

Response to comments of Referee #2 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.

5 *General comments:*

This paper presents a new 3D atmospheric radiative transfer model based on Monte-Carlo Method.

*It presents the methods commonly used to track the photons through the atmosphere and to compute the reflectances. Several
10 validation cases are then presented showing that the MONKI code can correctly reproduce previous results. Finally, a simulation of the Earth and Venus atmosphere were computed and analysed, demonstrating that the code is able of handling different optical properties.*

The paper is well written and clear. However, it does not really contribute to anything new.

15 We thank the reviewer for this comment. We agree that MONKI is not the first three-dimensional Monte Carlo radiative transfer code for polarised light. However, the present paper does make a clear methodological contribution.

First, MONKI samples scattering directions from the full polarisation-dependent distribution, fully accounting for the polarisation history of the photon. This is fundamentally different from the classical Monte Carlo approach of Collins et al. (1972) used by, e.g., MYSTIC, MSCART, SPARTA, IVMCM, and the backward mode of SMART-G, in which polarisation is neglected in the scattering-direction sampling and the resulting approximation is corrected afterwards by weight factors. García
20 Muñoz and Mills (2015) did take polarisation fully into account during the sampling in their backward Monte Carlo code, and showed that the classical approach can lead to poor convergence in optically thick and strongly polarising atmospheres. 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.

25 To the best of our understanding, MONKI is the first Monte Carlo code that consistently uses polarisation-dependent sampling successfully in both forward and backward modes.

In the revised paper, we have included Figs. 5 and 6b (Figs. 1 and 2 below), which now also show results obtained with the classical approach in MONKI. MONKI converges well in both forward and backward modes, whereas the classical approach shows large variance and apparent bias in finite simulations. We have included Appendix G9, which explains the formulae

30 involved in the classical approach and why it does not converge for thick polarising atmospheres.

Second, 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

35 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 Marchuk et al. (1980), Deutschmann (2015), and Wang et al. (2019), who included polarisation but did not start their derivation 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

40 units in 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.

Third, the paper presents a precomputation strategy for optical paths to the detector, which improves computational efficiency without changing the result. To our knowledge, this feature has not been described in this form for polarised local-estimation

45 Monte Carlo radiative transfer.

We have revised the manuscript to make these contributions more explicit. The novelty of the paper therefore lies not merely in presenting another Monte Carlo code, but in showing that exact polarised direction sampling can be implemented in both forward and backward Monte Carlo modes, in demonstrating the resulting robust convergence for optically thick and strongly polarising atmospheres, and in providing a complete and unified theoretical framework for polarised Monte Carlo radiative

50 transfer.

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*

55 *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."

In the conclusion of the article, three contributions of the MONKI code are listed, but are not convincing as they stand : 1- line 481 "common limitation of Monte Carlo codes is their failure to converge in optically thick and strongly polarising atmospheres". Can the authors be more specific about the values beyond which the convergence does not occur and give an example of such atmosphere.

We have added the convergence history when using the classical approach as used by, e.g., MYSTIC, to Fig. 2 below. As can be seen, with a Rayleigh-scattering optical thickness of 4, the classical approach approaches the correct value, albeit with slower convergence, but with an optical thickness of 16 severe problems occur. An example of a planet with such a thick Rayleigh-scattering atmosphere is Venus, with a surface pressure of approximately 92 bar (see Fig. 9 of the paper). Indeed, for a detector in space, the thick clouds high in the atmosphere often scatter the light more strongly than the gas (depending on

the wavelength, and the illumination and viewing geometry), as shown in Fig. 13 of the paper. However, a detector below the clouds (mounted on a probe or located on the surface) would be more sensitive to scattering by the gas and requires simulations by an accurate code such as MONKI.

