Response to comments of Referee #1 on "MONKI: a three-dimensional Monte Carlo simulator for transfer of polarised light in planetary atmospheres" by Victor Trees et al.

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We thank the reviewer for his/her careful reading and for the comments and suggestions, which have improved the manuscript. Below, we give in *blue italic*the reviewer's comment, in black our response, in *black italic* copied text from the manuscript, and in *red italic*the changed or new text in the manuscript.

First of all, I apologize to the authors and the editor(s) for the delay in producing this referee report.

The manuscript describes a new implementation of the Monte Carlo (MC) method to solve the vector radiative transfer equation. The manuscript confirms recent evidence that MC methods can combine both flexibility and accuracy. The first had long been clear, and indeed MC methods had been the usual choice for complex geometries. The second attribute, however, had been less obvious to the radiative transfer community. The current paper gives further evidence that MC methods are "exact" and, when properly implemented, can achieve arbitrary accuracies if one is willing to pay the cost of running sufficiently long simulations. In my opinion, this is the main point of the paper and I believe it's an important one.

The manuscript provides enough context to understand the implementation of the MC method, and demonstrates sufficiently its performance with comparisons against standard benchmark cases. This said, my main criticism of the manuscript, however, is that the implementation is based on "intuition", i.e. on tracking what happens to the simulated photons at each collision event. That makes it difficult to understand, for example, why neglecting the polarization state of the photon may lead to solutions that fail to convergence. In the same vein, it's difficult to understand why the implementation neglects variance reduction techniques. The integral formulation described in Garcia Munoz & Mills, 2015 (based on O'Brien, JQSRT, 1992) gives a more straightforward framework to tackle these issues.

We thank the reviewer for these important comments. We agree that an implementation-level description based on following simulated photons through successive collision events is intuitive, but does not by itself provide the clearest framework for understanding why certain Monte Carlo formulations converge and others do not. We have therefore substantially revised the manuscript in this respect.

In particular, we added Appendices G and H, in which we derive the forward and backward Monte Carlo equations for polarised radiative transfer directly from the vector radiative transfer equation, including the analytical formulation used to sample the polarised scattering direction. This addition strengthens the methodological contribution of the paper, because it provides a complete and unified theoretical framework for polarised Monte Carlo radiative transfer in both forward and backward modes, rather than only an implementation-oriented description of the code. Related derivations exist in the literature, for example in Marshak and Davis (2005) and Deutschmann et al. (2011), who neglected polarisation, or in Marchuk et al. (1980), Deutschmann (2015), and Wang et al. (2019), who included polarisation but did not start their derivations from the vector radiative transfer equation and also neglected polarisation-dependent sampling of the scattering direction. In addition, those derivations are distributed across different chapters, sometimes omit intermediate derivation steps, or have inconsistent physical units in their equations. Therefore, they do not provide the same complete and internally consistent derivation in the form presented here. We believe this framework is useful not only for understanding the implementation of MONKI itself, but also for readers who wish to validate or extend polarised Monte Carlo radiative transfer methods.

We also added a dedicated subappendix, App. G9, in which we discuss the classical or alternative sampling approach often used in Monte Carlo codes, such as MYSTIC. There we show explicitly that, in this approach, the scattering direction is sampled from the PDF corresponding to unpolarised incident radiation, after which a correction factor is applied. This subappendix makes clear why neglecting the incident photon's polarisation state during the sampling step can lead to large variance, apparent bias in finite simulations, and poor convergence in optically thick and strongly polarising atmospheres.

In addition, the revised manuscript now demonstrates this point numerically in new Figs. 5 and 6b by comparing MONKI with this classical alternative approach (see also Figs. 2 and 3 below). These new results show that MONKI converges well in both forward and backward modes for optically thick and strongly polarising atmospheres, whereas the classical approach shows apparent bias in finite simulations and poor convergence. García Muñoz and Mills (2015) already demonstrated this for a backward Monte Carlo formulation. Other Monte Carlo codes that take into account polarisation-dependent sampling of scattering directions are 3DMCPOL (Cornet et al., 2010), SMART-G (Ramon et al., 2019), and the code of Bartel and Hielscher (2000), but only do so in forward mode. To the best of our knowledge, MONKI is the first Monte Carlo code that consistently uses polarisation-dependent sampling successfully in both forward and backward modes.

