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Modification of Monte Carlo codes for use with sharply peaked phase functions

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Monte Carlo simulation is one of the commonly used methods of computing radiative transport through scattering media. However, Monte Carlo programs must be revalidated for each new situation that is significantly different from those studied in the past. In a previous work Zardecki and Gerstl compared a Gaussian beam transmission, which was computed by using a small-angle approximation (SAA) solution to the radiative transfer equation, with the transmission that was computed by using the Monte Carlo computer program MSCAT in the EOSAEL package. The results from the two methods are in general agreement, but not in all cases. The two methods yield different transmittances for those cases for which the aerosol phase function is sharply peaked. This would indicate that the failure is in the angular scattering algorithm of the Monte Carlo program, which uses the same lookup table method as the early codes of Collins and Wells. In this note a modification of the lookup table method that will work with sharply peaked phase functions is presented.

A Monte Carlo radiative transfer program works by generating three-dimensional random-walk trajectories for photons, starting at a source and leading to a detector, taking the optical characteristics of both into account. A photon trajectory consists of a series of linear translations of random length, each of which, except for the last, is followed by a change in flight direction. The new flight direction is selected by standard numerical procedures for generating random numbers, using the phase function as a probability density. The scattering angle is generated by inverting the following for $\theta$:

$$U = \frac{\int_{0}^{\theta} P(\cos \theta) d\Omega}{\int_{\frac{\pi}{2}}^{\frac{\pi}{2}} P(\cos \theta) d\Omega}.$$  

This problem can be studied by continuing the comparison begun by Tam and Zardecki. Tam and Zardecki obtained their approximate solution to the radiative transfer equation for a Gaussian phase function of the form

$$P(\cos \theta) = A \exp(-\alpha^2 \theta^2).$$

(In practice $A$ and $\alpha$ are found by doing a least-squares fit to the forward peak of an aerosol phase function if a distinct forward peak is present.) Thus, in order to make a comparison, the same Gaussian phase function must be used to generate the lookup table used in the Monte Carlo program.

The situation for the comparison is the following: A source with a Gaussian beam is aimed directly at a 1-cm-radius circular detector located 23 m away. The initial beam spread is taken to be 5.9 $\mu$rad and its...
becomes more peaked, as can be seen by the asymptote which ideally decreases as the aerosol phase function is incident upon the detector without attenuation. The lower level of the unattenuated transmittance. (Were these transmittances to include direct transmission also in between is assumed to have an extinction coefficient of 217.75 km$^{-1}$ so that the source-to-detector optical depth is 5. The width of the phase function is the only variable in the calculations. Without absorption, transmission loss is caused by beam spreading, which ideally decreases as the aerosol phase function becomes more peaked, as can be seen by the asymptotic approach of the scattered transmittance to the level of the unattenuated transmittance. (Were these transmittances to include direct transmission also there would be a lower asymptote at 7.75 $\times$ 10$^{-4}$ for a unit power source.) In Fig. 1 Monte Carlo, solutions are plotted as points and the SAA solutions are plotted as a solid curve.

First, consider what happens when the width of the phase function becomes less than the spacing between the lookup table angles. By using the lookup table angles provided by EOSAEL, we find that the Monte Carlo code clearly fails to work at all at $\alpha$ = 200 rad$^{-1}$, which corresponds to a phase function width of $\sim$ 0.29 deg. The significance of this number can be appreciated from the fact that the first three scattering angles in the EOSAEL phase function tables are 0, 0.5, and 1 deg. If $1/\alpha$ = 0.29 deg, then only 10% of the generated scattering angles will be greater than 0.58 deg. Thus, once the phase function is narrower than half the value of the first tabulated angle, the photon scattering angles will be generated according to a uniform distribution that is independent of the phase function width.

This failure can be moved to larger values of $\alpha$ by manually picking lookup table angles that are closer together, as was done in Refs. 5 and 6, and which is also provided as an option in the EOSAEL Mie scattering program. This is a time-consuming, error-prone, hit-and-miss procedure. What is needed is an adjustment of the spacing of the discrete angles (actually, cosines of angles) so that the tabulated and actual cumulative phase functions are more nearly the same.

An adaptive quadrature makes such adjustments of the angle spacing automatically. The Mie scattering program in EOSAEL has been modified to be used with the adaptive quadrature PSIMP found in Shampine and Allen.\(^7\) The EOSAEL Mie code can be run so that it calculates a phase function at any single prescribed angle. Thus the Mie code is easy to set up as a subroutine of the adaptive quadrature to be called in place of a function evaluation. The output of this new code is the phase function and the cumulative phase function evaluated at the cosine angles chosen by the adaptive quadrature. The tabulated values thus generated are used in the Monte Carlo code, which has been modified to accept them.