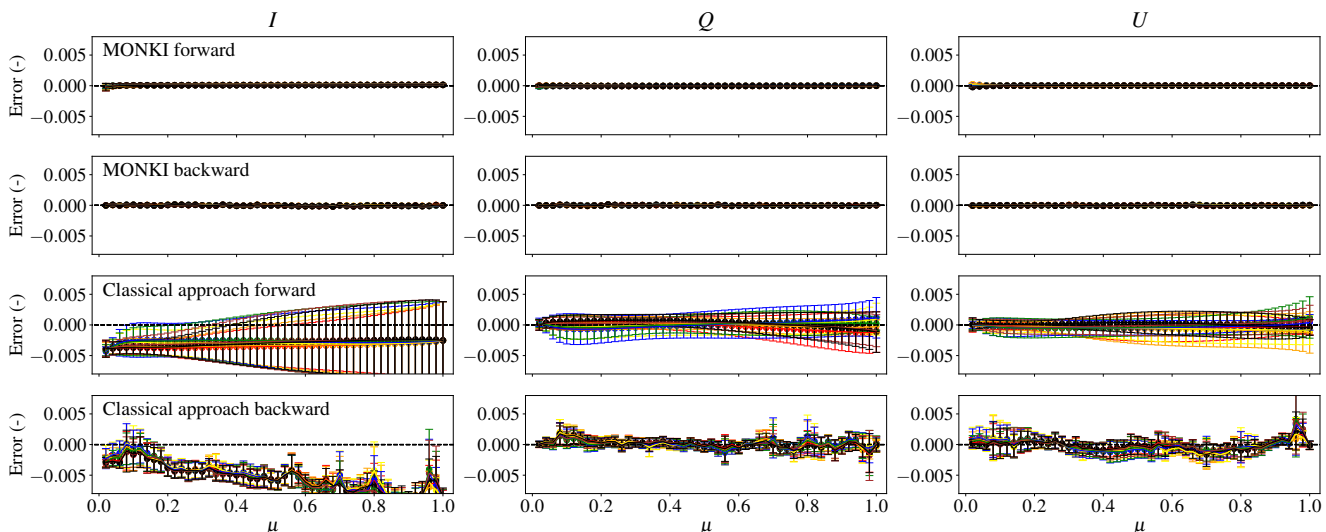


Figure 1. Differences between the MONKI results and those of Natraj and Hovenier, for MONKI in the forward mode (first row) and in the backward mode (second row), fully taking into account polarisation of light when sampling scattering directions. The third and fourth rows show the results when using 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.

2- "The current version of MONKI does not use variance reduction techniques". I suppose other codes may choose whether or not to use variance reduction technique, which are often necessary to achieve convergence in complex 3D atmospheres. So, it does not appear to be a real advantage.

100 MONKI does indeed not use other variance reduction techniques than the local estimation method. We agree that not having the option of extra variance reduction techniques may not be an advantage for users who use MONKI only as a tool. However, this design choice has advantages for us as code developers and for users who want to understand the details of the code, as explained on line 489: "By omitting those variance reduction techniques, MONKI produces unbiased results while preserving readability and simplicity, and thus adaptability when future extensions of the code are to be implemented." Simultaneously, we
 105 have presented an alternative method to speed up the simulations, as explained on line 491: "Instead of using such techniques, we increase the number of photons to achieve higher precision when needed."