We therefore believe that the revised manuscript now addresses the reviewer's concern more satisfactorily. The added Appendices G and H provide the formal integral framework that was missing from the original version, and App. G9 shows explicitly why neglecting the photon's polarisation state during the sampling step can lead to large variance, apparent bias in finite simulations, and poor convergence. Combined with the new comparison in Figs. 5 and 6b, this makes the rationale of the implementation much clearer and places it in the broader methodological framework suggested by the reviewer.

We added the following sentences to the abstract: *"Unlike classical Monte Carlo approaches that rely on post-sampling weight corrections and can therefore produce rare but disproportionately large photon weights, MONKI samples scattering directions* *from the full polarisation-dependent distribution, consistently in both forward and backward Monte Carlo modes. We provide the corresponding theoretical framework in the appendices. Because of this exact polarised sampling approach, the code converges robustly for optically thick and/or strongly polarising atmospheres."*

And to the introduction, line 87: *"Other Monte Carlo codes that take into account polarisation-dependent sampling of scattering directions are 3DMCPOL (Cornet et al., 2010), SMART-G (Ramon et al., 2019), and the code of Bartel and Hielscher (2000), but only do so in forward mode."*

And to the introduction, line 95: *"By fully tracking the polarisation state history of photons along their trajectories and sampling scattering directions from the corresponding polarisation-dependent distribution, MONKI converges in both forward and backward modes, including for optically thick and strongly polarising planetary atmospheres. The code has been written in modern Fortran. In addition to presenting the code itself, this paper provides, we believe for the first time, a complete derivation of the underlying forward and backward Monte Carlo equations and polarisation-dependent sampling formulae, thereby offering a unified theoretical framework for readers who wish to understand, validate, or extend polarised Monte Carlo radiative transfer methods."*

And we modified line 98 of the introduction: *"The appendices contain detailed explanations of the formulae implemented in MONKI, together with the derivation of the forward and backward Monte Carlo equations for polarised radiative transfer."*

We changed the paragraph in the Conclusion starting on line 480 into:

"Although MONKI is not the first code of its kind, it has fundamental methodological differences from other Monte Carlo codes. A common limitation of Monte Carlo codes is their failure to converge in optically thick and strongly polarising atmospheres. This issue arises when approximations are made in the sampling of scattering directions, by neglecting the photon's polarisation state and correcting afterwards by weight factors. MONKI instead samples scattering directions from the full polarisation-dependent distribution while fully tracking the polarisation history of each photon along its trajectory. As demonstrated in this paper, this exact polarised sampling approach converges in both forward and backward modes, including for optically thick and strongly polarising planetary atmospheres. In addition, the appendices provide a complete derivation of the corresponding forward and backward Monte Carlo equations and polarisation-dependent sampling formulae, thereby offering a unified theoretical framework for polarised Monte Carlo radiative transfer."

The manuscript is very well written. References in the manuscript seem complete.

I didn't check, but the MC implementation appears to be publicly available, which will help further disseminate the ideas developed here.

The code is indeed publicly available, and we agree that this will help further disseminate the ideas developed here.

I recommend the manuscript for publication, after addressing the following very minor comments.

Methods. It took me a while to figure out that the MC implementation is valid only for plane-parallel atmospheres, perhaps because the introduction mentions the application of polarimetry to disk-integrated observations. I suggest making it clear in the Introduction (#1) or Methods (#2) sections.

In the introduction, we changed line 90 from *'MONKI can perform simulations in both forward and backward modes (with reversed photon directions) for horizontally homogeneous and inhomogeneous (3D cloudy) scenes.'* into *'MONKI can perform simulations in both forward and backward modes (with reversed photon directions) for horizontally homogeneous and inhomogeneous (3D cloudy) plane-parallel atmospheres.'*

** line 16. w.r.t. is not standard, I think.*

We changed *'w.r.t.'* into *'with respect to'*

** line 20. "at the top of at the atmosphere". Language issue.*

We changed '*at the top of at the atmosphere (TOA)*' into *'at the top of the atmosphere (TOA)'*

** Fig. 1. In my printout, angles theta' and phi' become corrupt. It may just be a problem with my pdf reader though. Further, it would help if you could show the actual geometry of the problem, with the cells in both the x and y directions. This would make it clearer that the current geometry is plane parallel.*

We thank the reviewer for pointing out that the angles became corrupt in their printout. We did not, however, encounter this problem. As requested, we made a sketch of the 3D rectangular computational domain, and a photon path in forward and backward mode as shown in Fig. 1. We have also added this figure to the paper.