The adaptive quadrature PSIMP works by first applying Simpson’s rule to an integration interval, bisecting that interval, reapplying Simpson’s rule to each subinterval, and then computing a difference between the sums. The process is repeated until the difference is less than some prescribed value. The result is that the integrand becomes evaluated at a fine mesh of points, where it is rapidly varying, and at a coarse mesh, where it is not. When the mesh points, integrand evaluations, and cumulative sums are used in the Monte Carlo code, the agreement with the small-angle solution is extended to $\alpha$ = 200 rad$^{-1}$.

In order to ascertain the cause of this disagreement between the SAA and adaptive Monte Carlo solutions, it is useful to determine the conditions for which the scattering algorithm reproduces the phase function. If the phase function is a Gaussian, then the random scattering angles generated from it ought to occur with a frequency distribution of the same Gaussian. The angular scattering subroutine was incorporated into a separate test program so that the distribution of the scattering cosine angles could be checked by using a $\chi^2$ goodness-of-fit test.\(^8\)

In Fig. 2 the plotted points are the $\chi^2$ test statistics calculated for each value of $\alpha$. The dashed line is the value that, if exceeded by the test statistic, means that the Gaussian hypothesis must be rejected. The test statistic of angles generated by using the fixed angles of EOSAEL are plotted as triangles in Fig. 2.

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Fig. 1. Fraction of transmitted, scattered light from a unit power source that is incident upon the detector aperture. Monte Carlo calculations are plotted as discrete points. Transmittances that are calculated by using the fixed-angle phase function lookup table of EOSAEL are plotted as open triangles. Transmittances that are calculated by using lookup table angles generated with the adaptive quadrature are plotted as filled circles for a single-precision Monte Carlo code and as open circles for a double-precision Monte Carlo code. The upper dashed line represents the fraction of power that is incident upon the detector without attenuation. The lower dashed curve is for the total (direct plus scattered) transmission. The apparent fit of the single-precision transmittances at 1500 and 2000 rad$^{-1}$ is fortuitous. There were not enough photon histories for convergence to occur.
Fig. 2. $\chi^2$ test for determining whether scattering angles have a Gaussian distribution. Triangles indicate the fixed-angle lookup table of EOSAEL. The $\times$'s indicate the single-precision adaptive quadrature. The filled circles indicate the angles that are chosen by using the double-precision adaptive quadrature program, with the angles being output to the test program single precision; the open circles indicate the double-precision test. The probability that the generated scattering angles are Gaussian is less than 5% for points lying above the dashed line.

Angles generated this way are not Gaussian for $\alpha > 20$ and are probably the reason why the EOSAEL Monte Carlo transmittances differ from the small-angle results in Fig. 1 even before the catastrophe at $\alpha = 200$ rad$^{-1}$. The relative differences plotted in Fig. 3 also indicate that the EOSAEL fixed-angle approach fails at $\alpha$ between 20 and 30 rad$^{-1}$.

If the lookup table is generated by using the adaptive quadrature then the scattering angles are Gaussian to $\alpha = 200$ rad$^{-1}$, as is clear in Fig. 2. The adaptive quadrature fails at this point because of round-off error. Neighboring cosines differ only in the seventh decimal place. A finer mesh can be generated if the adaptive quadrature is run with 16-decimal-digit (double-precision) accuracy. The lookup table generated at this accuracy yields scattering angles that are Gaussian to 3000 rad$^{-1}$, at which point the adaptive quadrature program fails. A Monte Carlo program that uses these angles in its lookup table would also have to be double precision. However, lookup table angles that are generated double precision yet $\chi^2$-tested at seven-decimal-digit (single-precision) accuracy generate scattering angles that are Gaussian to $\alpha = 700$ rad$^{-1}$. A lookup table so generated can be used in a single-precision version of the Monte Carlo code, yielding a profit of faster execution than the double-precision version.