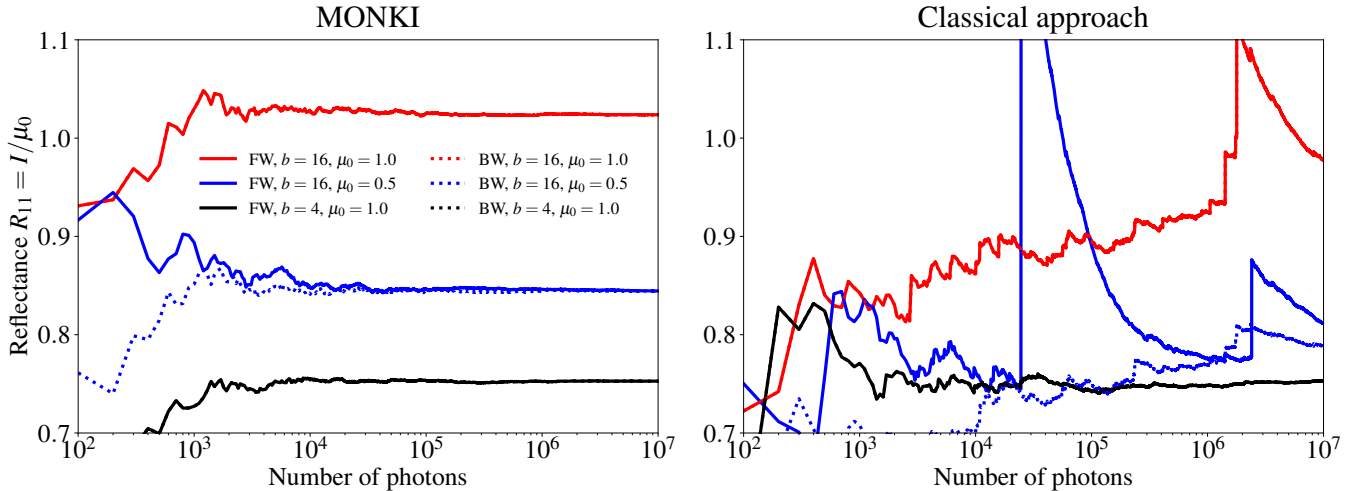


Figure 2. Left figure: convergence history of the TOA reflectance, R_{11} , by MONKI in forward mode (solid lines) and backward mode (dotted lines) for a Rayleigh scattering atmosphere with $b = 4$ and $\mu_0 = 1.0$ (black), $b = 16$ and $\mu_0 = 0.5$ (blue), and $b = 16$ and $\mu_0 = 1.0$ (red). The 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.

3- *“In order to speed up MONKI’s simulations, we implemented and presented a precomputation approach for optical paths to the detector.”. This may be a new method for obtaining converging results more quickly but quantitative values showing the gain in computational speed have to be added to the article. Note that adaptive grid was already introduced in Villefranque et al. (2019)*

The speed improvement obtained with the precomputation approach depends strongly on the number of grid cells (layers and columns) used in the simulations. More grid cells can give more potential speed improvement, but only if (most of) those grid cells are cloud-free. In addition, the potential speed improvement increases with the number of simultaneous zenith angles (viewing zenith angles in forward mode, and solar zenith angles in backward mode) that are computed, but only if (most of) those optical paths are cloud-free. Therefore, it is difficult to give a single number for the speed improvement. As an example, however, we have added the following footnote to the last sentence of the precomputation approach section:

‘The speed increases with the number of cloud-free grid cells and viewing directions. For example, for the cloudy Earth sample signal of Fig. 11, for $\theta_0 = \varphi = \varphi_0 = 0^\circ$ and 90 viewing zenith angles simultaneously, the speed improvement is a factor 1.9.’

We thank the reviewer for mentioning the adaptive-grid method of Villefranque et al. (2019). Our precomputation approach is fundamentally different. In MONKI, the original atmospheric grid is not modified: photons are still propagated through the same grid during the Monte Carlo simulation. Our speed-up applies only to the evaluation of the optical path from a scattering or surface event to the detector in the local-estimation step. For paths that are cloud- and aerosol-free, we precompute the

125 detector optical thickness and thereby avoid repeated event-to-detector propagations. In contrast, Villefranque et al. accelerate
the ray tracing through the full 3-D volume itself by means of hierarchical adaptive grids. In principle, our optical-path pre-
computation could be combined with such an adaptive-grid strategy in future work.

130 *4 - “MONKI can import different particle scattering matrices and can, in principle, also simulate light scattered by non-
spherical aerosol particles and ice clouds”. The same applies for other code as long as optical properties are known.*

We thank the reviewer for pointing this out. We do not claim that the ability to simulate light scattered by non-spherical parti-
cles is unique to MONKI.

135 *To increase the novelty of the paper, I would recommend to go deeply in the analysis of the methods used to sample the
scattering direction at each interaction presented in appendices E and F. I may be wrong, but it seems to me that the rejection
method is not commonly used in Monte-Carlo Atmospheric radiative transfer. A deeper analysis of this method comparing to
the conventionnal one (tabulated cumulative distribution function) in terms of accuracy, convergence and computation time,
could be valuable to increase the interest of this publication for the community.*

140 We thank the reviewer for this helpful suggestion. We agree that the choice of sampling method deserves clarification. In the
present work, however, the main methodological point is not the generic comparison between acceptance-rejection sampling
and tabulated inverse-CDF sampling as numerical techniques, but the fact that the scattering direction is sampled from the full
polarisation-dependent probability distribution, rather than from an approximate distribution corrected afterwards by weight
factors.

