] and in addition contains many useful extensions. However, the double-precision complex arithmetic functions requiring a declaration of COMPLEX*16 variables are not supported by the IBM Professional FORTRAN. It was therefore necessary to break up the FORTRAN statements related to the computations of $A_n(mx)$ and $W_n(x)$, and eventually those of $a_n(x, m)$ and $b_n(x, m)$ so that the real and imaginary parts can be evaluated separately using REAL*8 variables. Because this was the only change required for downloading of the DBMIE subroutine, the porting, which includes successful compiling and executing, took a minimum of time.

Demonstration program

The DBMIE subroutine as downloaded for execution on a PS/2 can be used for a sphere with any value size parameter. However, it can return scattering results for a maximum of 200 different scattering angles when supplementary directions are included. Of course, one can go through the subroutine repeatedly with different sets of scattering angles, and can build up a table for several thousand values of the scattering angle. Such a procedure would have to be used, since the scattering curves over the 0–180° range can contain up to x minima and maxima. A satisfactory display of a curve with 100 oscillations requires at least 500 points. Because we currently have only a 640-by-480-pel display for our workstation, some arbitrary decisions and trade-offs had to be made. Hence, the panels were designed to accept spheres with size parameter no greater than 100. Even with this moderate upper limit, the curves displayed for large values of the parameter x do not faithfully represent all fine details.

The material used in the following discussion comprises display panels of the contents of an IBM 8513 color display at the PS/2 workstation. The absence of colors in reproduction is generally acceptable except for the curves representing specific intensity vs scattering angle and degree of polarization vs scattering angle, which are shown with identifying symbols. Even in these cases, a user familiar with the physical problem will find no difficulty in identifying the curves.

The panel shown in Figure 1 provides a definition of the size parameter, and reminds the user that the

Table 1 CPU time as a function of size parameter

Size Parameter	Number of Double-Precision Instructions	CPU Time (s)
1	22 K	0.28
5	50 K	0.55
10	78 K	0.82
50	263 K	2.69
100	475 K	4.83
500	2.1 M	21.47
1000	4.2 M	42.02

refractive index of the material of the sphere is a complex quantity. Furthermore, after performing all needed calculations using double-precision arithmetic procedures, the variations of specific intensity and degree of polarization as a function of the scattering angle will be presented for a sphere illuminated by unpolarized (natural) radiation. The curves are plotted, with each having 181 data points.

Table 1 shows the number of floating-point instructions required to compute all four Stokes parameters at 181 different angular positions as the size parameter is varied from 1 to 1000. Because of the use of the downward-recurrence procedure, the number of instructions also depends to some extent upon the value of the refractive index. Furthermore, use of this procedure and the need to have a subroutine capable of providing reliable results for diverse conditions lead to a considerable computational overhead for the small-sized spheres. It may be noted that the values presented in Table 1 do not include instructions for the computations of the specific intensity and the degree of polarization from the Stokes parameters, and those required for the generation of graphs in an easy-to-follow format.

There are three input parameters: the size parameter of the sphere and the real, as well as the imaginary, part of the refractive index of its material. These options permit holding any of these two parameters constant, and stepping through a series of frames for the third parameter, each increasing it by a fixed amount in the user-specified range.

The user may select either a manual or an automatic mode for the display of the frames of results in a graphic format. Under the manual mode, the user must press the enter key to start computations for the next frame. If the automatic mode is selected, the computations for the next frame are started after a lapse of five seconds.

The typical scattering patterns which may be displayed are shown in Figures 2 through 4. The results shown in Figure 2 are for a very small particle (molecular size range). This is a typical Rayleigh scattering pattern, with the specific intensity decreasing by a factor of two as one proceeds from the forward (or backward) direction to the middle. The degree of polarization of the scattered radiation is zero in the forward and backward directions, but is 100 percent in the directions at right angles to that of the incident radiation. For a size parameter of 10 representing a cloud droplet illuminated by the visible light (Figure 3, $m = 1.3333 - 0.0i$), both curves depict about 10 pronounced minima and maxima. The curve for specific intensity vs scattering angle is the one starting in the 1000–10 000 range on the left side of the diagram, decreasing rapidly, and then, after several oscillations, establishing itself in the 5–20 range (use the left scale). The strong specific-intensity maximum in the forward direction is due to diffraction. The remaining oscillations are the result of interference among the waves reflected and refracted by the sphere, and those traveling on its surface. When some absorption is introduced (Figure 4, $m = 1.3333 - 0.1i$), one finds a significant decrease in the amplitude of oscillations in the curve representing specific intensity vs scattering angle.

