

### Response to Reviewer #3

We are very grateful to the reviewers for taking the time to carefully review our manuscript. We respond to each reviewer's comments below. We have added line references to the positions in the tracked changes manuscript where we have made changes.

*Regarding this manuscript, I want to make some comments that are actually not mandatory for the authors. They can take into account my comments or not. If not, the article can be published in its current form. Over time, the authors have made an important contribution in this field so that now, they do not have to be hindered by technical details.*

We thank the reviewer for their helpful comments and their suggestions for future development of our method. We have addressed the comments below.

*I do not understand why the side domains have periodic boundaries. A domain with these conditions is a domain that repeats itself infinitely in both directions. But, for example,  $D_3$  is connected with  $D_1$ . In my opinion, a heterogeneous 3D domain embedded within a horizontally infinite medium can be modeled with periodic and open boundary conditions. In Fig. 8 of Evans' paper it is shown that for a Gaussian cloud, the flux computed with periodic boundaries for a 12-km domain agrees with that computed for open boundaries for a 3 km domain. Thus, in the case of periodic boundaries, the domain must be larger to diminish the contribution of the incoming radiance at the domain edges. That's all. However, because you need the domain  $D_3$  to model the position of a sensor outside the cloud domain, I would consider that the domains  $D_3$  and  $D_1$  are connected by continuity, and I would impose open boundary condition on the left boundary of  $D_3$ . In other words, I would consider the computational domain  $D_3 \cup D_1 \cup D_7$  as a whole, and impose open boundary conditions on the left boundary of  $D_3$  and the right boundary of  $D_7$ .*

This comment raised an important issue, which is that the physical reasoning for the formulation of the open boundary conditions is actually missing from our paper. We have added several sentences on this to the manuscript which we believe clarify this issue.

Line 443:

“The periodic boundary conditions in the auxiliary domains ensure that the RT solution in each auxiliary domain is independent of the 3D domain so that the system of RTs is solvable. This approximation neglects multiple scattering interactions between the heterogeneous medium ( $D_1$ ) and the auxiliary domains. As a result, open horizontal boundary conditions are an approximate treatment of the RT solution for a heterogeneous medium embedded in a horizontally homogeneous medium. Features like cloud and surface adjacency effects cannot be modelled unless the domain of 3D radiative transfer is sufficiently large enough to resolve them.”

The technical issue is that, while the radiance at the boundary between  $D_3$  and  $D_1$  is continuous in the directions incoming towards  $D_1$ , it is not continuous in the outgoing directions from  $D_1$ . If we make  $D_1$  bigger, so that we resolve more of the plane-parallel medium with 3D radiative transfer, then this discontinuity will lessen, and the approximation of the RT with open horizontal boundary conditions will be more accurate. The example in Fig. 8 of Evans' paper is non-scattering as it is in the longwave and uses a black surface. In contrast to a scattering medium, the open horizontal boundary conditions provide an exact solution of the 3D RT for Evans' example even when the open horizontal boundary conditions are imposed right at cloud edge.

*In the case of satellite measurements, the main problem is the discretization of the domain above the clouds, which is usually meant up to 50-60 km. To connect the two domains (clear and cloudy), the idea used by Pincus and Evans for the parallelization of SHDOM can be used (the two domains communicate with each other through the boundary conditions).*

We agree that a treatment of the atmosphere is important either through explicitly resolving the full vertical column and making use of additional computational resources or by making use of approximate atmospheric correction methods given the weak atmospheric scattering at wavelengths typical for cloud remote sensing. We do intend to implement MPI-based parallelization for our method, which would be very valuable for multi-layered cloud scenes. The computational tradeoffs between the different approaches are a forward modelling issue beyond the scope of this paper and we opt not to discuss these ideas within the manuscript.

*I understand that the authors are fans of Martin. Indeed, Martin is an exceptional mathematician and his formalism is a mathematical delicacy. However, I think that it cannot be easily understood by a physicist or an engineer. For this reason, I want to suggest you to use a formalism that is more appropriate to Evans' implementation. By transforming Evans' implementation into a mathematical language, it is very easy to linearize the model's equations. In this way, different approximations for derivatives calculation, including the single-scattering approximation, become very clear.*

We agree that the mathematical formalism is quite formal and dense, but it has several benefits. The first benefit is that we are able to link the formalism of Martin et al. (2014) with the work of Levis et al. (2015, 2020) making the physical consequences of the approximate Jacobian calculation clearer. Secondly, Evans (1998) has only a very short description of the open boundary conditions and does not mention the influence of the boundary condition on the radiance calculation that occurs in the SHDOM code. If open boundary conditions may be more widely used for remote sensing retrievals using 3D radiative transfer, then it is worth describing this aspect of the model in detail. Thirdly, it is not possible to explain the much-reduced accuracy of the approximate Jacobian for the optical properties at the domain edge when using open boundary conditions without invoking the concept of a coupled system of RTEs. The description of the coupling is most clear when a precise, formal treatment is used rather than invoking high level analogies like in Evans (1998) (e.g. the concept of "independent scans") that are ambiguous in their meaning.

Because of these benefits, we have opted not to change the formalism within the manuscript. Instead, we have added a reference to other more pragmatic descriptions and clarified the relationship between our formalism and the details of implementation:

Line 381: “For a more pragmatic description of the essence of the approximate Jacobian calculation that does not include the treatment of the boundary conditions presented here, readers may refer to Levis et al. (2020). Our treatment focuses on the continuous problem rather than the details of numerical implementation such as delta-M scaling of the optical properties except where conceptually necessary. Pertinent details on the numerical implementation related to the delta-M scaling and TMS correction in SHDOM can be found elsewhere (Evans, 1998; Doicu and Efremenko, 2019) and in Appendices A and C.”