145 We have therefore revised the manuscript to analyse this point more deeply. In particular, Appendices G and H and the
new Figs. 1 and 2 (Figs. 5 and 6b in the new paper) now compare MONKI’s exact polarised sampling approach with the
classical alternative approach, and show the consequences for bias and convergence in optically thick and strongly polarising
atmospheres. This increases the novelty of the paper (see also the reply to the first comment above).

150 Regarding the specific use of the acceptance-rejection method in Appendices E and F: for Rayleigh scattering, we use this
method because obtaining the CDF, and especially its inverse, for the full joint polarised PDF is not straightforward when the
polarisation of the incident beam is taken into account. For Mie scattering, we likewise use acceptance-rejection, but with an
envelope function constructed to closely follow the strongly forward-peaked distribution and thus maintain a high acceptance
rate. Moreover, in that case the proposal distribution itself is sampled using the inverse transform method. The adopted sampling
strategy is therefore chosen for practicality and efficiency in the context of the full polarised PDF.

155 A systematic benchmark of acceptance-rejection sampling versus tabulated inverse-CDF sampling in terms of computation
time, convergence, and implementation cost would certainly be of interest, but we consider that to be a separate algorithmic
study that falls outside the main scope of the present paper. The focus of the present manuscript is on the exact polarised
sampling formulation itself and its consequences for convergence and accuracy, which we now discuss more explicitly in the
revised paper.

160 *In summary, I understand that the authors wish to publish this article to have a reference to cite it for further study or when it will be used by other scientific teams as the code is freely available, which is important to mention. Nevertheless, I would recommend to try to improve the paper by taking the above comments into account.*

Specific comments :

165 – *Equation of line 137 : This is correct only in the principal plane, ie when the scattered radiation is in the same plane of the incident radiation.*

We have changed the sentence on line 135 as follows: "When $U = 0$, we can use an alternative definition that includes the direction of polarisation:" -> '*For observations in the principal plane, i.e. the vertical plane containing the local zenith direction and the incident solar beam, the viewing direction lies in the same vertical plane as the incident radiation. In this case (with relative azimuth angles of 0° or 180°), the principal plane coincides with the scattering plane. If the local atmosphere-surface system is horizontally homogeneous, symmetry implies that $U = 0$, and we can use the signed degree of linear polarisation...*'

170 – *To avoid confusion, in Equation (10) and (13), authors should be more precise by indicating the direction of the incident radiation and of the view (for eq 10) or scattered (eq 13) direction.*

175 We thank this suggestion. For readability, we did not add the angle dependencies of the incident light. In fact, the incident light depends on the full geometry of the preceding photon trajectory. In the first paragraph of Sect. 2.3, we have added: '*Since \bar{I} changes along the photon trajectory, its dependence on position, direction, and previous events is omitted for readability.*' We also clearly state below the equation that \bar{I}' (with a prime) refers to the incident light. For the signal contribution W , we have added the ω^\bullet dependence notation to emphasize that W can be computed simultaneously for multiple detector angles.

180 – *Section 2.6, line 274 : does it means that the χ matrix need to be stored and each scattering in the reverse mode to be apply at the end of the incident Stokes vector ?*

In the backward mode, the multiplication by the phase matrices is indeed applied effectively at the end, before multiplying by the incident Stokes vector. However, the individual phase matrices do not need to be stored. Instead, their cumulative effect is incorporated progressively in the detector-response matrix, which is updated at each scattering event, as explained in the backward mode section of the paper.

185 – *Section 3.1, Table 1: The results are in forward or backward mode ? Can you add the absolute and relative difference in the Table*

The results are for MONKI in forward mode. We have clarified this in the caption:

190 "*Comparison of the TOA radiances computed using MONKI in forward mode with ...*"

In addition, we modified the text on line 302 as follows:

"The MONKI simulations were done in forward mode and used 10^7 photons, ..."