Table 1 shows the timings for a size parameter range of 1 to 1000. The PS/2 Model 80 is 4.6 times faster than the IBM 360 Model 50 and 7.3 times faster than the PC AT for the computations published in Reference 8.

The calculations using the PS/2 Model 80 were compared to those published in Reference 8 for both real and imaginary refractive index cases, and the results compared exactly to five significant figures.

Concluding remarks

The demonstration program described in the preceding sections clearly shows that a PS/2 Model 80 with the math coprocessor is suitable for obtaining solutions of fairly sophisticated technical problems in standalone office or classroom environments. Since several millions of floating-point instructions can be executed in a matter of minutes, and equations can be easily programmed in Professional FORTRAN, it can be used as a powerful teaching tool in many disciplines. For such activities, it is essential for the potential users to become familiar with a panel system such as TRYLON and GKS. Since the user does not always look for a solution in a matter of minutes,

Figure 2 Variations of the specific intensity (lower curve), and the degree of polarization (upper curve) as a function of the scattering angle for a very small (molecular-range) particle

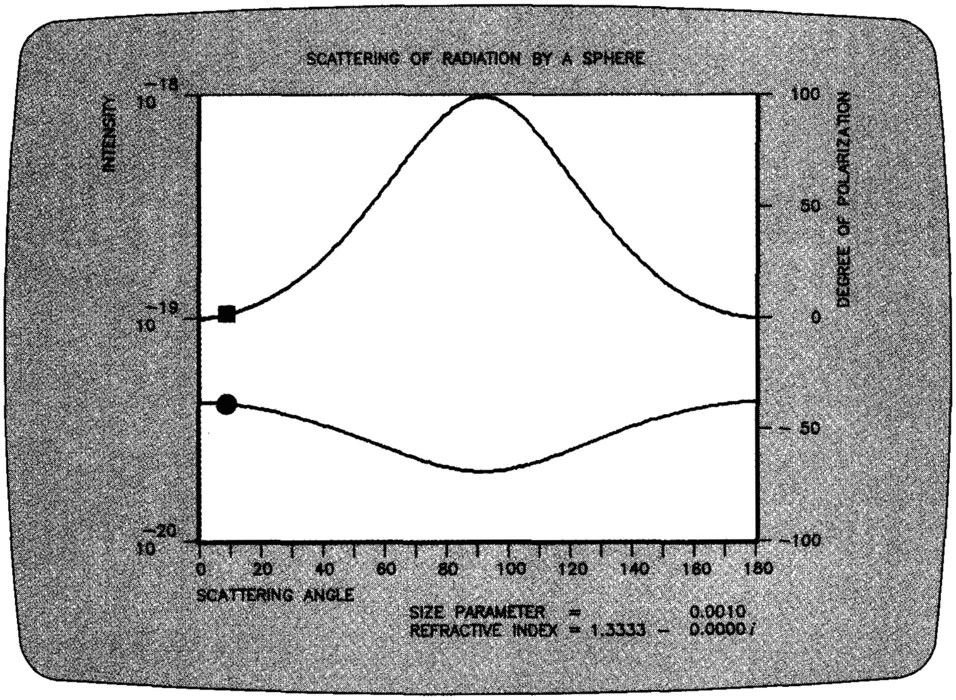


Figure 3 Variations of the specific intensity (the curve starting in the 1000–10 000) range on the left side, eventually settling down in the 5–20 range (use the scale on the left side of the diagram), and the degree of polarization as a function of the scattering angle for a sphere with size parameter 10. The material is water with no absorption; $m = 1.3333 - 0.0i$.