** In Methods section, please state how V>0 is defined.*

We added the following explanation to Stokes vector introduction of the Method section: *'In particular, for $Q > 0$ ($Q < 0$), the direction of polarisation is parallel (perpendicular) to the reference plane. For $U > 0$ ($U < 0$), the direction of polarisation is rotated by $+45°$ ($-45°$) from the direction parallel to the reference plane, with positive rotations defined as anti-clockwise when looking in the propagation direction of the light. For $V > 0$, there is an excess of right-handed circular polarisation, that is, the electric field vector rotates clockwise when looking in the propagation direction of the light.'*

** line 166. Having the code decide between scattering by a gas molecule or an aerosol particle (or different types of them, if different aerosol types coexist) is inefficient in a MC method. It would be notably faster if the optical (scattering, absorption) properties are properly averaged and assigned to "average" particles. Could the authors please comment on this?*

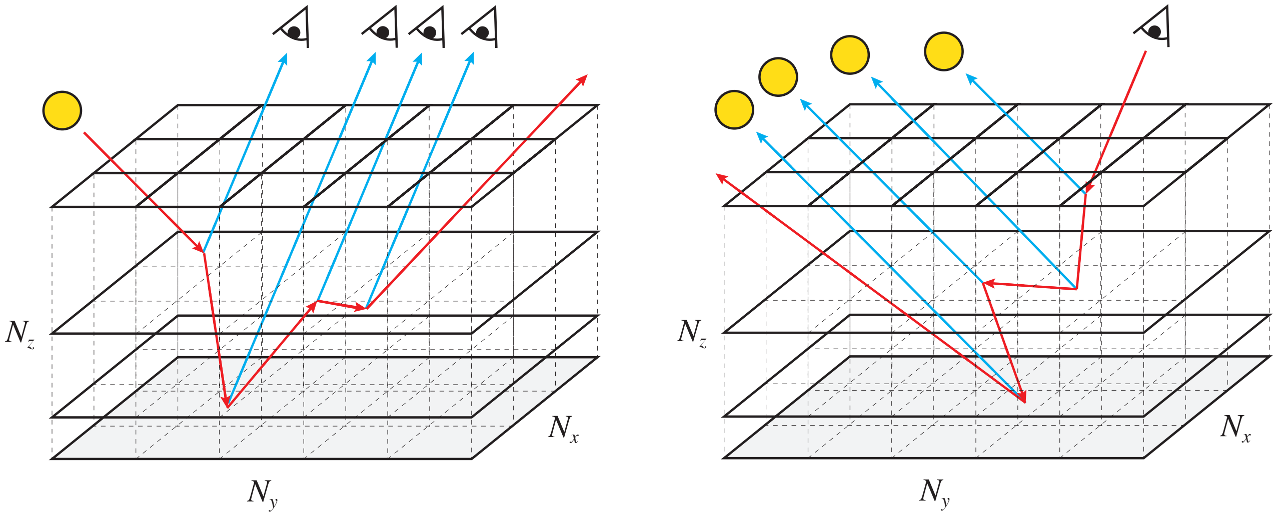

Figure 1. Sketches of the 3D computational domain of MONKI and of a photon trajectory (red arrows) in forward mode (left) and backward mode (right). Here, the numbers of columns in the x and y directions are $N_x = 3$ and $N_y = 5$, respectively, while $N_z = 3$ is the number of layers. The domain is periodic in the horizontal directions. At every scattering event (i.e. each change in direction of the red arrow), the probability of scattering toward the detector (in forward mode) or toward the Sun (in backward mode) is computed using the local estimation method (blue arrows).

We thank the reviewer for this suggestion. Indeed, the separation of photon paths into gas or aerosol (type) scattering is, in terms of path sampling, less efficient than considering average optical properties (phase matrices and single scattering albedos, weighted by their relative scattering optical thicknesses).