In addition, we have now included the comparison tables with de Haan et al. (1987) for MONKI's backward mode as well; see Tables S4 to S7 of the supplement.

195 We have decided not to include the differences in the tables, because in principle that information would be redundant and would make the tables unnecessarily large. We note that almost all differences fall within two standard deviations of the Monte Carlo noise, and will converge further to the exact result of de Haan et al. (1987) with an increasing number of photons.

– *Section 3.3, Figure 6 : Why do you use the standard deviation of 3DMCPOL and not the one of MYSTIC that it is used to calculate the difference*

200

We use the standard deviation of 3DMCPOL for consistency with Fig. 10 of Emde et al. (2018). (See the caption of their Fig. 10: "The grey area in the difference plots corresponds to 2σ of 3DMCPOL (Monte Carlo model without variance reduction).").

– *Section 3.3, Figure 6: Why divided the results by $1000/E_0$ and not using the same quantity than in the IPRT comparison (Emde et al. 2018) ?*

205

We use the same quantity as used in the IPRT comparison. See the caption of Fig. 10 of Emde et al. (2018): "The Stokes vector components are normalised to $1000/E_0$."

– *Section 4 : I do not know Venus atmosphere, is it common to have clouds between 50 and 70 km ? Do you have some references to support the configuration ?*

210

Yes, the clouds on Venus are approximately located between 50 and 70 km altitude. See, e.g., Fig. 6 of Haus et al. (2015). We have modified the sentence on line 423 as follows:

"The cloud in the Venus model extends from 50 to 70 km, with a vertically homogeneous optical thickness $b^a = 30$ (see Haus et al., 2015, for more detailed Venus cloud models)."

– *Appendices E and F describe how the rejection method is used for the Rayleigh and Mie scattering instead of the inverse CDF method using tabulated values as is usually done. Have the two methods been compared in terms of accuracy and computation time. These can be an interesting result to add in the paper. See my general comments.*

215

We indeed use rejection sampling and, in the case of Mie scattering, also inverse sampling from the CDF of the envelope function. This choice is dictated by the form of the probability density function that has to be sampled (Eq. D7), which depends on the incident state of polarisation and on multiple elements of the single-scattering matrix. For this full polarisation-dependent PDF, deriving a tabulated cumulative distribution function, and especially its inverse, is not straightforward. For that reason, we do not currently have an inverse-CDF formulation for the same fully polarised sampling problem, and therefore cannot provide a direct benchmark of rejection sampling versus inverse-CDF sampling for this case.

220

225 We note, however, that the main methodological point of the paper is not a generic comparison between two numerical sampling techniques, but the fact that the scattering direction is sampled from the full polarisation-dependent distribution. In the revised manuscript, we have therefore focused the additional analysis on this point, by comparing MONKI's exact polarised sampling approach with the classical alternative approach and by showing the consequences for bias and convergence.

230 – *Line 505. MONKY is designed to support the preparatory studies for the aforementioned spectropolarimetric missions, which means calculating radiances at different wavelengths. However, no information is given on how the multispectral properties of the atmosphere including gas absorption and particles scattering will be accounted for.*

The multispectral properties of the atmosphere, including gas absorption and particle scattering, enter the simulation via the wavelength-dependent input absorption and scattering cross-sections, as described by Eqs. A10, A12, A16, and A17 in Appendix A. We have added the following sentence to the conclusion, line 500:

235 *"For Earth applications, MONKI uses the same method as DAK (Doubling-Adding KNMI) to compute the input atmospheric optical properties. MONKI can handle spectral variations of those properties, producing simulated spectra by so-called line-by-line computations."*

Typos :

240 *line 58 : delete "and"*

We have kept "and" here because it reflects the distinction between errors in the geometric albedo and errors in the locally reflected radiances.

Reference :

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Villefranque, N., Fournier, R., Couvreur, F., Blanco, S., Céline, C., Eymet, V., et al. (2019). A path-tracing Monte Carlo library for 3-D radiative transfer in highly resolved cloudy atmospheres. Journal of Advances in Modeling Earth Systems, 11. <https://doi.org/10.1029/2018MS001602>

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