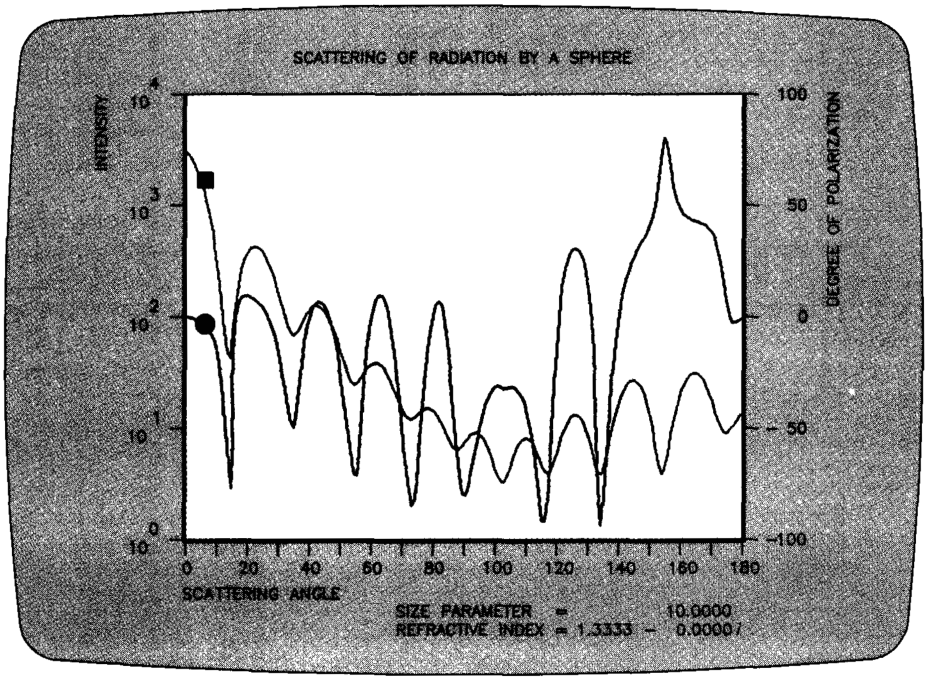
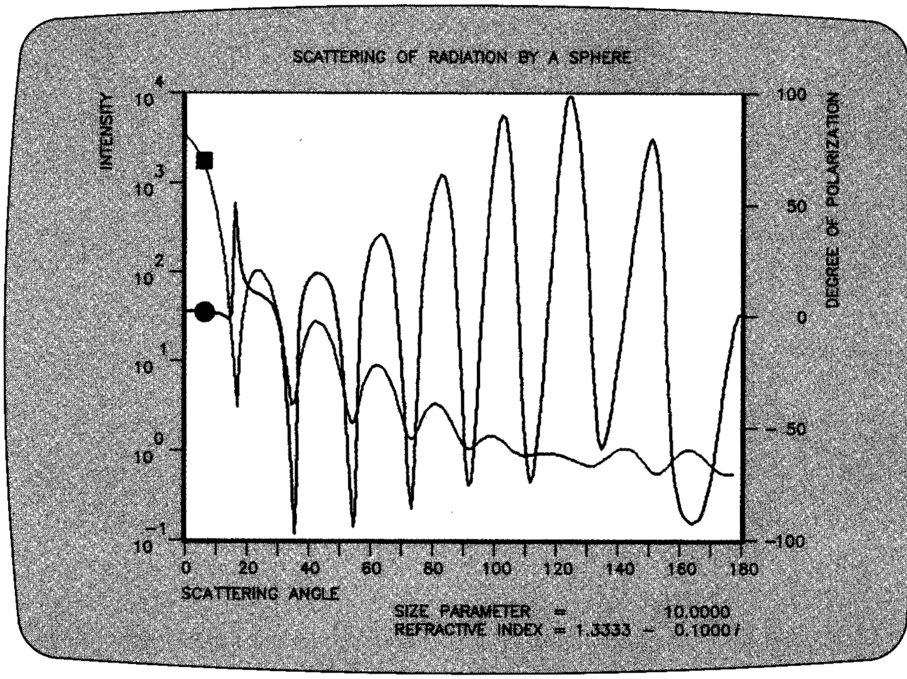


Figure 4 Variations of the specific intensity (see caption of Figure 3 for identification) and the degree of polarization as a function of the scattering angle for a sphere with size parameter 10. The material is water with some absorption; $m = 1.3333 - 0.1i$.



a research problem requiring execution of several hundred million instructions can also be programmed and executed on this model. The availability of the OS/2 operating system can be expected to ease some of the restrictions on the program size. Thus, a PS/2 Model 80 can also be used for graduate-level studies.

Acknowledgments

We take this opportunity to express our sincere thanks to our colleagues Dr. Alan H. Karp for providing the results shown in Table 1, and Dr. Baxter H. Armstrong for carefully reading the first draft of the manuscript and making very helpful comments.

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Reprint Order No. G321-5343.