However, the dominant computational cost lies in sampling scattering directions from the single-scattering phase matrix. The construction and sampling of cumulative distribution functions (CDFs) for aerosol phase matrices are computationally expensive. In MONKI, these CDFs are precomputed once per aerosol type and are independent of local number densities (see Appendix F of the MONKI paper). If gas and multiple aerosol types were mixed into an effective scatterer, the phase matrix, and thus its CDF, would in general differ for each grid cell due to spatially varying composition, especially in 3D inhomogeneous scenes. This would require either storing a large number of CDFs or recomputing them on the fly, both of which are computationally inefficient.

Moreover, Rayleigh scattering is treated separately using an efficient rejection-sampling approach (Appendix E of the MONKI paper). Mixing Rayleigh and aerosol scattering into a single phase matrix would remove this simplicity without a clear performance gain.

For these reasons, we chose to sample gas and aerosol scattering events separately, which offers a favourable balance between computational efficiency, memory usage, and algorithmic clarity.

** pg. 8. Footnote. Setting w=1e-16 to terminate a simulation seems unnecessarily stringent. My guess is that the calculation converges for w 1e-6. Could the authors please confirm this statement?*

Indeed, using a larger cut-off value for w would reduce the computation time. However, this would also introduce a small negative bias in the simulated radiances, because photons would then be terminated prematurely rather than being followed until their weight becomes numerically negligible. The magnitude of this bias is proportional to the chosen cut-off value. In this paper, we aimed to present numerically unbiased results, and therefore chose the smallest practical value, $w = 10^{-16}$, close to machine precision.

** pg. 9. Just wondering, how easy would it be to extend the surface treatment to non-Lambertian reflection?*

There are two ways to implement non-Lambertian surface reflection in a Monte Carlo code (see, e.g., Mayer, 2009).

The first and simplest approach is to sample the reflection direction from a simple angular distribution (i.e., isotropic and cosine-weighted over the hemisphere, as in Appendix C) and to scale the photon weight (and, when including polarisation, the normalised Stokes vector) by the surface BRDF (or surface reflection matrix) evaluated for the chosen incident and reflected directions. This approach is unbiased but may lead to large variance when the BRDF is strongly peaked (e.g., for specular reflection from a flat water surface), because directions close to the specular peak are only rarely sampled, while those rare events carry very large weights.

A more efficient, but more complex, approach is to interpret the reflected intensity as a probability density function and to sample the reflection angles from the corresponding cumulative distribution functions. This can be done using direct inversion if an analytic CDF exists (as for Lambertian reflection; Appendix C), via rejection sampling (Appendix E), or by using precomputed CDF tables (Appendix F), analogous to the treatment of atmospheric scattering already implemented in MONKI. Consequently, extending MONKI to non-Lambertian surfaces mainly requires providing a suitable PDF (based on the reflected intensity, Appendix D) and applying the corresponding reflection matrix to update the photon's Stokes vector.

** line 261. "In the backward mode, every photon that is not completely absorbed contributes to the result, assuming that the light source is at an infinite distance." I was a bit puzzled to read this. My understanding is that the backward model works best when the observer has a narrow entry cone or, equivalently, when the observer is very far. For the backward implementation, it is no problem if the star subtends a finite solid angle.*

In MONKI we use the local estimation method. For each scattering or surface reflection event, the contribution to the signal is computed from the probability of scattering toward the detector direction, multiplied by the direct transmittance along that path. When the detector is at infinite distance in forward mode, we compute the radiance in a single viewing direction, represented by a collimated bundle of plane-parallel rays. In this case, every scattering location can, in principle, be connected to the detector in that viewing direction, and the corresponding scattering probability can be evaluated for all events. When the detector is at a finite distance in forward mode, it has a specific location in 3D space and a finite field of view. Then, some scattering locations may lie outside the detector's field of view and cannot be connected to the detector by a straight line, and those events do not