In summary at this point, the Monte Carlo code that uses the EOSAEL fixed angles is good only to $\alpha = 20$ rad$^{-1}$, while the use of lookup table angles picked with the single-precision adaptive quadrature is good to $\alpha = 200$ rad$^{-1}$, to 700 rad$^{-1}$ with angles picked with the double-precision adaptive quadrature but used with the single-precision Monte Carlo code, and to 3000 rad$^{-1}$ by generating the lookup table angles double precision and using them in a double-precision Monte Carlo code. The relative differences between the SAA and the Monte Carlo transmittances plotted in Fig. 3 and the transmittances of Fig. 1 show that the double-precision-generated lookup table angles extend the usefulness of the Monte Carlo code to at least $\alpha = 1000$ rad$^{-1}$. The single-precision Monte Carlo code has produced physically impossible transmittances for $\alpha > 1000$ rad$^{-1}$ and so should not be trusted for $\alpha > 700$ rad$^{-1}$. Whether there is any advantage in running the Monte Carlo code double precision for $\alpha$ between 1000 and 3000 rad$^{-1}$ is not clear, because of the tens to hundreds of millions of photon histories needed for convergence for these large values of $\alpha$.

The U-shaped pattern in Fig. 3 is caused first for small $\alpha$ by the failure of the SAA and for large $\alpha$ by poor convergence caused by the tremendous increase in the number of photon histories needed for convergence. To 40 rad$^{-1}$, no more than $10^6$ histories are needed for convergence, whereas $10^8$ histories are estimated to be needed for $\alpha = 1000$ rad$^{-1}$. Convergence is a subjective estimate because the transmittance, as it is being computed, is a nonmonotonic function of the number of photon histories that follows an irregular sawtooth pattern, which makes it difficult to predict what the final value of the transmittance will be. The convergence problem needs to be studied. On the other hand, poor convergence may
Table 1. Representative Phase Function Widths

<table>
<thead>
<tr>
<th>References and Conditions for Aerosol</th>
<th>α (rad⁻¹)</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elliot¹⁰</td>
<td>Mean Diameter (μm)</td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>15</td>
<td>1.85</td>
</tr>
<tr>
<td>F</td>
<td>20</td>
<td>9.39</td>
</tr>
<tr>
<td>G</td>
<td>24</td>
<td>12.9</td>
</tr>
<tr>
<td>Longtin et al.¹¹</td>
<td>Mode Radius (μm)</td>
<td>ln(σ)</td>
</tr>
<tr>
<td>0 m/s</td>
<td>50</td>
<td>6.24</td>
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<tr>
<td>10 m/s</td>
<td>71</td>
<td>7.76</td>
</tr>
<tr>
<td>20 m/s</td>
<td>102</td>
<td>9.28</td>
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<tr>
<td>30 m/s</td>
<td>130</td>
<td>10.6</td>
</tr>
<tr>
<td>Zardecki²</td>
<td>12.5 mm/h rain</td>
<td>1030</td>
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</tbody>
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EOMASS²

<table>
<thead>
<tr>
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</tr>
</thead>
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<tr>
<td>Maritime Arctic</td>
</tr>
<tr>
<td>Maritime Arctic</td>
</tr>
<tr>
<td>Maritime Polar</td>
</tr>
<tr>
<td>Continental Polar</td>
</tr>
</tbody>
</table>

²The aerosol size characteristics are from the references.
³σ is the width of the log-normal size distribution.
⁴Ref. 2.

be a consequence of using the Gaussian phase function, which is defined for small angles only.

Since the validity of the Monte Carlo results is restricted to phase functions of certain widths it is important to know which modes are appropriate for aerosols of a given size. Since α is not a common measure of phase function width it would be helpful to relate α to asymmetry factor g. An estimate of the relationship can be made by fitting the Gaussian phase function to the forward diffraction peak of the Henyey–Greenstein phase function. Obtaining a set of such fitted points of α and g and fitting them with a second-order regression curve yields the relation

\[
-\ln \alpha = 0.318 + 1.287 \ln(1-g) + 0.0398 \ln^2(1-g).
\]

(3)

This equation was used to obtain the estimate of α in Table 1 for the well-characterized aerosols of Elliot.¹⁰ The Gaussian phase function inverse widths for the blowing sand model of Longtin et al.¹¹ were made by making a least-squares fit to the phase functions calculated with a Mie scattering program by using the log-normal size distribution parameters listed in Table 1. Graphic fits were made only to the phase functions of the EOMASS database, which exhibit strong, narrow peaks in the forward direction. Gaussian widths for other aerosols are listed in the Tam–Zardecki paper.²

The fixed-angle lookup table method used for the EOMASS Monte Carlo code does not appear to have much utility. For most cases the best approach is to generate the lookup table angles by using the double-precision adaptive quadrature with a double-precision Mie code and by using a truncated version of these cosine angles with the single-precision Monte Carlo code.

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References