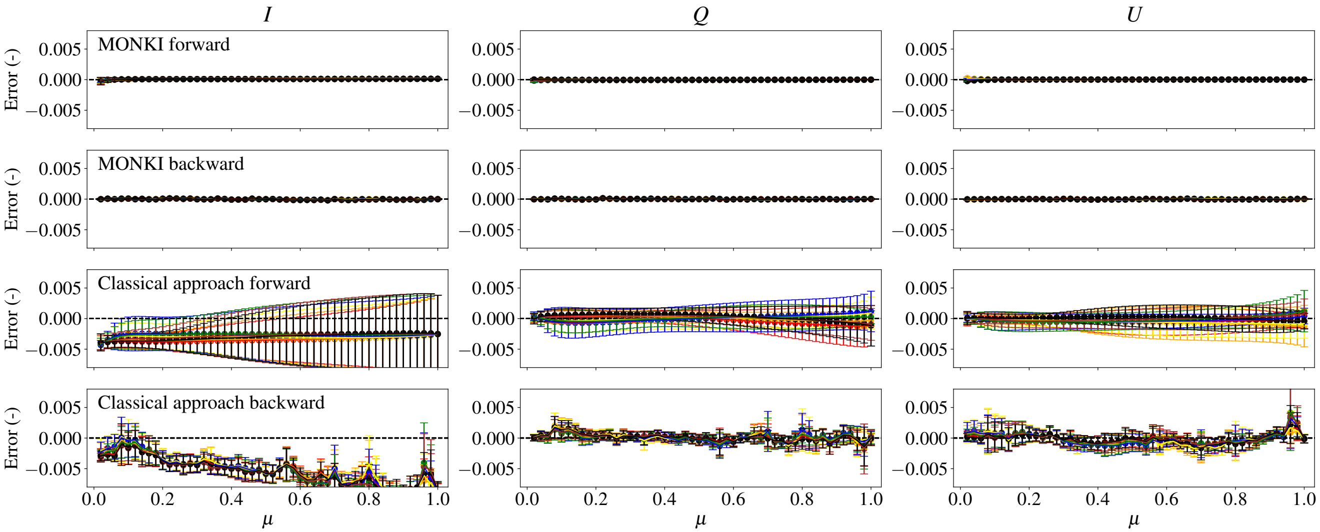

Figure 2. Differences between the MONKI results and those of Natraj and Hovenier, for MONKI in forward mode (first row) and in backward mode (second row), fully taking into account polarisation of light when sampling scattering directions. The third and fourth rows show the results when using instead the classical scattering direction sampling approach in MONKI, as used by, e.g., MYSTIC (see App. G9). The error bars indicate the ±2 standard deviations of the simulated results. Those error bars, and the seven different colours referring to the different values of φ, are virtually indistinguishable for the MONKI forward and backward modes.

contribute in forward mode. In backward mode this geometric restriction does not occur, because photons are launched from the detector itself.

Finally, the statement in the manuscript refers to the illumination geometry: MONKI assumes a collimated light source at infinite distance such that in backward mode all scattering locations are directly illuminated and can, in principle, be connected to the light source direction and contribute.

We revised the first paragraph of the backward mode section: *'MONKI can be used in both forward and backward modes. In backward mode, photon paths are traced from the detector towards the light source (the Sun), as illustrated in Fig. 1. The detector radiance Stokes vector is again computed using the local estimation method, here with the option to evaluate multiple solar zenith angles ϑ_0 at a fixed solar azimuth angle φ_0 simultaneously.*

The backward mode is particularly useful when the detector is at a finite distance from, or even inside, the atmosphere-surface system. Although this application is not treated in the present paper, it is important for future extensions of MONKI to spherical atmospheres in combination with a detector at a finite distance. In such cases, the path from a scattering event to the detector depends on the location of the event, and the detector cannot be represented by a single collimated viewing direction throughout the domain. Consequently, in forward mode, only a small fraction of photons launched from the source would reach the detector's field of view, severely limiting the code's efficiency. In backward mode, by contrast, photons are launched from

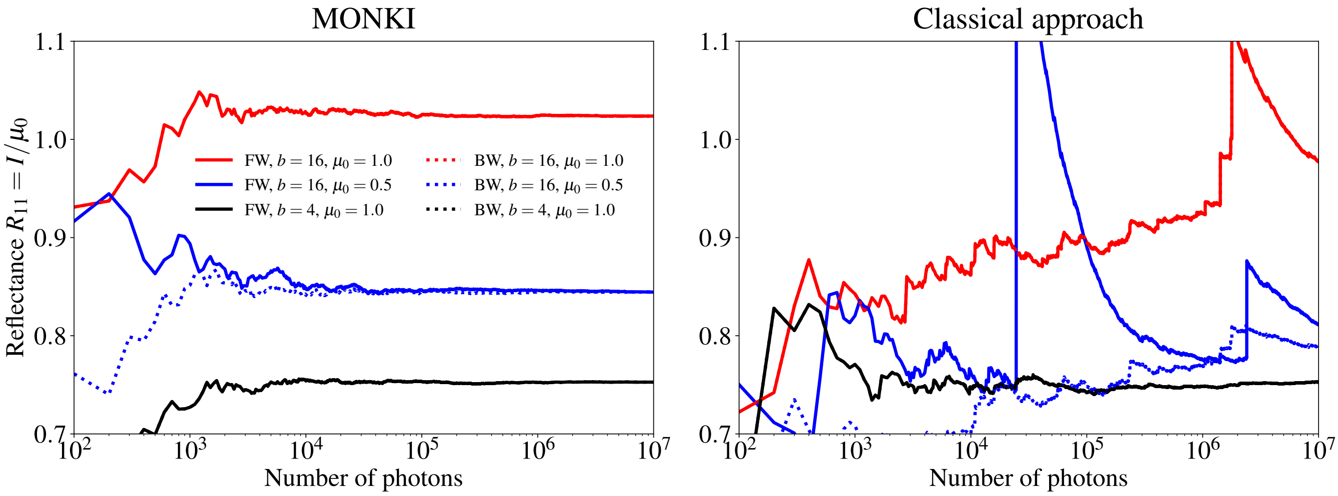

Figure 3. Left figure: convergence history of the TOA reflectance, R_{11}, by MONKI in forward mode (solid lines) and backward mode (dotted lines) for a Rayleigh scattering atmosphere with $b = 4$ and $\mu_0 = 1.0$ (black), $b = 16$ and $\mu_0 = 0.5$ (blue), and $b = 16$ and $\mu_0 = 1.0$ (red). The viewing geometry is nadir ($\mu = 1.0$). For $\mu_0 = 1.0$, the solid and dotted lines overlap. Right figure: similar, but using the classical scattering direction sampling approach in MONKI, as used by, e.g., MYSTIC (see App. G9). The jumps are caused by infrequent but large photon weights.

the detector, so that all traced photon paths lie within its field of view. Assuming collimated illumination from a light source at infinite distance, every backward-traced photon that is not completely absorbed can, in principle, be connected to the source direction and therefore contributes to the local estimate. We refer to Appendix G8 for the derivation of the backward Monte Carlo equations for polarised light as used in this section.'

** line 324. Did the authors "switch off" the direction sampling based on the polarization state of the photon and, in that case, did they run into problems to converge the model? I feel curious to know the answer.*

We have included Fig. 2 below in the paper, which shows the differences between the MONKI results and the benchmark results for the thick Rayleigh atmospheres of Natraj and Hovenier (2012), in forward and backward modes (top two rows). The two bottom rows show the results obtained when "switching off" the direction sampling based on the polarisation state of the photon. More precisely, we use there the classical approach in MONKI, as is also used in MYSTIC: neglecting the polarisation state of the incident photon when sampling a new scattering direction, and correcting for this neglect by adjusting the photon's weighting factor. We have included the new subappendix G9 in the paper, explaining the formulae involved in this classical approach and why it may fail to converge for optically thick and strongly polarising atmospheres.

The reason for the larger apparent bias and variance in the classical approach is its poor convergence for these cases, as pointed out by García Muñoz and Mills (2015). We added the following paragraph to Section 3.2:

'MONKI fully accounts for the photon's polarisation history when sampling scattering directions. However, when the classical scattering-direction sampling approach is used in MONKI instead, Fig. 2 (two bottom rows) shows clear deviations and a much larger variance. The classical approach (see Collins et al., 1972) neglects the polarisation state of the incident photon when sampling a new scattering direction, and corrects for this neglect by adjusting the photon's weighting factor (see Appendix G9). Examples of codes that use this approach are MYSTIC (Emde et al., 2010), MSCART (Wang et al., 2017, 2019), SPARTA (Barlakas et al., 2016), IVMCM (Gay et al., 2010), and the backward mode of SMART-G (Ramon et al., 2019). García Muñoz and Mills (2015) pointed out that for thick, strongly polarising atmospheres, such as those used by Natraj and Hovenier (2012), those codes may fail to converge. This is because, upon multiple scattering, these correction factors are multiplied repeatedly. In the unlikely event that a photon path contains several strongly polarising scattering directions, this can produce infrequent but very large photon weights (see Appendix G9).'

We also demonstrate the non-convergence of the classical approach by adding the convergence history of that approach to Fig. 3 above.

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